Full wwPDB X-ray Structure Validation Report (i)

Dec 16, 2023 – 08:22 am GMT

PDB ID	:	4AQY
Title	:	Structure of ribosome-apramycin complexes
Authors	:	Matt, T.; Ng, C.L.; Lang, K.; Sha, S.H.; Akbergenov, R.; Shcherbakov, D.; Meyer, M.; Duscha, S.; Xie, J.; Dubbaka, S.R.; Perez-Fernandez, D.; Vasella, A.; Ramakrishnan, V.; Schacht, J.; Bottger, E.C.
Deposited on	:	2012-04-20
Resolution	:	3.50 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:

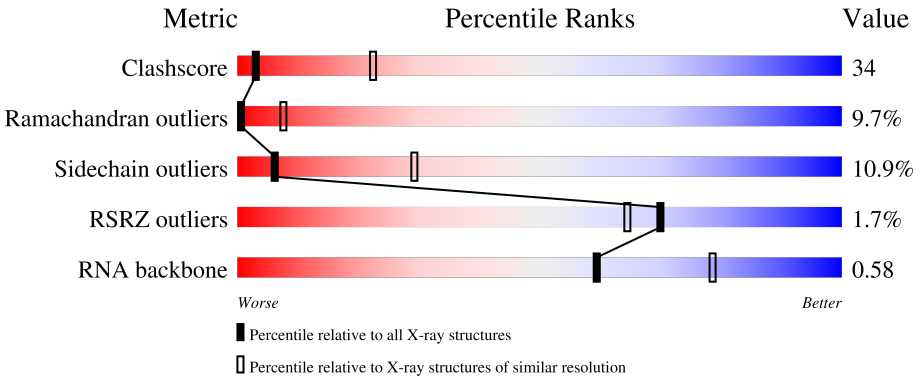
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)
RNA backbone	3102	1002 (4.00-3.00)

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	1522	36% 51% 11%
2	B	256	2% 21% 52% 17% 9%
3	C	239	20% 47% 17% 14%
4	D	208	4% 34% 53% 13%

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Mol	Chain	Length	Quality of chain
5	E	161	33% 50% 9% 7%
6	F	101	32% 61% 7%
7	G	155	37% 53% 10%
8	H	138	40% 47% 12%
9	I	128	30% 58% 11%
10	J	104	16% 16% 57% 19% 6%
11	K	129	35% 50% 7% 8%
12	L	135	34% 47% 12% 7%
13	M	126	7% 29% 54% 15%
14	N	60	3% 15% 67% 18%
15	O	88	41% 49% 10%
16	P	88	31% 55% 9% 6%
17	Q	104	4% 39% 47% 12%
18	R	88	6% 27% 44% 10% 17%
19	S	92	28% 46% 13% 13%
20	T	106	38% 43% 11% 7%
21	V	26	8% 58% 31% 8%
22	W	6	17% 17% 50% 33%
23	Z	15	7% 7% 20% 47% 27%

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
24	MG	A	2548	-	-	-	X
24	MG	A	2549	-	-	-	X
24	MG	A	2550	-	-	-	X
24	MG	A	2554	-	-	-	X
24	MG	A	2555	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	MG	A	2557	-	-	-	X
24	MG	A	2562	-	-	-	X
24	MG	A	2563	-	-	-	X
24	MG	A	2565	-	-	-	X
24	MG	A	2580	-	-	-	X
24	MG	A	2582	-	-	-	X
24	MG	A	2584	-	-	-	X
24	MG	A	2600	-	-	-	X
24	MG	A	2609	-	-	-	X
24	MG	A	2613	-	-	-	X
24	MG	A	2615	-	-	-	X
24	MG	A	2618	-	-	-	X
24	MG	A	2624	-	-	-	X
24	MG	A	2626	-	-	-	X
24	MG	A	2631	-	-	-	X
24	MG	A	2634	-	-	-	X
24	MG	A	2644	-	-	-	X
24	MG	A	2653	-	-	-	X
24	MG	A	2661	-	-	-	X
24	MG	A	2662	-	-	-	X
24	MG	A	2663	-	-	-	X
24	MG	A	2667	-	-	-	X
24	MG	A	2683	-	-	-	X
24	MG	A	2684	-	-	-	X
24	MG	A	2687	-	-	-	X
24	MG	A	2689	-	-	-	X
24	MG	A	2696	-	-	-	X
24	MG	A	2698	-	-	-	X
24	MG	A	2701	-	-	-	X
24	MG	A	2708	-	-	-	X
24	MG	A	2714	-	-	-	X
24	MG	A	2716	-	-	-	X
24	MG	A	2722	-	-	-	X
24	MG	A	2725	-	-	-	X
24	MG	A	2726	-	-	-	X
24	MG	A	2728	-	-	-	X
24	MG	A	2731	-	-	-	X
24	MG	A	2735	-	-	-	X
24	MG	A	2739	-	-	-	X
24	MG	A	2740	-	-	-	X
24	MG	A	2741	-	-	-	X
24	MG	A	2742	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	MG	A	2744	-	-	-	X
24	MG	A	2747	-	-	-	X
24	MG	S	1143	-	-	-	X
25	K	A	2670	-	-	-	X
25	K	A	2672	-	-	-	X
25	K	A	2675	-	-	-	X
25	K	A	2680	-	-	-	X
25	K	A	2682	-	-	-	X

2 Entry composition (i)

There are 28 unique types of molecules in this entry. The entry contains 52514 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 RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	A	1510	32446	14444	6006	10488	1508	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	1702	1066	339	290	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	842	531	155	153	3	0	0	0

- Molecule 7 is a protein called 30S RIBOSOMAL PROTEIN S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	155	Total	C	N	O	S	0	0	0
			1256	781	252	217	6			

- Molecule 8 is a protein called 30S RIBOSOMAL PROTEIN S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	138	Total	C	N	O	S	0	0	0
			1115	705	215	192	3			

- Molecule 9 is a protein called 30S RIBOSOMAL PROTEIN S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	I	127	Total	C	N	O	0	0	0
			1010	639	198	173			

- Molecule 10 is a protein called 30S RIBOSOMAL PROTEIN S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	98	Total	C	N	O	S	0	0	0
			794	499	156	138	1			

- Molecule 11 is a protein called 30S RIBOSOMAL PROTEIN S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	119	Total	C	N	O	S	0	0	0
			884	549	168	164	3			

- Molecule 12 is a protein called 30S RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	125	Total	C	N	O	S	0	0	1
			971	611	196	163	1			

- Molecule 13 is a protein called 30S RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	125	Total	C	N	O	S	0	0	0
			996	617	207	170	2			

- Molecule 14 is a protein called 30S RIBOSOMAL PROTEIN S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	60	Total	C	N	O	S	0	0	0
			491	312	104	71	4			

- Molecule 15 is a protein called 30S RIBOSOMAL PROTEIN S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	O	88	Total	C	N	O	S	0	0	0
			733	459	147	125	2			

- Molecule 16 is a protein called 30S RIBOSOMAL PROTEIN S16.

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

- Molecule 17 is a protein called 30S RIBOSOMAL PROTEIN S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	104	Total	C	N	O	S	0	0	0
			856	547	161	146	2			

- Molecule 18 is a protein called 30S RIBOSOMAL PROTEIN S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	R	73	Total	C	N	O	0	0	0
			596	380	118	98			

- Molecule 19 is a protein called 30S RIBOSOMAL PROTEIN S19.

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

- Molecule 20 is a protein called 30S RIBOSOMAL PROTEIN S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	T	99	Total	C	N	O	S	0	0	0
			761	469	162	128	2			

- Molecule 21 is a protein called 30S RIBOSOMAL PROTEIN THX.

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

- Molecule 22 is a RNA chain called 5'-R(*UP*UP*CP*AP*AP*AP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	W	6	Total 123	C 57	N 22	O 39	P 5	0	0	0

- Molecule 23 is a RNA chain called 5'-R(*GP*GP*GP*AP*UP*UP*GP*AP*AP*AP*AP* UP*CP*CP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	Z	15	Total 319	C 144	N 60	O 101	P 14	0	0	0

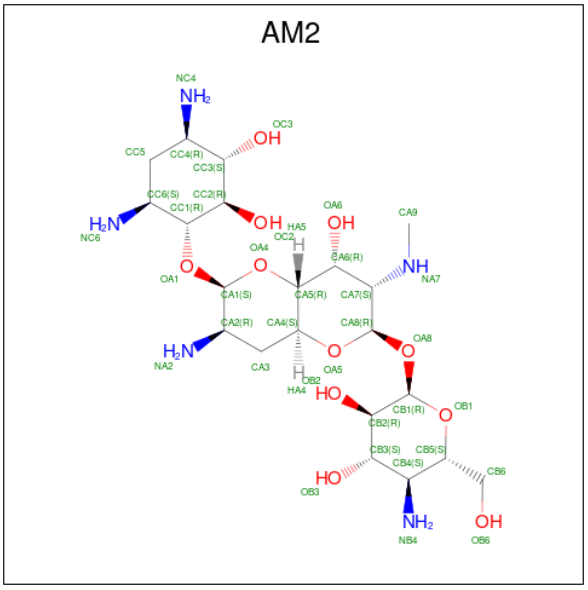
- Molecule 24 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	A	190	Total 190	Mg 190	0	0
24	D	1	Total 1	Mg 1	0	0
24	F	1	Total 1	Mg 1	0	0
24	G	2	Total 2	Mg 2	0	0
24	H	1	Total 1	Mg 1	0	0
24	J	1	Total 1	Mg 1	0	0
24	K	1	Total 1	Mg 1	0	0
24	L	1	Total 1	Mg 1	0	0
24	M	1	Total 1	Mg 1	0	0
24	S	1	Total 1	Mg 1	0	0
24	W	2	Total 2	Mg 2	0	0
24	Z	1	Total 1	Mg 1	0	0

- Molecule 25 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	14	Total K 14 14	0	0
25	V	1	Total K 1 1	0	0

- Molecule 26 is APRAMYCIN (three-letter code: AM2) (formula: $C_{21}H_{41}N_5O_{11}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C N O 37 21 5 11	0	0
26	A	1	Total C N O 37 21 5 11	0	0
26	A	1	Total C N O 37 21 5 11	0	0
26	A	1	Total C N O 37 21 5 11	0	0
26	A	1	Total C N O 37 21 5 11	0	0

- Molecule 27 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 28 is water.

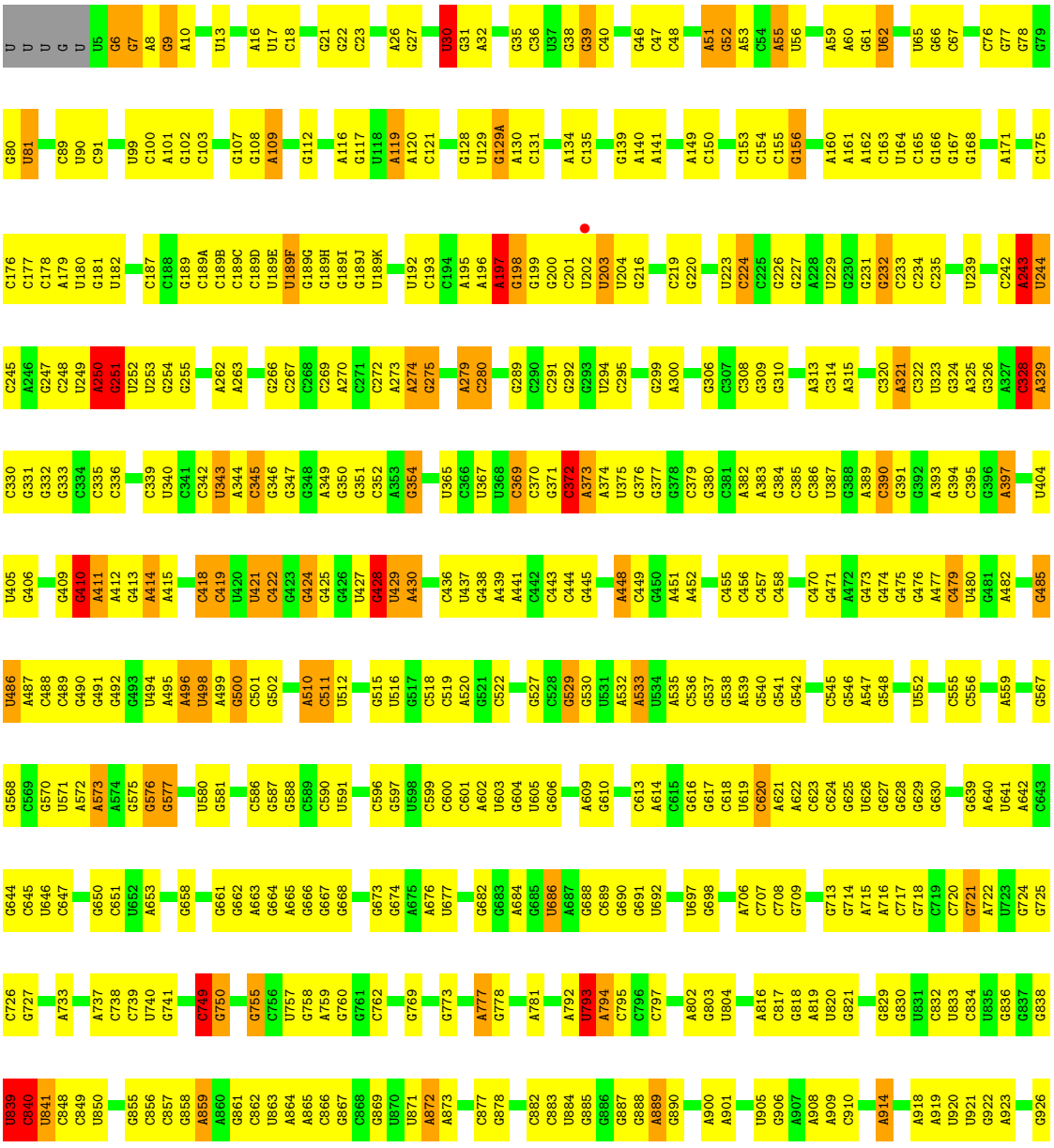
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	A	1	Total O 1 1	0	0

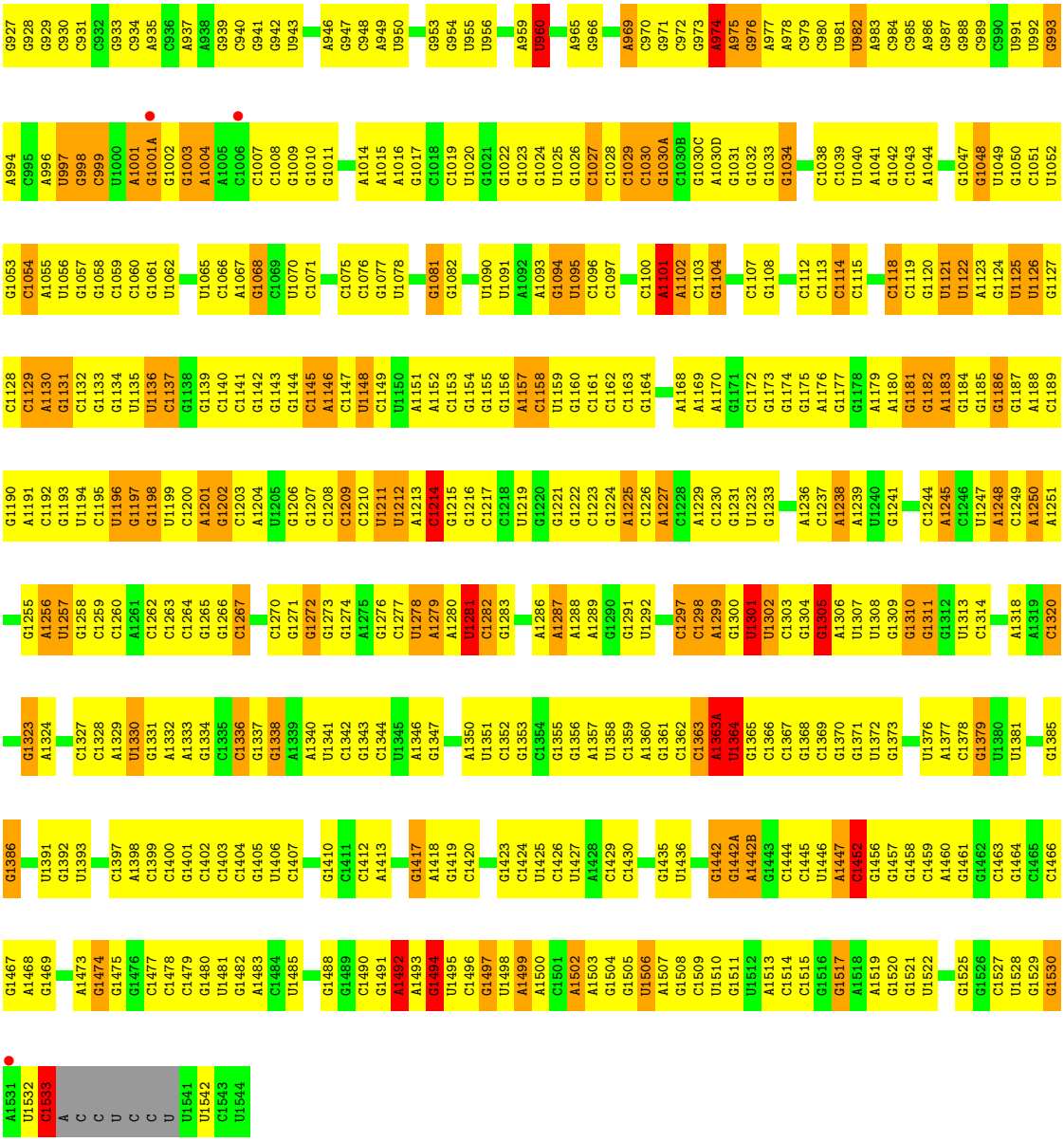
3 Residue-property plots (i)

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 RIBOSOMAL RNA

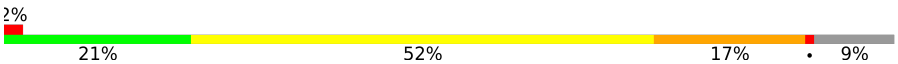
Chain A:

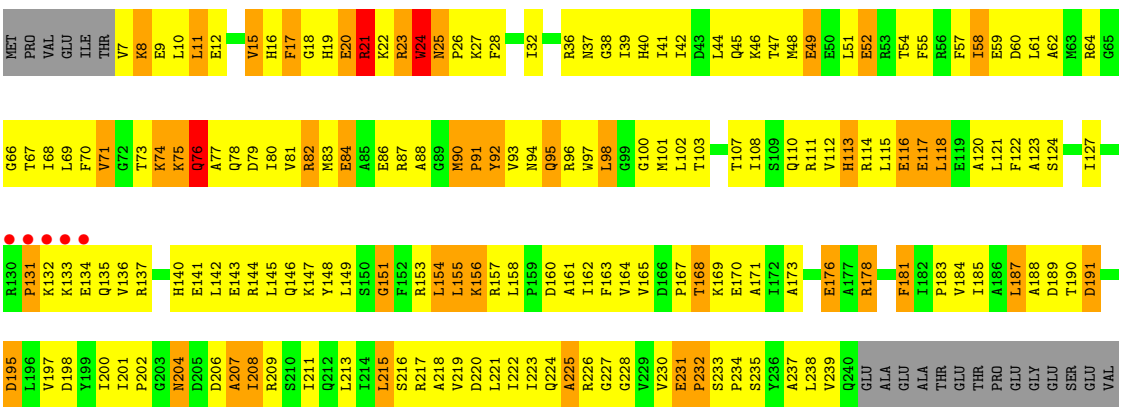




• Molecule 2: 30S RIBOSOMAL PROTEIN S2

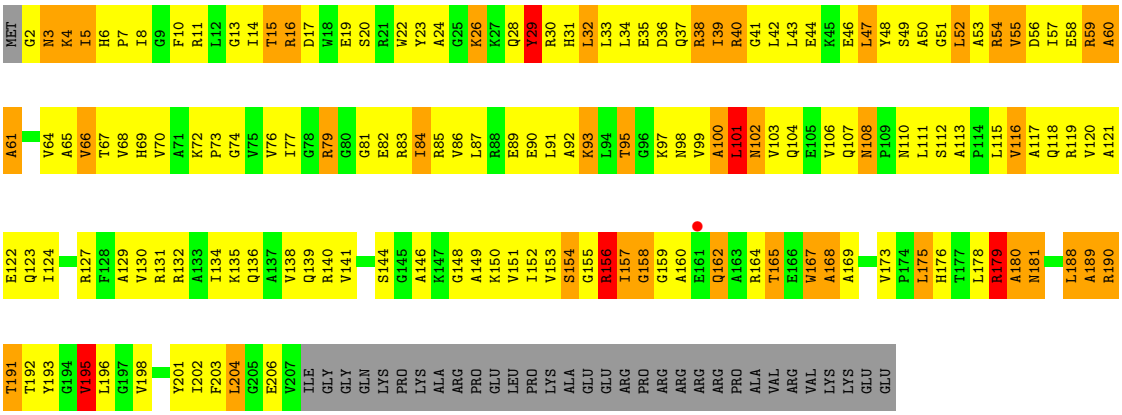
Chain B:





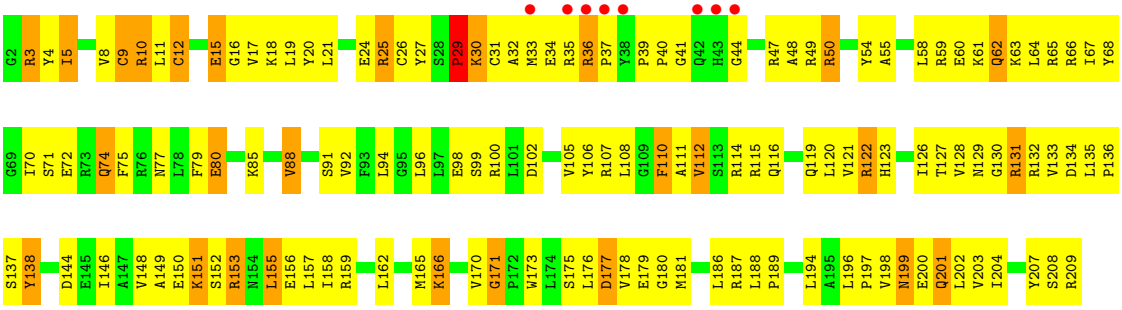
• Molecule 3: 30S RIBOSOMAL PROTEIN S3

Chain C:



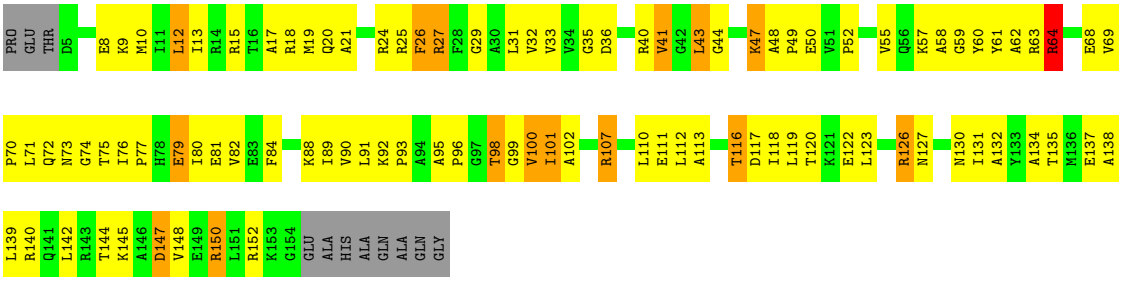
• Molecule 4: 30S RIBOSOMAL PROTEIN S4

Chain D:



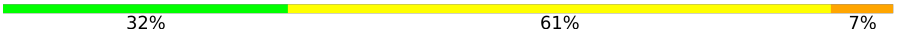
• Molecule 5: 30S RIBOSOMAL PROTEIN S5

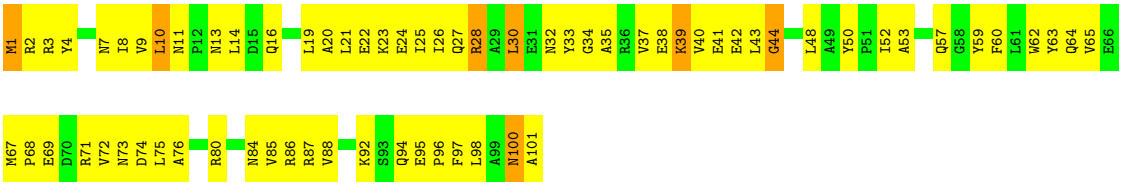
Chain E:



• Molecule 6: 30S RIBOSOMAL PROTEIN S6

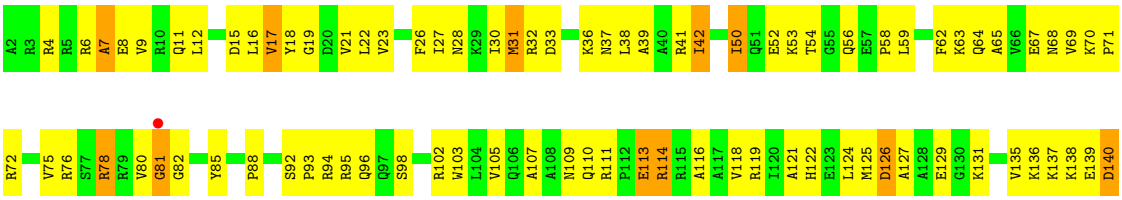
Chain F:

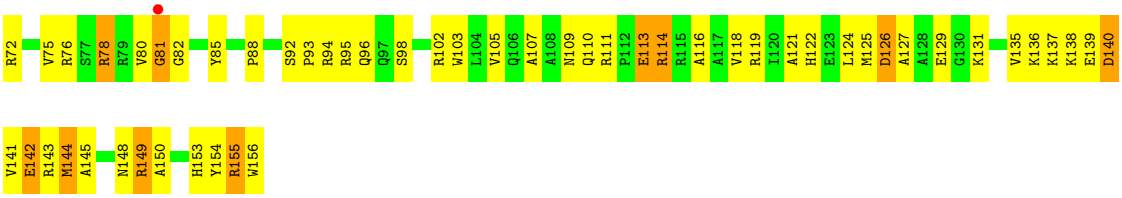




• Molecule 7: 30S RIBOSOMAL PROTEIN S7

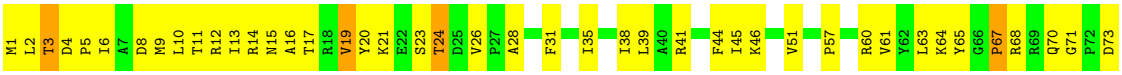
Chain G:





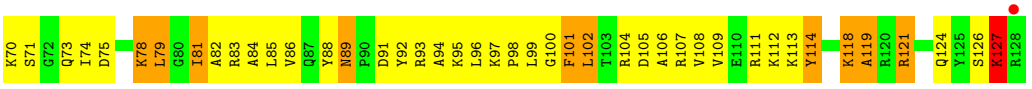
• Molecule 8: 30S RIBOSOMAL PROTEIN S8

Chain H:



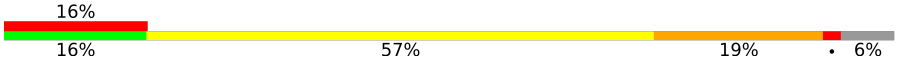
• Molecule 9: 30S RIBOSOMAL PROTEIN S9

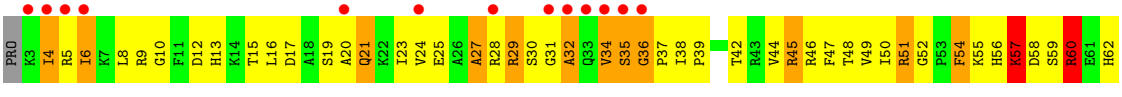
Chain I:

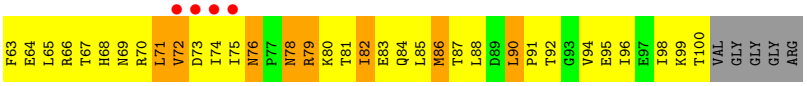


• Molecule 10: 30S RIBOSOMAL PROTEIN S10

Chain J:

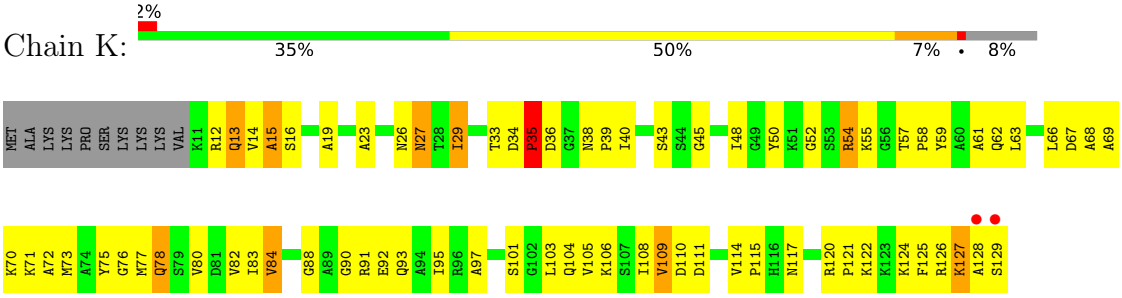






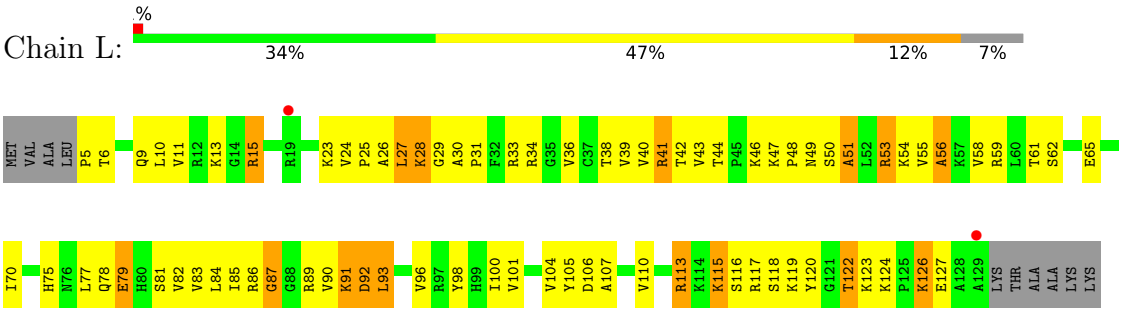
• Molecule 11: 30S RIBOSOMAL PROTEIN S11

Chain K:



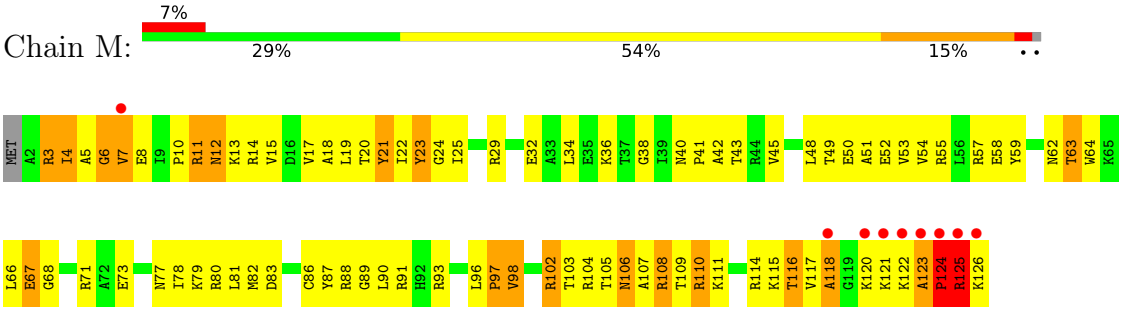
• Molecule 12: 30S RIBOSOMAL PROTEIN S12

Chain L:



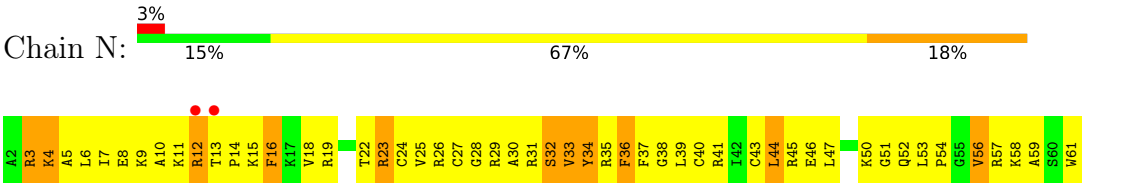
• Molecule 13: 30S RIBOSOMAL PROTEIN S13

Chain M:



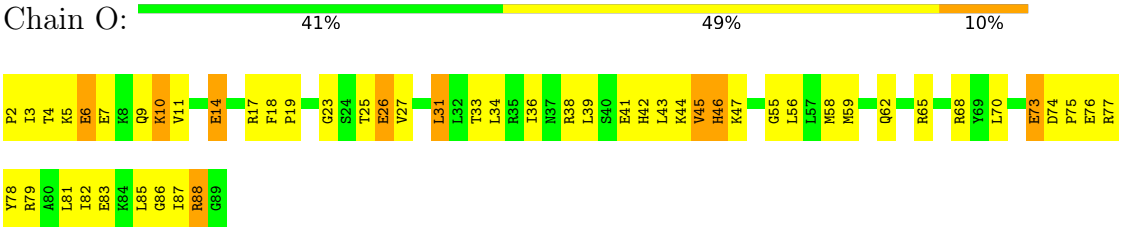
• Molecule 14: 30S RIBOSOMAL PROTEIN S14

Chain N:



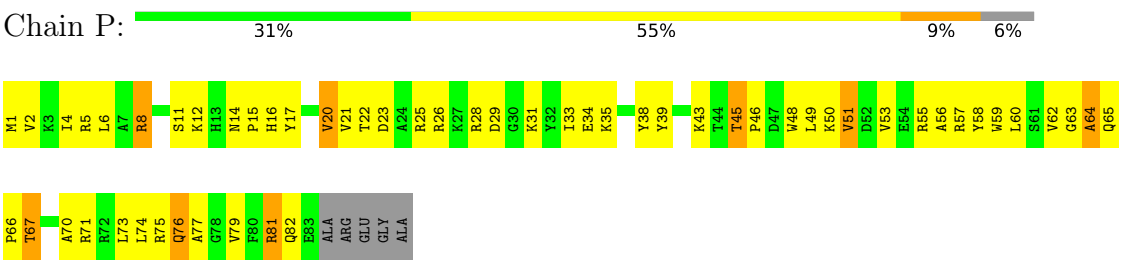
• Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain O:



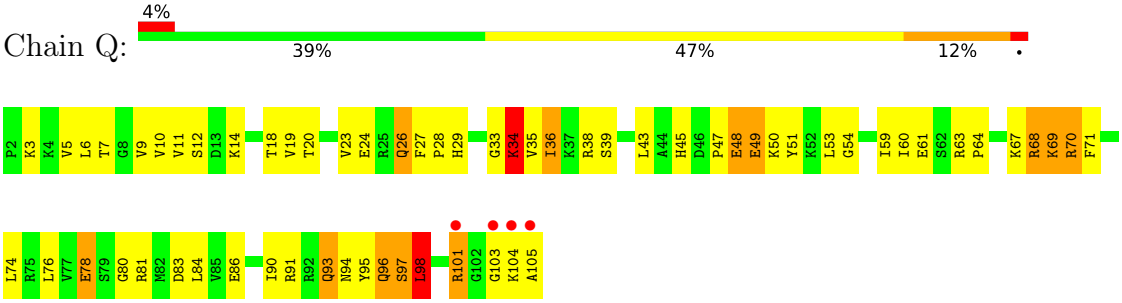
• Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain P:



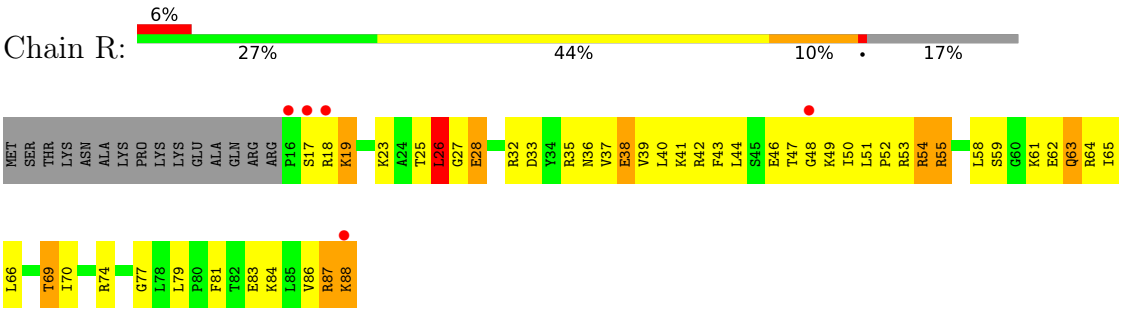
• Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain Q:



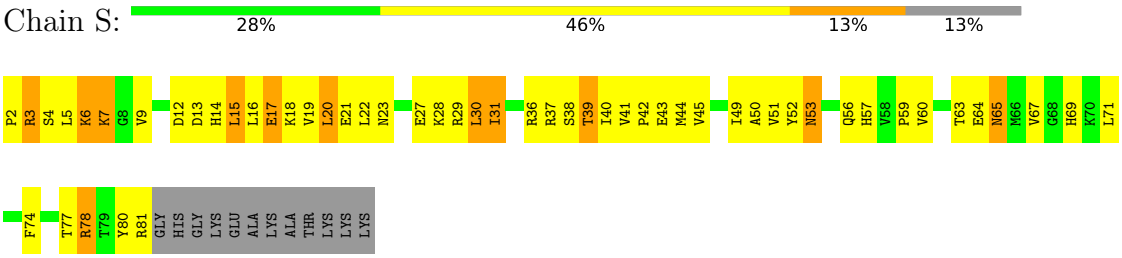
• Molecule 18: 30S RIBOSOMAL PROTEIN S18

Chain R:



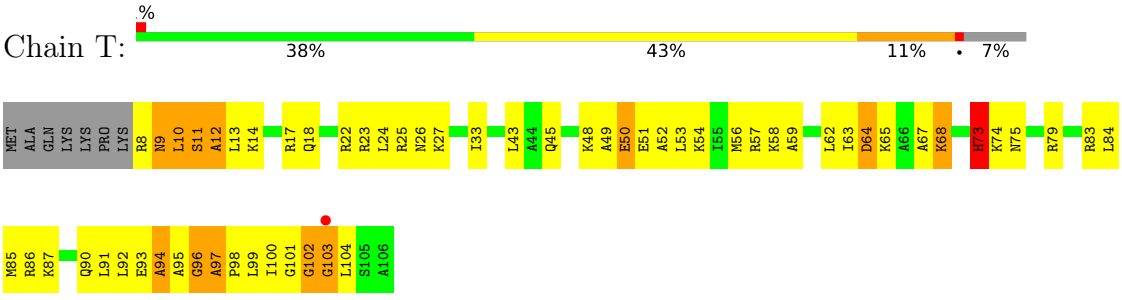
• Molecule 19: 30S RIBOSOMAL PROTEIN S19

Chain S:



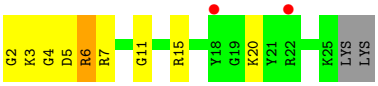
• Molecule 20: 30S RIBOSOMAL PROTEIN S20

Chain T:



• Molecule 21: 30S RIBOSOMAL PROTEIN THX

Chain V:

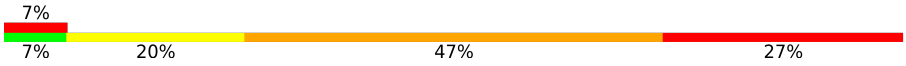


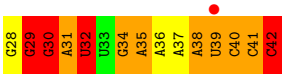
• Molecule 22: 5'-R(*UP*UP*CP*AP*AP*AP)-3'

Chain W:

• Molecule 23: 5'-R(*GP*GP*GP*AP*UP*UP*GP*AP*AP*AP*AP*UP*CP*CP*C)-3'

Chain Z:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	402.18Å 402.18Å 175.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.50 39.77 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (40.00-3.50) 99.8 (39.77-3.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.25 (at 3.48Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.193 , 0.235 0.199 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	119.8	Xtriage
Anisotropy	0.253	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 127.8	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	0.94	EDS
Total number of atoms	52514	wwPDB-VP
Average B, all atoms (Å^2)	126.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.45% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: K, ZN, AM2, MG

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	0.51	8/36318 (0.0%)	0.74	31/56682 (0.1%)
2	B	0.37	0/1935	0.68	0/2609
3	C	0.39	0/1636	0.67	0/2205
4	D	0.36	0/1732	0.65	0/2318
5	E	0.43	0/1162	0.74	1/1564 (0.1%)
6	F	0.33	0/855	0.62	0/1154
7	G	0.37	0/1275	0.60	0/1709
8	H	0.42	0/1135	0.75	0/1527
9	I	0.37	0/1028	0.68	0/1378
10	J	0.38	0/807	0.66	0/1085
11	K	0.37	0/899	0.67	0/1213
12	L	0.46	0/987	0.75	0/1322
13	M	0.36	0/1007	0.67	0/1347
14	N	0.42	0/500	0.69	0/664
15	O	0.35	0/744	0.59	0/992
16	P	0.41	0/716	0.71	0/963
17	Q	0.41	0/869	0.71	0/1159
18	R	0.34	0/602	0.62	0/799
19	S	0.35	0/661	0.66	0/890
20	T	0.40	0/763	0.75	1/1006 (0.1%)
21	V	0.48	0/212	0.63	0/277
22	W	2.62	10/137 (7.3%)	0.91	1/211 (0.5%)
23	Z	1.61	1/357 (0.3%)	0.93	1/555 (0.2%)
All	All	0.50	19/56337 (0.0%)	0.72	35/83629 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	8	22
22	W	0	1
23	Z	0	3
All	All	8	26

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1533	C	N1-C2	15.01	1.55	1.40
1	A	1533	C	C4-C5	13.16	1.53	1.43
22	W	6	A	C5-C4	12.22	1.47	1.38
22	W	6	A	N9-C8	11.21	1.46	1.37
22	W	6	A	C2-N3	10.77	1.43	1.33
22	W	6	A	N1-C2	9.96	1.43	1.34
1	A	1533	C	C2-O2	9.72	1.33	1.24
22	W	6	A	C6-N1	9.08	1.42	1.35
1	A	1533	C	N3-C4	8.82	1.40	1.33
22	W	6	A	N3-C4	8.57	1.40	1.34
22	W	6	A	C5-C6	8.23	1.48	1.41
1	A	1533	C	C2-N3	8.07	1.42	1.35
1	A	1533	C	C4-N4	7.47	1.40	1.33
22	W	6	A	N7-C5	7.11	1.43	1.39
1	A	1533	C	C5-C6	6.42	1.39	1.34
22	W	6	A	C8-N7	6.23	1.35	1.31
1	A	1533	C	N1-C6	6.12	1.40	1.37
22	W	6	A	N9-C4	5.79	1.41	1.37
23	Z	42	C	N1-C2	5.25	1.45	1.40

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1363(A)	A	C2'-C3'-O3'	9.91	131.30	109.50
1	A	243	A	C2'-C3'-O3'	9.00	129.30	109.50
1	A	1452	C	C2'-C3'-O3'	8.70	128.64	109.50
1	A	410	G	C2'-C3'-O3'	8.31	127.78	109.50
1	A	119	A	C2'-C3'-O3'	7.75	126.55	109.50
1	A	51	A	C2'-C3'-O3'	7.56	126.13	109.50
1	A	30	U	N1-C1'-C2'	7.27	123.45	114.00
22	W	6	A	C2'-C3'-O3'	6.81	124.59	113.70
1	A	328	C	N1-C1'-C2'	6.80	122.84	114.00
1	A	793	U	C2'-C3'-O3'	6.54	124.16	113.70
1	A	428	G	N9-C1'-C2'	6.42	122.35	114.00
1	A	372	C	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	1214	C	N1-C1'-C2'	6.12	121.96	114.00
1	A	686	U	N1-C1'-C2'	6.09	121.92	114.00
20	T	12	ALA	N-CA-C	-5.93	94.98	111.00
1	A	1305	G	N9-C1'-C2'	5.92	121.69	114.00
1	A	30	U	C5'-C4'-C3'	5.76	125.21	116.00
1	A	840	C	N1-C1'-C2'	5.73	121.45	114.00
1	A	749	C	N1-C1'-C2'	-5.69	105.74	112.00
1	A	793	U	N1-C1'-C2'	5.69	121.40	114.00
1	A	1502	A	N9-C1'-C2'	5.64	121.33	114.00
1	A	1299	A	N9-C1'-C2'	5.55	121.21	114.00
1	A	203	U	O4'-C1'-N1	5.53	112.62	108.20
1	A	1301	U	N1-C1'-C2'	5.41	121.03	114.00
1	A	839	U	N1-C1'-C2'	5.40	121.02	114.00
5	E	64	ARG	N-CA-C	-5.38	96.47	111.00
1	A	197	A	N9-C1'-C2'	5.36	120.96	114.00
1	A	1488	G	C5'-C4'-C3'	-5.32	107.49	116.00
1	A	974	A	N9-C1'-C2'	5.30	120.89	114.00
1	A	686	U	O4'-C1'-N1	5.29	112.44	108.20
1	A	1305	G	C2'-C3'-O3'	5.18	121.98	113.70
1	A	577	G	C5'-C4'-C3'	-5.15	107.75	116.00
23	Z	30	G	C2'-C3'-O3'	5.06	121.80	113.70
1	A	1101	A	N9-C1'-C2'	5.03	120.54	114.00
1	A	960	U	N1-C1'-C2'	5.02	120.53	114.00

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	30	U	C4'
1	A	197	A	C4'
1	A	410	G	C3'
1	A	1181	G	C4'
1	A	1305	G	C3',C4'
1	A	1363(A)	A	C3'
1	A	1452	C	C3'

All (26) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1065	U	Sidechain
1	A	1094	G	Sidechain
1	A	112	G	Sidechain
1	A	1121	U	Sidechain

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Mol	Chain	Res	Type	Group
1	A	1186	G	Sidechain
1	A	1281	U	Sidechain
1	A	1310	G	Sidechain
1	A	1330	U	Sidechain
1	A	1364	U	Sidechain
1	A	1417	G	Sidechain
1	A	1492	A	Sidechain
1	A	1494	G	Sidechain
1	A	1533	C	Sidechain
1	A	239	U	Sidechain
1	A	250	A	Sidechain
1	A	251	G	Sidechain
1	A	424	G	Sidechain
1	A	516	U	Sidechain
1	A	529	G	Sidechain
1	A	575	G	Sidechain
1	A	740	U	Sidechain
1	A	773	G	Sidechain
22	W	1	U	Sidechain
23	Z	29	G	Sidechain
23	Z	32	U	Sidechain
23	Z	35	A	Sidechain

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	32446	0	16380	1059	0
2	B	1900	0	1951	285	0
3	C	1612	0	1677	243	0
4	D	1702	0	1762	184	0
5	E	1146	0	1207	115	0
6	F	842	0	857	89	0
7	G	1256	0	1295	94	0
8	H	1115	0	1177	92	0
9	I	1010	0	1043	122	0
10	J	794	0	840	146	0
11	K	884	0	904	92	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	L	971	0	1057	97	0
13	M	996	0	1072	107	0
14	N	491	0	529	90	0
15	O	733	0	771	61	0
16	P	700	0	720	68	0
17	Q	856	0	930	69	0
18	R	596	0	668	80	0
19	S	647	0	673	85	0
20	T	761	0	859	70	0
21	V	208	0	221	14	0
22	W	123	0	66	5	0
23	Z	319	0	164	32	0
24	A	190	0	0	0	0
24	D	1	0	0	0	0
24	F	1	0	0	0	0
24	G	2	0	0	0	0
24	H	1	0	0	0	0
24	J	1	0	0	0	0
24	K	1	0	0	0	0
24	L	1	0	0	0	0
24	M	1	0	0	0	0
24	S	1	0	0	0	0
24	W	2	0	0	0	0
24	Z	1	0	0	0	0
25	A	14	0	0	0	0
25	V	1	0	0	0	0
26	A	185	0	205	9	0
27	D	1	0	0	0	0
27	N	1	0	0	0	0
28	A	1	0	0	0	0
All	All	52514	0	37028	3057	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 34.

All (3057) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1113:C:C2'	1:A:1114:C:H5'	1.60	1.28
1:A:1147:C:H2'	1:A:1148:U:H5"	1.25	1.12
4:D:98:GLU:HG2	4:D:189:PRO:HG3	1.32	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1271:G:H2'	1:A:1272:G:H5"	1.22	1.11
1:A:972:C:H4'	10:J:57:LYS:HG2	1.30	1.10
1:A:1244:C:H2'	1:A:1245:A:H5"	1.28	1.10
4:D:62:GLN:HA	4:D:62:GLN:HE21	1.14	1.09
3:C:79:ARG:H	3:C:79:ARG:HD3	1.17	1.08
6:F:30:LEU:HB3	6:F:35:ALA:HB3	1.21	1.08
20:T:50:GLU:HA	20:T:100:ILE:HD11	1.27	1.08
1:A:243:A:H4'	1:A:244:U:H5'	1.29	1.07
2:B:91:PRO:HG3	2:B:154:LEU:HB2	1.30	1.07
1:A:1047:G:H2'	1:A:1048:G:H5"	1.35	1.07
14:N:26:ARG:HH12	14:N:47:LEU:HD21	1.18	1.07
19:S:39:THR:HG22	19:S:40:ILE:H	1.11	1.07
19:S:28:LYS:HG3	19:S:29:ARG:H	1.20	1.06
1:A:991:U:H3	1:A:1212:U:H1'	1.17	1.06
3:C:26:LYS:H	3:C:26:LYS:HD3	1.18	1.06
6:F:28:ARG:HH11	6:F:28:ARG:HB2	1.17	1.05
3:C:44:GLU:HA	3:C:52:LEU:HD21	1.35	1.05
1:A:1157:A:H5'	1:A:1158:C:C6	1.92	1.04
1:A:1047:G:C2'	1:A:1048:G:H5"	1.88	1.04
10:J:49:VAL:HG13	14:N:41:ARG:HB2	1.37	1.03
1:A:1029:C:H3'	1:A:1030:C:H5"	1.40	1.03
2:B:116:GLU:HA	2:B:153:ARG:HH22	1.18	1.02
5:E:101:ILE:HD13	5:E:119:LEU:HD23	1.40	1.02
4:D:187:ARG:NE	4:D:188:LEU:H	1.56	1.02
1:A:498:U:H2'	1:A:499:A:H5"	1.41	1.02
3:C:64:VAL:HB	3:C:99:VAL:HG21	1.43	1.01
1:A:1113:C:H2'	1:A:1114:C:H5'	1.01	1.00
2:B:18:GLY:HA2	2:B:42:ILE:HG12	1.40	0.99
3:C:91:LEU:HD11	3:C:99:VAL:HG23	1.44	0.99
1:A:1115:C:H42	1:A:1185:G:H1	1.05	0.99
4:D:187:ARG:HE	4:D:188:LEU:H	1.11	0.98
1:A:329:A:C5	1:A:332:G:C6	2.52	0.97
1:A:991:U:N3	1:A:1212:U:H1'	1.79	0.97
1:A:1113:C:C2'	1:A:1114:C:C5'	2.43	0.97
1:A:329:A:C8	1:A:332:G:O6	2.17	0.97
1:A:1314:C:OP2	19:S:6:LYS:HD3	1.65	0.97
1:A:223:U:H2'	1:A:224:C:H5"	1.42	0.97
9:I:127:LYS:H	9:I:127:LYS:HD2	1.28	0.96
18:R:38:GLU:HA	18:R:41:LYS:HE2	1.45	0.96
9:I:114:TYR:HD2	10:J:60:ARG:HB2	1.27	0.96
10:J:79:ARG:HH11	10:J:79:ARG:HA	1.30	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:8:LEU:HD12	10:J:20:ALA:HB2	1.45	0.96
3:C:83:ARG:HA	3:C:86:VAL:HG23	1.47	0.96
23:Z:30:G:H2'	23:Z:31:A:H8	1.31	0.96
4:D:3:ARG:HH21	4:D:74:GLN:HG3	1.30	0.95
1:A:1158:C:H3'	1:A:1158:C:O2	1.65	0.95
10:J:4:ILE:HD13	10:J:4:ILE:H	1.30	0.95
9:I:3:GLN:HA	9:I:3:GLN:HE21	1.32	0.95
1:A:998:G:H3'	1:A:999:C:H5"	1.46	0.94
1:A:1271:G:C2'	1:A:1272:G:H5"	1.96	0.94
1:A:1502:A:H2	1:A:1505:G:H1	1.14	0.94
1:A:996:A:H3'	1:A:997:U:H5"	1.50	0.93
3:C:14:ILE:HG22	3:C:15:THR:H	1.33	0.93
12:L:55:VAL:HG12	12:L:56:ALA:H	1.33	0.93
1:A:1147:C:C2'	1:A:1148:U:H5"	1.99	0.93
1:A:141:A:H1'	1:A:182:U:O2	1.69	0.92
2:B:7:VAL:HG12	2:B:8:LYS:H	1.33	0.92
10:J:29:ARG:HB2	10:J:29:ARG:HH11	1.33	0.92
10:J:32:ALA:HB3	10:J:75:ILE:HG23	1.48	0.92
1:A:1129:C:O2'	1:A:1131:G:H5"	1.70	0.92
9:I:9:ARG:HG2	9:I:14:VAL:HG12	1.52	0.92
23:Z:30:G:H2'	23:Z:31:A:C8	2.04	0.91
2:B:103:THR:HG23	2:B:176:GLU:OE1	1.70	0.91
18:R:55:ARG:NH1	18:R:55:ARG:HB3	1.85	0.91
1:A:1115:C:O2'	14:N:61:TRP:HB2	1.68	0.91
23:Z:34:G:H2'	23:Z:35:A:C8	2.06	0.91
1:A:1115:C:H1'	14:N:61:TRP:HA	1.50	0.91
3:C:130:VAL:O	3:C:134:ILE:HG12	1.72	0.90
1:A:155:C:H2'	1:A:156:G:H5"	1.53	0.90
2:B:98:LEU:HD23	2:B:98:LEU:H	1.33	0.90
3:C:157:ILE:HG21	3:C:164:ARG:HH21	1.37	0.90
4:D:50:ARG:NH1	4:D:50:ARG:HB3	1.85	0.90
4:D:199:ASN:HD21	4:D:201:GLN:HB2	1.36	0.89
1:A:1244:C:C2'	1:A:1245:A:H5"	2.01	0.89
9:I:97:LYS:HA	9:I:102:LEU:HD13	1.54	0.89
1:A:586:C:H2'	1:A:587:G:H5"	1.54	0.89
18:R:59:SER:HB3	18:R:62:GLU:HG3	1.55	0.88
1:A:477:A:H2'	1:A:479:C:H5"	1.56	0.88
3:C:93:LYS:HE2	3:C:93:LYS:HA	1.55	0.88
9:I:17:VAL:HG22	9:I:63:ILE:HD12	1.52	0.88
1:A:1473:A:H2'	1:A:1474:G:H5"	1.56	0.88
13:M:117:VAL:HG12	13:M:118:ALA:H	1.37	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:82:ARG:HA	2:B:92:TYR:CE2	2.09	0.87
1:A:479:C:H5'	1:A:479:C:H6	1.39	0.87
4:D:121:VAL:HG22	4:D:126:ILE:HD12	1.55	0.87
4:D:150:GLU:HG2	4:D:153:ARG:NH2	1.90	0.87
1:A:1060:C:C5	3:C:2:GLY:HA3	2.09	0.87
2:B:218:ALA:O	2:B:222:ILE:HG13	1.75	0.87
1:A:1250:A:H4'	9:I:68:GLY:H	1.38	0.87
1:A:38:G:H22	1:A:397:A:H5'	1.40	0.86
1:A:135:C:O2	16:P:1:MET:HB2	1.73	0.86
1:A:329:A:N7	1:A:332:G:C6	2.43	0.86
1:A:1038:C:H2'	1:A:1039:C:C6	2.11	0.86
4:D:64:LEU:HD12	4:D:75:PHE:HZ	1.40	0.86
11:K:54:ARG:HB3	11:K:54:ARG:HH11	1.40	0.86
1:A:1022:G:H2'	1:A:1023:G:H8	1.41	0.86
1:A:1301:U:H3'	1:A:1302:U:H5'	1.57	0.86
2:B:78:GLN:HE22	2:B:96:ARG:HH12	1.21	0.86
1:A:1103:C:H2'	1:A:1104:G:H5"	1.57	0.86
1:A:939:G:H5"	7:G:102:ARG:NH2	1.91	0.85
1:A:1144:G:H21	1:A:1146:A:H62	1.20	0.85
10:J:31:GLY:HA2	10:J:78:ASN:HD22	1.40	0.85
14:N:26:ARG:HG3	14:N:27:CYS:H	1.41	0.85
8:H:17:THR:HG22	8:H:63:LEU:HD13	1.56	0.85
3:C:108:ASN:HD21	3:C:144:SER:HB2	1.41	0.85
1:A:1314:C:C5	19:S:6:LYS:HE2	2.11	0.85
11:K:54:ARG:O	11:K:57:THR:HG22	1.77	0.85
19:S:42:PRO:O	19:S:45:VAL:HG23	1.77	0.85
3:C:79:ARG:HE	3:C:82:GLU:HG2	1.41	0.84
13:M:91:ARG:HB2	13:M:98:VAL:HG23	1.58	0.84
1:A:1132:C:H2'	1:A:1133:G:C8	2.11	0.84
7:G:54:THR:HG22	7:G:56:GLN:H	1.43	0.84
13:M:15:VAL:HG23	13:M:43:THR:O	1.76	0.84
1:A:1247:U:H2'	1:A:1248:A:H5"	1.58	0.84
10:J:94:VAL:HG12	10:J:95:GLU:H	1.42	0.84
18:R:47:THR:HA	18:R:83:GLU:HB2	1.58	0.84
1:A:1047:G:H2'	1:A:1048:G:C5'	2.08	0.83
11:K:54:ARG:HB3	11:K:54:ARG:NH1	1.93	0.83
12:L:83:VAL:HG21	12:L:100:ILE:HG23	1.60	0.83
1:A:877:C:O2	8:H:3:THR:HG21	1.76	0.83
1:A:1247:U:C2'	1:A:1248:A:H5"	2.07	0.83
5:E:15:ARG:HD3	5:E:26:PHE:CD1	2.13	0.83
19:S:39:THR:HG22	19:S:40:ILE:N	1.91	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:43:LEU:HD11	5:E:132:ALA:HB1	1.60	0.83
9:I:127:LYS:HB2	13:M:126:LYS:NZ	1.93	0.83
16:P:6:LEU:HB3	16:P:17:TYR:HD2	1.42	0.83
1:A:838:G:H2'	1:A:839:U:H5"	1.60	0.83
13:M:34:LEU:HD13	13:M:41:PRO:HA	1.61	0.83
2:B:16:HIS:HA	2:B:204:ASN:OD1	1.79	0.83
20:T:50:GLU:O	20:T:100:ILE:HG13	1.79	0.83
1:A:1113:C:H2'	1:A:1114:C:C5'	1.98	0.82
4:D:105:VAL:HG21	4:D:126:ILE:HD13	1.60	0.82
10:J:32:ALA:HB3	10:J:75:ILE:CG2	2.08	0.82
13:M:62:ASN:O	13:M:63:THR:HB	1.79	0.82
13:M:81:LEU:HD22	13:M:88:ARG:HH21	1.44	0.82
19:S:28:LYS:HG3	19:S:29:ARG:N	1.94	0.82
1:A:231:G:H2'	1:A:232:G:H5"	1.61	0.82
2:B:223:ILE:HG21	2:B:230:VAL:HG22	1.59	0.82
3:C:26:LYS:H	3:C:26:LYS:CD	1.90	0.82
1:A:1001(A):G:H2'	1:A:1002:G:O4'	1.80	0.82
1:A:9:G:OP1	5:E:122:GLU:HG3	1.79	0.82
1:A:62:U:O2'	1:A:379:C:H1'	1.80	0.82
2:B:76:GLN:HG3	2:B:206:ASP:OD1	1.79	0.82
3:C:59:ARG:HH12	3:C:97:LYS:HE2	1.44	0.82
6:F:26:ILE:HG21	6:F:63:TYR:CE2	2.15	0.82
10:J:27:ALA:HB2	10:J:85:LEU:HD21	1.62	0.82
19:S:52:TYR:HA	19:S:56:GLN:O	1.80	0.82
9:I:53:VAL:HG21	9:I:85:LEU:HD21	1.61	0.82
1:A:1163:C:H2'	1:A:1164:G:H8	1.42	0.82
2:B:116:GLU:HA	2:B:153:ARG:NH2	1.95	0.82
4:D:187:ARG:HE	4:D:188:LEU:N	1.77	0.82
19:S:28:LYS:CG	19:S:29:ARG:H	1.93	0.82
5:E:101:ILE:HD12	5:E:118:ILE:O	1.79	0.81
20:T:73:HIS:O	20:T:74:LYS:HG2	1.80	0.81
10:J:4:ILE:HD13	10:J:4:ILE:N	1.95	0.81
1:A:223:U:C2'	1:A:224:C:H5"	2.11	0.81
3:C:110:ASN:ND2	3:C:140:ARG:HB3	1.95	0.81
17:Q:78:GLU:OE2	17:Q:81:ARG:HD2	1.79	0.81
1:A:1101:A:H4'	1:A:1102:A:O5'	1.80	0.81
3:C:155:GLY:O	3:C:156:ARG:HB2	1.78	0.81
10:J:6:ILE:HD11	10:J:73:ASP:H	1.44	0.81
3:C:131:ARG:O	3:C:135:LYS:HG3	1.81	0.81
1:A:718:G:H5'	11:K:117:ASN:ND2	1.95	0.81
21:V:6:ARG:NE	21:V:15:ARG:HH12	1.79	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1210:C:H3'	1:A:1211:U:H5"	1.62	0.81
2:B:136:VAL:O	2:B:140:HIS:HB2	1.80	0.81
3:C:26:LYS:HD3	3:C:26:LYS:N	1.96	0.81
11:K:84:VAL:HG23	11:K:110:ASP:HA	1.63	0.80
2:B:19:HIS:NE2	2:B:206:ASP:HB3	1.95	0.80
2:B:116:GLU:HG2	2:B:153:ARG:NH1	1.96	0.80
10:J:94:VAL:HG12	10:J:95:GLU:N	1.96	0.80
3:C:79:ARG:H	3:C:79:ARG:CD	1.95	0.80
8:H:20:TYR:HE2	8:H:75:ARG:HD2	1.45	0.80
5:E:150:ARG:HH11	5:E:150:ARG:CB	1.95	0.80
1:A:1158:C:O2	1:A:1158:C:C3'	2.30	0.80
8:H:51:VAL:HG21	8:H:60:ARG:NH2	1.95	0.80
1:A:954:G:H2'	1:A:955:U:C6	2.17	0.80
1:A:1048:G:H5'	1:A:1048:G:H8	1.45	0.80
2:B:19:HIS:HE2	2:B:206:ASP:HB3	1.46	0.80
19:S:63:THR:HG22	19:S:64:GLU:H	1.46	0.79
1:A:1121:U:O2'	1:A:1122:U:H5'	1.80	0.79
4:D:62:GLN:HA	4:D:62:GLN:NE2	1.96	0.79
20:T:56:MET:HG3	20:T:84:LEU:CD1	2.12	0.79
2:B:71:VAL:O	2:B:165:VAL:HG23	1.81	0.79
4:D:158:ILE:H	4:D:158:ILE:HD12	1.48	0.79
1:A:232:G:H5'	1:A:232:G:H8	1.46	0.79
1:A:243:A:C4'	1:A:244:U:H5'	2.12	0.79
1:A:1060:C:H5"	10:J:51:ARG:HG2	1.62	0.79
1:A:1115:C:H1'	14:N:61:TRP:CA	2.11	0.79
4:D:153:ARG:HG2	4:D:181:MET:CE	2.12	0.79
4:D:162:LEU:HD13	4:D:181:MET:HG2	1.63	0.79
12:L:117:ARG:HD2	12:L:123:LYS:O	1.82	0.79
1:A:1125:U:H5"	1:A:1126:U:H5	1.46	0.79
1:A:1157:A:H5'	1:A:1158:C:N1	1.96	0.79
12:L:110:VAL:HG21	12:L:113:ARG:HG3	1.63	0.79
17:Q:63:ARG:HG2	17:Q:64:PRO:HD2	1.65	0.79
1:A:1491:G:H21	26:A:3001:AM2:HB61	1.46	0.79
1:A:427:U:H3'	1:A:428:G:H5"	1.65	0.79
1:A:1163:C:H2'	1:A:1164:G:C8	2.18	0.79
9:I:99:LEU:HB3	9:I:101:PHE:HE1	1.48	0.79
9:I:114:TYR:CD2	10:J:60:ARG:HB2	2.16	0.79
3:C:132:ARG:HA	3:C:135:LYS:HE2	1.63	0.79
1:A:888:G:H3'	1:A:889:A:H5"	1.63	0.78
1:A:984:C:H2'	1:A:985:C:H6	1.49	0.78
14:N:32:SER:HB2	14:N:40:CYS:HB2	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:32:ARG:HH21	18:R:65:ILE:HD12	1.47	0.78
2:B:10:LEU:HD23	2:B:11:LEU:HG	1.65	0.78
14:N:26:ARG:NH1	14:N:47:LEU:HD21	1.97	0.78
2:B:219:VAL:HA	2:B:222:ILE:HD12	1.65	0.78
18:R:55:ARG:HB3	18:R:55:ARG:HH11	1.46	0.78
1:A:498:U:C2'	1:A:499:A:H5"	2.12	0.78
3:C:70:VAL:O	3:C:106:VAL:HG23	1.82	0.78
12:L:27:LEU:HG	12:L:28:LYS:H	1.49	0.78
1:A:1029:C:C3'	1:A:1030:C:H5"	2.12	0.78
5:E:127:ASN:HD22	5:E:130:ASN:ND2	1.81	0.78
1:A:129(A):G:O2'	1:A:189(F):U:H2'	1.84	0.77
20:T:68:LYS:HE3	20:T:68:LYS:HA	1.65	0.77
4:D:176:LEU:HG	4:D:177:ASP:H	1.48	0.77
9:I:99:LEU:HB3	9:I:101:PHE:CE1	2.19	0.77
19:S:63:THR:HB	19:S:65:ASN:HD21	1.49	0.77
1:A:344:A:H3'	1:A:345:C:H5"	1.66	0.77
3:C:79:ARG:NE	3:C:82:GLU:HG2	2.00	0.77
18:R:25:THR:O	18:R:26:LEU:HB2	1.82	0.77
1:A:1113:C:O2'	1:A:1114:C:C5'	2.32	0.77
1:A:250:A:H1'	1:A:252:U:C6	2.20	0.77
1:A:231:G:C2'	1:A:232:G:H5"	2.14	0.77
4:D:64:LEU:HD12	4:D:75:PHE:CZ	2.18	0.77
9:I:70:LYS:O	9:I:74:ILE:HG13	1.84	0.77
16:P:74:LEU:O	16:P:79:VAL:HG23	1.84	0.77
1:A:155:C:C2'	1:A:156:G:H5"	2.15	0.77
1:A:1125:U:H5"	1:A:1126:U:C5	2.20	0.77
6:F:37:VAL:HA	6:F:65:VAL:HG12	1.67	0.77
1:A:1226:C:N4	13:M:104:ARG:HD2	2.00	0.77
1:A:1115:C:N4	1:A:1185:G:H1	1.83	0.76
1:A:1502:A:H2	1:A:1505:G:N1	1.83	0.76
2:B:140:HIS:HA	2:B:143:GLU:HG2	1.67	0.76
4:D:112:VAL:HG23	4:D:116:GLN:OE1	1.82	0.76
3:C:179:ARG:O	3:C:181:ASN:N	2.18	0.76
7:G:26:PHE:CE2	7:G:30:ILE:HD11	2.21	0.76
1:A:1391:U:H2'	1:A:1392:G:C8	2.20	0.76
10:J:29:ARG:HB2	10:J:29:ARG:NH1	2.01	0.76
10:J:50:ILE:H	10:J:50:ILE:HD12	1.49	0.76
1:A:329:A:N6	1:A:332:G:C2	2.54	0.76
1:A:1057:G:H5"	3:C:154:SER:OG	1.86	0.76
3:C:179:ARG:HG2	3:C:180:ALA:N	2.00	0.76
1:A:1263:C:H2'	1:A:1264:C:C6	2.20	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:989:C:H42	1:A:1216:G:H1	1.30	0.75
7:G:15:ASP:O	7:G:19:GLY:HA2	1.84	0.75
1:A:196:A:H2'	1:A:197:A:H5"	1.68	0.75
1:A:522:C:H41	12:L:53:ARG:HH22	1.32	0.75
4:D:79:PHE:HE1	4:D:204:ILE:HD13	1.52	0.75
1:A:1216:G:H5"	14:N:5:ALA:CB	2.16	0.75
4:D:3:ARG:NH2	4:D:70:ILE:HG13	2.02	0.75
8:H:51:VAL:HG11	8:H:60:ARG:HB2	1.67	0.75
8:H:80:ILE:N	8:H:80:ILE:HD12	2.01	0.75
1:A:385:C:H2'	1:A:386:C:H6	1.49	0.75
13:M:52:GLU:HG2	13:M:55:ARG:HH21	1.52	0.75
16:P:4:ILE:HG13	16:P:64:ALA:HB1	1.67	0.75
5:E:79:GLU:HG3	5:E:93:PRO:HD2	1.66	0.75
12:L:5:PRO:HG2	12:L:10:LEU:HD11	1.67	0.75
6:F:28:ARG:HB2	6:F:28:ARG:NH1	1.98	0.75
20:T:53:LEU:HD11	20:T:104:LEU:HD12	1.68	0.75
19:S:20:LEU:HA	19:S:23:ASN:HD22	1.50	0.75
1:A:1038:C:H2'	1:A:1039:C:H6	1.50	0.74
1:A:1142:G:H2'	1:A:1143:G:O4'	1.87	0.74
2:B:59:GLU:HB2	2:B:221:LEU:HD11	1.68	0.74
3:C:102:ASN:N	3:C:102:ASN:HD22	1.85	0.74
15:O:87:ILE:HG22	15:O:88:ARG:N	2.02	0.74
2:B:95:GLN:HE21	2:B:147:LYS:HG3	1.51	0.74
5:E:101:ILE:HD12	5:E:101:ILE:H	1.52	0.74
8:H:1:MET:HG2	8:H:2:LEU:H	1.52	0.74
3:C:64:VAL:CB	3:C:99:VAL:HG21	2.17	0.74
5:E:150:ARG:HH11	5:E:150:ARG:HB3	1.53	0.74
3:C:14:ILE:HG22	3:C:15:THR:N	2.02	0.74
1:A:1157:A:H4'	1:A:1158:C:O5'	1.86	0.74
5:E:81:GLU:HG3	5:E:90:VAL:HG22	1.68	0.74
23:Z:30:G:C2'	23:Z:31:A:H8	2.01	0.74
1:A:998:G:C3'	1:A:999:C:H5"	2.18	0.74
1:A:1227:A:H5'	13:M:111:LYS:HZ3	1.52	0.74
1:A:1250:A:H4'	9:I:68:GLY:N	2.02	0.74
1:A:1281:U:H5'	1:A:1282:C:H5	1.53	0.74
19:S:63:THR:HB	19:S:65:ASN:ND2	2.01	0.74
9:I:102:LEU:HD12	9:I:102:LEU:N	2.01	0.74
23:Z:34:G:H2'	23:Z:35:A:H8	1.50	0.74
2:B:111:ARG:HB3	2:B:149:LEU:HD11	1.69	0.74
14:N:12:ARG:O	14:N:14:PRO:HD3	1.87	0.74
10:J:8:LEU:HB3	10:J:16:LEU:HD22	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:720:C:H3'	1:A:721:G:H5"	1.68	0.73
1:A:1276:G:H2'	1:A:1277:C:H5"	1.70	0.73
1:A:1369:C:H2'	1:A:1370:G:C8	2.23	0.73
9:I:42:ARG:HH21	9:I:71:SER:HB2	1.52	0.73
17:Q:101:ARG:HA	17:Q:101:ARG:HE	1.52	0.73
1:A:1161:C:H2'	1:A:1162:C:C6	2.24	0.73
2:B:124:SER:O	2:B:127:ILE:HG13	1.87	0.73
5:E:69:VAL:HG21	5:E:113:ALA:HB1	1.70	0.73
10:J:81:THR:C	10:J:83:GLU:H	1.91	0.73
11:K:124:LYS:HD3	11:K:125:PHE:HE1	1.53	0.73
23:Z:39:U:H2'	23:Z:40:C:C6	2.23	0.73
1:A:954:G:H2'	1:A:955:U:H6	1.54	0.73
4:D:50:ARG:HB3	4:D:50:ARG:HH11	1.52	0.73
5:E:101:ILE:CD1	5:E:119:LEU:HD23	2.16	0.73
6:F:48:LEU:HG	6:F:57:GLN:HA	1.70	0.73
1:A:984:C:H2'	1:A:985:C:C6	2.23	0.73
1:A:1132:C:H2'	1:A:1133:G:H8	1.53	0.73
3:C:42:LEU:O	3:C:42:LEU:HD23	1.88	0.73
3:C:180:ALA:O	3:C:181:ASN:HB3	1.87	0.73
11:K:23:ALA:HB1	11:K:88:GLY:HA3	1.71	0.73
3:C:64:VAL:HB	3:C:99:VAL:CG2	2.17	0.73
1:A:996:A:C3'	1:A:997:U:H5"	2.19	0.73
1:A:21:G:H2'	1:A:22:G:C8	2.23	0.73
2:B:118:LEU:HD12	2:B:142:LEU:HD21	1.69	0.73
10:J:37:PRO:HA	10:J:72:VAL:HG22	1.69	0.73
10:J:49:VAL:O	10:J:60:ARG:HA	1.88	0.73
17:Q:67:LYS:HA	17:Q:70:ARG:HH12	1.54	0.73
19:S:22:LEU:HD13	19:S:28:LYS:HG2	1.71	0.73
1:A:342:C:H3'	1:A:343:U:H5"	1.71	0.73
2:B:78:GLN:NE2	2:B:96:ARG:HH12	1.86	0.73
13:M:108:ARG:NH1	13:M:114:ARG:HG2	2.03	0.73
1:A:477:A:C2'	1:A:479:C:H5"	2.19	0.72
1:A:676:A:H1'	11:K:115:PRO:HB3	1.71	0.72
1:A:1157:A:H5'	1:A:1158:C:C5	2.23	0.72
26:A:3001:AM2:HA93	26:A:3001:AM2:HB5	1.69	0.72
2:B:69:LEU:HD23	2:B:70:PHE:N	2.04	0.72
3:C:34:LEU:O	3:C:38:ARG:HG3	1.89	0.72
1:A:428:G:H1'	1:A:430:A:C8	2.23	0.72
1:A:1133:G:H2'	1:A:1134:G:H8	1.54	0.72
1:A:1420:C:H42	1:A:1480:G:H1	1.37	0.72
2:B:217:ARG:HA	2:B:220:ASP:OD2	1.87	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:6:GLY:HA3	9:I:83:ARG:HB2	1.71	0.72
19:S:63:THR:HG22	19:S:64:GLU:N	2.04	0.72
1:A:718:G:H5'	11:K:117:ASN:HD22	1.53	0.72
4:D:3:ARG:HH21	4:D:74:GLN:CG	2.00	0.72
3:C:91:LEU:HD21	3:C:99:VAL:H	1.54	0.72
1:A:38:G:N2	1:A:397:A:H5'	2.04	0.72
1:A:1264:C:H2'	1:A:1265:G:C8	2.25	0.72
2:B:91:PRO:HG2	2:B:155:LEU:HG	1.70	0.72
6:F:30:LEU:HB3	6:F:35:ALA:CB	2.13	0.72
1:A:1151:A:HO2'	1:A:1152:A:H8	1.35	0.72
1:A:576:G:H3'	1:A:577:G:C5'	2.20	0.72
2:B:69:LEU:HD12	2:B:155:LEU:HD11	1.71	0.72
2:B:101:MET:HA	2:B:108:ILE:HG21	1.72	0.72
12:L:41:ARG:HG3	12:L:42:THR:N	2.01	0.72
14:N:23:ARG:NH1	14:N:30:ALA:HB2	2.04	0.72
1:A:1417:G:OP2	26:A:3005:AM2:NC6	2.22	0.72
1:A:1053:G:HO2'	1:A:1199:U:H5	1.38	0.72
2:B:68:ILE:HG13	2:B:161:ALA:HB3	1.72	0.72
18:R:26:LEU:HD13	18:R:27:GLY:H	1.54	0.72
2:B:80:ILE:HG21	2:B:211:ILE:HG22	1.70	0.71
20:T:49:ALA:O	20:T:53:LEU:HD23	1.90	0.71
1:A:1113:C:O2'	1:A:1114:C:H5"	1.90	0.71
1:A:1256:A:O3'	1:A:1257:U:H4'	1.90	0.71
1:A:1399:C:H4'	1:A:1400:C:H5"	1.71	0.71
8:H:103:VAL:HG21	8:H:109:ILE:O	1.91	0.71
15:O:18:PHE:HB2	15:O:19:PRO:HD2	1.72	0.71
1:A:1262:C:H2'	1:A:1263:C:C6	2.26	0.71
4:D:24:GLU:O	4:D:25:ARG:HB3	1.91	0.71
11:K:95:ILE:HD12	11:K:95:ILE:H	1.55	0.71
19:S:39:THR:CG2	19:S:40:ILE:H	1.94	0.71
4:D:110:PHE:HD1	4:D:110:PHE:H	1.37	0.71
16:P:76:GLN:O	16:P:76:GLN:HG2	1.90	0.71
1:A:269:C:H2'	1:A:270:A:H8	1.56	0.71
1:A:329:A:C8	1:A:332:G:C6	2.77	0.71
3:C:83:ARG:C	3:C:85:ARG:H	1.91	0.71
12:L:93:LEU:HD23	12:L:93:LEU:H	1.55	0.71
3:C:19:GLU:HG2	3:C:54:ARG:NH1	2.04	0.71
15:O:27:VAL:HG12	15:O:31:LEU:HD22	1.73	0.71
1:A:479:C:H6	1:A:479:C:C5'	2.01	0.71
2:B:132:LYS:HA	2:B:135:GLN:HB2	1.72	0.71
7:G:50:ILE:HG21	7:G:58:PRO:HA	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:5:ARG:O	10:J:98:ILE:HA	1.90	0.71
26:A:3005:AM2:HC61	26:A:3005:AM2:HA21	1.39	0.71
3:C:23:TYR:CD1	3:C:24:ALA:N	2.58	0.71
8:H:79:VAL:HB	8:H:80:ILE:HD12	1.73	0.71
11:K:78:GLN:O	11:K:103:LEU:HD23	1.90	0.71
1:A:376:G:H2'	1:A:377:G:H8	1.56	0.71
3:C:55:VAL:O	3:C:55:VAL:HG12	1.90	0.71
2:B:115:LEU:HD12	2:B:145:LEU:HD22	1.72	0.70
8:H:46:LYS:HG3	8:H:64:LYS:HB2	1.72	0.70
8:H:64:LYS:HG2	8:H:79:VAL:HG21	1.72	0.70
9:I:48:GLU:N	9:I:49:PRO:HD2	2.05	0.70
1:A:180:U:C2'	1:A:181:G:H5'	2.21	0.70
1:A:692:U:OP1	11:K:124:LYS:HE2	1.90	0.70
8:H:51:VAL:CG1	8:H:60:ARG:HB2	2.20	0.70
14:N:40:CYS:O	14:N:44:LEU:HB3	1.92	0.70
1:A:1297:C:O2	1:A:1297:C:H2'	1.89	0.70
3:C:43:LEU:HD21	3:C:68:VAL:HG21	1.73	0.70
10:J:62:HIS:HB3	14:N:59:ALA:HB3	1.73	0.70
13:M:10:PRO:HB2	13:M:18:ALA:HB1	1.72	0.70
12:L:24:VAL:O	12:L:24:VAL:HG12	1.91	0.70
1:A:329:A:C6	1:A:332:G:C2	2.79	0.70
1:A:840:C:H4'	1:A:841:U:H5	1.56	0.70
1:A:1264:C:H2'	1:A:1265:G:H8	1.57	0.70
14:N:26:ARG:HH12	14:N:47:LEU:CD2	1.99	0.70
1:A:421:U:H5'	1:A:422:C:OP2	1.92	0.70
1:A:1114:C:O2	1:A:1115:C:C6	2.45	0.70
4:D:155:LEU:HB3	4:D:158:ILE:HD13	1.73	0.70
2:B:97:TRP:HZ2	2:B:102:LEU:HD13	1.57	0.70
13:M:40:ASN:HD22	13:M:41:PRO:CD	2.05	0.70
1:A:1010:G:H2'	1:A:1011:G:H8	1.56	0.70
4:D:62:GLN:HE21	4:D:62:GLN:CA	1.97	0.70
6:F:50:TYR:CE1	18:R:77:GLY:HA2	2.27	0.70
9:I:127:LYS:HB2	13:M:126:LYS:HZ2	1.54	0.70
3:C:58:GLU:HB3	10:J:92:THR:HG21	1.73	0.69
3:C:129:ALA:HB3	3:C:132:ARG:NH1	2.06	0.69
4:D:63:LYS:HD2	4:D:198:VAL:HG22	1.74	0.69
12:L:83:VAL:CG2	12:L:100:ILE:HG23	2.21	0.69
19:S:77:THR:HG22	19:S:78:ARG:N	2.05	0.69
1:A:866:C:H2'	1:A:867:G:H5'	1.74	0.69
15:O:81:LEU:HD22	15:O:85:LEU:HD12	1.74	0.69
1:A:1196:U:H4'	1:A:1197:G:H5"	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:15:LEU:HA	19:S:18:LYS:HB2	1.72	0.69
2:B:116:GLU:HG2	2:B:153:ARG:HH12	1.55	0.69
1:A:586:C:C2'	1:A:587:G:H5"	2.22	0.69
1:A:1356:G:H2'	1:A:1357:A:C8	2.28	0.69
1:A:1532:U:H2'	1:A:1533:C:C6	2.27	0.69
10:J:38:ILE:HG13	10:J:71:LEU:HB3	1.73	0.69
5:E:102:ALA:HB2	5:E:120:THR:HB	1.74	0.69
11:K:34:ASP:O	11:K:36:ASP:N	2.26	0.69
21:V:6:ARG:CZ	21:V:15:ARG:HH12	2.04	0.69
1:A:479:C:H5'	1:A:479:C:C6	2.27	0.69
7:G:52:GLU:O	7:G:54:THR:N	2.26	0.69
10:J:27:ALA:HB1	10:J:74:ILE:HD13	1.73	0.69
11:K:14:VAL:HG21	11:K:40:ILE:HD13	1.74	0.69
12:L:38:THR:HG22	12:L:39:VAL:HG23	1.75	0.69
16:P:34:GLU:OE2	16:P:55:ARG:HD3	1.91	0.69
1:A:371:G:O2'	1:A:372:C:H5'	1.92	0.69
15:O:5:LYS:H	15:O:5:LYS:HD2	1.57	0.69
2:B:178:ARG:HB3	2:B:178:ARG:HH11	1.58	0.69
5:E:150:ARG:HH11	5:E:150:ARG:CG	2.05	0.69
8:H:113:SER:HB2	8:H:134:ILE:HD11	1.75	0.69
13:M:15:VAL:HG21	13:M:48:LEU:HD21	1.74	0.69
1:A:448:A:OP2	1:A:485:G:N2	2.27	0.68
1:A:1190:G:OP1	3:C:4:LYS:HA	1.93	0.68
9:I:9:ARG:CG	9:I:14:VAL:HG12	2.22	0.68
1:A:8:A:N6	4:D:209:ARG:HA	2.09	0.68
15:O:6:GLU:H	15:O:6:GLU:CD	1.94	0.68
1:A:613:C:O2'	1:A:614:A:H5'	1.92	0.68
1:A:1347:G:N2	1:A:1373:G:H2'	2.09	0.68
1:A:229:U:H5"	16:P:33:ILE:HD13	1.75	0.68
1:A:576:G:H3'	1:A:577:G:H5'	1.74	0.68
1:A:1125:U:H3	10:J:5:ARG:HH21	1.40	0.68
1:A:1330:U:H2'	1:A:1331:G:H5'	1.74	0.68
1:A:1473:A:C2'	1:A:1474:G:H5"	2.23	0.68
11:K:14:VAL:HG21	11:K:40:ILE:CD1	2.22	0.68
17:Q:7:THR:O	17:Q:23:VAL:HG13	1.94	0.68
4:D:128:VAL:HG12	4:D:129:ASN:ND2	2.09	0.68
8:H:3:THR:HG23	8:H:4:ASP:H	1.59	0.68
18:R:46:GLU:H	18:R:46:GLU:CD	1.96	0.68
19:S:30:LEU:HD11	19:S:50:ALA:HB2	1.76	0.68
2:B:7:VAL:HG21	2:B:220:ASP:HB2	1.76	0.68
13:M:19:LEU:O	13:M:22:ILE:HG13	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1113:C:O2'	1:A:1114:C:H5'	1.92	0.68
1:A:1022:G:H2'	1:A:1023:G:C8	2.28	0.68
14:N:14:PRO:O	14:N:15:LYS:HB2	1.93	0.68
20:T:96:GLY:O	20:T:97:ALA:HB3	1.95	0.68
1:A:1103:C:C2'	1:A:1104:G:H5"	2.25	0.67
3:C:134:ILE:HG23	3:C:151:VAL:HB	1.76	0.67
1:A:981:U:H3'	1:A:982:U:H5"	1.74	0.67
1:A:1491:G:H5"	12:L:46:LYS:HG3	1.76	0.67
3:C:118:GLN:O	3:C:122:GLU:HB2	1.93	0.67
13:M:40:ASN:HD22	13:M:41:PRO:HD2	1.58	0.67
1:A:1039:C:H2'	1:A:1040:U:C6	2.29	0.67
1:A:1281:U:H5'	1:A:1282:C:C5	2.29	0.67
3:C:58:GLU:HB2	3:C:65:ALA:HB2	1.76	0.67
4:D:4:TYR:O	4:D:5:ILE:HB	1.94	0.67
12:L:28:LYS:C	12:L:30:ALA:H	1.98	0.67
13:M:117:VAL:HG12	13:M:118:ALA:N	2.09	0.67
16:P:6:LEU:HB3	16:P:17:TYR:CD2	2.29	0.67
1:A:291:C:O2'	1:A:292:G:H5'	1.95	0.67
1:A:1041:A:H2'	1:A:1042:G:H8	1.59	0.67
3:C:53:ALA:O	3:C:54:ARG:HB2	1.94	0.67
10:J:5:ARG:HA	10:J:73:ASP:OD1	1.94	0.67
20:T:14:LYS:O	20:T:18:GLN:HG3	1.94	0.67
4:D:189:PRO:HB2	4:D:194:LEU:HD21	1.76	0.67
8:H:85:ARG:HD3	8:H:86:ILE:N	2.09	0.67
1:A:369:C:O2	1:A:369:C:H2'	1.93	0.67
2:B:87:ARG:NH1	2:B:233:SER:HB3	2.09	0.67
3:C:8:ILE:HG23	3:C:16:ARG:HG2	1.76	0.67
3:C:59:ARG:NH1	3:C:97:LYS:HE2	2.10	0.67
4:D:187:ARG:NE	4:D:188:LEU:N	2.37	0.67
8:H:45:ILE:HD12	8:H:61:VAL:HG13	1.75	0.67
18:R:17:SER:HA	18:R:19:LYS:NZ	2.10	0.67
1:A:839:U:O2	1:A:839:U:H2'	1.94	0.67
13:M:49:THR:HG22	13:M:51:ALA:H	1.59	0.67
20:T:73:HIS:C	20:T:74:LYS:HG2	2.15	0.67
1:A:1210:C:C3'	1:A:1211:U:H5"	2.26	0.66
19:S:3:ARG:HG2	19:S:3:ARG:HH11	1.59	0.66
19:S:12:ASP:H	19:S:38:SER:HB3	1.60	0.66
1:A:342:C:C3'	1:A:343:U:H5"	2.24	0.66
3:C:64:VAL:HG12	3:C:66:VAL:HG23	1.76	0.66
4:D:150:GLU:HA	4:D:153:ARG:HH21	1.59	0.66
13:M:81:LEU:O	13:M:86:CYS:HB3	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Z:39:U:O2'	23:Z:40:C:H5'	1.95	0.66
1:A:1003:G:H2'	1:A:1003:G:N3	2.10	0.66
1:A:1040:U:H2'	1:A:1041:A:C8	2.29	0.66
3:C:47:LEU:H	3:C:47:LEU:HD12	1.60	0.66
21:V:5:ASP:O	21:V:11:GLY:HA3	1.96	0.66
4:D:209:ARG:HG2	4:D:209:ARG:HH11	1.59	0.66
13:M:54:VAL:O	13:M:58:GLU:HG2	1.96	0.66
1:A:664:G:H22	1:A:741:G:H1	1.42	0.66
1:A:997:U:H3'	1:A:998:G:H5"	1.75	0.66
1:A:1009:G:O2'	1:A:1010:G:H5'	1.96	0.66
18:R:55:ARG:HH11	18:R:55:ARG:CB	2.08	0.66
20:T:10:LEU:H	20:T:13:LEU:HD11	1.60	0.66
1:A:389:A:H2'	1:A:390:C:H5'	1.77	0.66
1:A:628:G:H2'	1:A:629:G:C8	2.30	0.66
1:A:1051:C:H2'	1:A:1052:U:H6	1.61	0.66
2:B:82:ARG:HA	2:B:92:TYR:HE2	1.57	0.66
6:F:50:TYR:HE1	18:R:77:GLY:HA2	1.61	0.66
8:H:13:ILE:O	8:H:17:THR:HG23	1.95	0.66
10:J:42:THR:HG23	10:J:67:THR:O	1.96	0.66
1:A:1310:G:O2'	1:A:1311:G:O5'	2.13	0.66
1:A:1366:C:H2'	1:A:1367:C:H6	1.61	0.66
2:B:142:LEU:HB3	2:B:146:GLN:OE1	1.95	0.66
8:H:86:ILE:HG22	8:H:87:SER:N	2.09	0.66
10:J:31:GLY:HA2	10:J:78:ASN:ND2	2.10	0.66
1:A:1255:G:H3'	1:A:1279:A:H61	1.59	0.66
3:C:107:GLN:O	3:C:108:ASN:HB2	1.95	0.66
4:D:170:VAL:HG22	4:D:171:GLY:N	2.09	0.66
8:H:84:ARG:HH11	8:H:84:ARG:HG3	1.61	0.66
1:A:192:U:H2'	1:A:193:C:H6	1.59	0.66
1:A:343:U:H5'	1:A:343:U:H6	1.61	0.66
14:N:25:VAL:HG12	14:N:39:LEU:HD23	1.75	0.66
15:O:87:ILE:HG22	15:O:88:ARG:H	1.59	0.66
1:A:1039:C:H2'	1:A:1040:U:H6	1.60	0.65
2:B:115:LEU:HD23	2:B:153:ARG:HH21	1.61	0.65
7:G:85:TYR:HD2	7:G:154:TYR:HE2	1.44	0.65
1:A:329:A:N7	1:A:332:G:O6	2.26	0.65
1:A:1201:A:H4'	1:A:1202:G:O5'	1.95	0.65
2:B:15:VAL:HG12	2:B:16:HIS:H	1.60	0.65
2:B:24:TRP:HA	2:B:190:THR:HG22	1.77	0.65
6:F:48:LEU:HD13	6:F:52:ILE:HD12	1.78	0.65
17:Q:68:ARG:O	17:Q:69:LYS:HB2	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:51:LEU:HD22	2:B:55:PHE:HE1	1.62	0.65
3:C:43:LEU:CD2	3:C:47:LEU:HD22	2.26	0.65
18:R:36:ASN:OD1	18:R:39:VAL:HG12	1.95	0.65
23:Z:28:G:H2'	23:Z:29:G:C5	2.31	0.65
1:A:1435:G:H2'	1:A:1436:U:C6	2.31	0.65
14:N:29:ARG:HG2	14:N:29:ARG:HH11	1.60	0.65
1:A:196:A:C2'	1:A:197:A:H5"	2.25	0.65
3:C:19:GLU:HB3	3:C:40:ARG:HH22	1.62	0.65
1:A:1123:A:H4'	10:J:37:PRO:HD2	1.79	0.65
9:I:66:ARG:HB3	9:I:66:ARG:NH1	2.11	0.65
10:J:50:ILE:HD12	10:J:50:ILE:N	2.11	0.65
1:A:165:C:H2'	1:A:166:G:H8	1.60	0.65
2:B:132:LYS:O	2:B:136:VAL:HG23	1.96	0.65
5:E:57:LYS:HG2	5:E:61:TYR:CE2	2.32	0.65
1:A:269:C:H2'	1:A:270:A:C8	2.31	0.65
2:B:131:PRO:HB2	2:B:133:LYS:HB3	1.78	0.65
10:J:94:VAL:CG1	10:J:95:GLU:H	2.09	0.65
1:A:1193:G:O2'	1:A:1194:U:H5'	1.96	0.64
1:A:1292:U:P	7:G:41:ARG:HH22	2.21	0.64
2:B:102:LEU:N	2:B:102:LEU:HD12	2.12	0.64
3:C:134:ILE:O	3:C:138:VAL:HG23	1.97	0.64
7:G:54:THR:CG2	7:G:56:GLN:H	2.10	0.64
9:I:118:LYS:O	9:I:119:ALA:HB3	1.96	0.64
11:K:72:ALA:HB1	11:K:77:MET:HG3	1.79	0.64
1:A:1053:G:C3'	1:A:1054:C:H5'	2.27	0.64
1:A:1114:C:C2	1:A:1115:C:C5	2.85	0.64
6:F:40:VAL:HG22	6:F:41:GLU:N	2.12	0.64
2:B:7:VAL:N	2:B:221:LEU:HD23	2.12	0.64
2:B:167:PRO:HD3	2:B:188:ALA:HB2	1.79	0.64
16:P:11:SER:OG	16:P:14:ASN:HB3	1.98	0.64
1:A:9:G:H5"	5:E:122:GLU:OE1	1.96	0.64
1:A:946:A:H2'	1:A:947:G:C8	2.33	0.64
1:A:1001:A:O2'	1:A:1001(A):G:H5'	1.97	0.64
1:A:1014:A:C2	1:A:1219:U:H1'	2.33	0.64
1:A:1154:G:H2'	1:A:1155:G:H8	1.62	0.64
2:B:95:GLN:HE21	2:B:147:LYS:CG	2.10	0.64
3:C:110:ASN:HD21	3:C:140:ARG:HB3	1.59	0.64
4:D:150:GLU:HG2	4:D:153:ARG:HH21	1.61	0.64
7:G:92:SER:O	7:G:96:GLN:HG3	1.97	0.64
9:I:111:ARG:HG2	9:I:112:LYS:N	2.12	0.64
12:L:41:ARG:HG2	12:L:41:ARG:HH11	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:537:G:OP1	12:L:113:ARG:NH2	2.31	0.64
1:A:1158:C:C5	1:A:1160:G:C8	2.85	0.64
1:A:1251:A:H4'	9:I:12:GLU:OE2	1.97	0.64
1:A:1533:C:O5'	1:A:1533:C:H6	1.81	0.64
16:P:43:LYS:HA	16:P:48:TRP:HB3	1.78	0.64
20:T:90:GLN:HA	20:T:93:GLU:HG2	1.79	0.64
1:A:840:C:H4'	1:A:841:U:C5	2.32	0.64
1:A:1048:G:H5'	1:A:1048:G:C8	2.29	0.64
3:C:47:LEU:HD23	3:C:68:VAL:HG11	1.78	0.64
9:I:47:LEU:C	9:I:49:PRO:HD2	2.18	0.64
11:K:69:ALA:O	11:K:73:MET:HG2	1.97	0.64
12:L:24:VAL:HG13	12:L:98:TYR:HE2	1.61	0.64
20:T:57:ARG:HH22	20:T:100:ILE:HG21	1.62	0.64
20:T:93:GLU:OE1	20:T:93:GLU:HA	1.97	0.64
23:Z:39:U:C3'	23:Z:40:C:H5'	2.27	0.64
1:A:272:C:O2'	1:A:273:A:H5'	1.97	0.64
1:A:1152:A:OP1	10:J:68:HIS:ND1	2.31	0.64
1:A:1168:A:H2'	1:A:1169:A:O4'	1.97	0.64
1:A:1314:C:C6	19:S:6:LYS:HE2	2.33	0.64
2:B:167:PRO:CD	2:B:188:ALA:HB2	2.28	0.64
3:C:139:GLN:HA	3:C:139:GLN:NE2	2.12	0.64
6:F:10:LEU:CD1	6:F:59:TYR:HB3	2.28	0.64
9:I:79:LEU:O	9:I:83:ARG:HG3	1.98	0.64
19:S:13:ASP:HA	19:S:16:LEU:HB3	1.80	0.64
1:A:501:C:H2'	1:A:502:G:H8	1.62	0.64
1:A:1209:C:O2	1:A:1209:C:H2'	1.98	0.64
3:C:39:ILE:O	3:C:43:LEU:HB2	1.98	0.64
8:H:119:LEU:HD12	8:H:124:ALA:CA	2.28	0.64
8:H:119:LEU:HD12	8:H:124:ALA:HB2	1.78	0.64
17:Q:33:GLY:O	17:Q:34:LYS:C	2.34	0.64
12:L:110:VAL:CG2	12:L:113:ARG:HG3	2.28	0.64
20:T:102:GLY:O	20:T:104:LEU:N	2.30	0.64
1:A:155:C:C3'	1:A:156:G:H5"	2.28	0.63
1:A:1157:A:H5'	1:A:1158:C:C2	2.33	0.63
2:B:181:PHE:HD2	8:H:70:GLN:HB3	1.63	0.63
11:K:26:ASN:O	11:K:27:ASN:HB2	1.98	0.63
1:A:587:G:H5'	1:A:587:G:H8	1.63	0.63
6:F:87:ARG:HH11	6:F:87:ARG:HG3	1.63	0.63
10:J:8:LEU:HD21	10:J:96:ILE:HG12	1.79	0.63
12:L:6:THR:O	12:L:10:LEU:HD12	1.98	0.63
1:A:489:C:H2'	1:A:490:G:H8	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1222:G:OP1	19:S:77:THR:HG21	1.99	0.63
2:B:87:ARG:CZ	2:B:233:SER:HB3	2.28	0.63
3:C:123:GLN:HE22	3:C:140:ARG:HH22	1.47	0.63
8:H:31:PHE:O	8:H:35:ILE:HG12	1.98	0.63
1:A:189:G:H1	1:A:189(K):U:H3	1.44	0.63
10:J:51:ARG:HB3	10:J:59:SER:HB3	1.81	0.63
1:A:444:C:H2'	1:A:445:G:H8	1.63	0.63
1:A:1360:A:O2'	1:A:1361:G:H5'	1.97	0.63
2:B:95:GLN:HG3	2:B:147:LYS:O	1.98	0.63
5:E:81:GLU:CD	5:E:88:LYS:HE2	2.19	0.63
6:F:101:ALA:HB2	18:R:28:GLU:HA	1.80	0.63
17:Q:36:ILE:H	17:Q:36:ILE:HD13	1.62	0.63
2:B:66:GLY:HA2	2:B:160:ASP:OD2	1.98	0.63
4:D:108:LEU:HB3	4:D:110:PHE:HE1	1.64	0.63
7:G:54:THR:HG22	7:G:56:GLN:N	2.13	0.63
9:I:97:LYS:HA	9:I:102:LEU:CD1	2.29	0.63
14:N:24:CYS:HB3	14:N:28:GLY:H	1.64	0.63
15:O:10:LYS:HE2	15:O:10:LYS:O	1.98	0.63
1:A:580:U:H2'	1:A:581:G:O4'	1.98	0.63
2:B:82:ARG:O	2:B:86:GLU:HG3	1.99	0.63
5:E:48:ALA:HB1	5:E:49:PRO:HD2	1.80	0.63
1:A:1423:G:O2'	1:A:1424:C:H5'	1.98	0.63
3:C:110:ASN:O	3:C:111:LEU:HD23	1.99	0.63
13:M:105:THR:O	13:M:107:ALA:N	2.30	0.63
1:A:1095:U:H6	1:A:1095:U:H5'	1.63	0.63
1:A:1385:G:H2'	1:A:1386:G:H5"	1.81	0.63
2:B:97:TRP:HH2	2:B:176:GLU:OE2	1.79	0.63
4:D:158:ILE:H	4:D:158:ILE:CD1	2.11	0.63
6:F:67:MET:SD	6:F:72:VAL:HG22	2.39	0.63
9:I:126:SER:HB2	9:I:127:LYS:HD2	1.81	0.63
1:A:339:C:H2'	1:A:340:U:H6	1.62	0.62
1:A:539:A:H2'	1:A:540:G:C8	2.34	0.62
2:B:178:ARG:HH22	8:H:74:PRO:HB3	1.63	0.62
3:C:103:VAL:HG12	3:C:104:GLN:N	2.13	0.62
19:S:60:VAL:HG21	19:S:74:PHE:HB3	1.80	0.62
1:A:262:A:H4'	20:T:75:ASN:HD22	1.64	0.62
1:A:476:G:H2'	1:A:477:A:H8	1.63	0.62
1:A:1222:G:P	19:S:77:THR:HG21	2.38	0.62
13:M:81:LEU:HD22	13:M:88:ARG:NH2	2.12	0.62
1:A:983:A:H5'	14:N:3:ARG:NH1	2.13	0.62
2:B:167:PRO:O	2:B:171:ALA:N	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:107:GLN:H	3:C:107:GLN:CD	2.01	0.62
8:H:38:ILE:HG21	8:H:111:ILE:HG12	1.80	0.62
8:H:107:LEU:HD23	8:H:107:LEU:N	2.14	0.62
19:S:6:LYS:HB3	19:S:7:LYS:HE3	1.80	0.62
1:A:1114:C:C2'	1:A:1115:C:O5'	2.47	0.62
1:A:1405:G:O2'	1:A:1406:U:H5'	2.00	0.62
11:K:124:LYS:HD3	11:K:125:PHE:CE1	2.34	0.62
1:A:59:A:H1'	1:A:354:G:N2	2.15	0.62
1:A:178:C:O2'	1:A:179:A:H5'	2.00	0.62
1:A:759:A:H61	17:Q:94:ASN:HD21	1.47	0.62
1:A:872:A:O2'	1:A:873:A:H3'	1.99	0.62
2:B:114:ARG:O	2:B:114:ARG:HD3	2.00	0.62
19:S:30:LEU:HD12	19:S:31:ILE:H	1.65	0.62
1:A:35:G:H2'	1:A:36:C:C6	2.35	0.62
1:A:486:U:H2'	1:A:487:A:H8	1.65	0.62
1:A:545:C:H5"	4:D:72:GLU:HG3	1.81	0.62
6:F:2:ARG:NE	6:F:69:GLU:HG2	2.14	0.62
6:F:10:LEU:H	6:F:10:LEU:HD12	1.63	0.62
6:F:22:GLU:O	6:F:26:ILE:HG12	1.99	0.62
6:F:30:LEU:CB	6:F:35:ALA:HB3	2.14	0.62
23:Z:39:U:H2'	23:Z:40:C:C5	2.34	0.62
1:A:254:G:O2'	1:A:255:G:H5'	1.98	0.62
1:A:439:A:N6	1:A:496:A:H1'	2.14	0.62
4:D:153:ARG:HG2	4:D:181:MET:HE1	1.81	0.62
5:E:15:ARG:HD3	5:E:26:PHE:HD1	1.62	0.62
12:L:28:LYS:C	12:L:30:ALA:N	2.52	0.62
2:B:10:LEU:CD2	2:B:11:LEU:HG	2.30	0.62
2:B:95:GLN:C	2:B:96:ARG:HD2	2.20	0.62
12:L:24:VAL:HG13	12:L:98:TYR:CE2	2.35	0.62
13:M:3:ARG:HA	13:M:8:GLU:O	1.99	0.62
13:M:23:TYR:HB2	13:M:67:GLU:OE2	2.00	0.62
15:O:17:ARG:HG3	15:O:17:ARG:HH11	1.64	0.62
1:A:235:C:H1'	17:Q:61:GLU:OE2	1.99	0.62
1:A:620:C:N1	4:D:135:LEU:HD13	2.14	0.62
1:A:976:G:H5"	1:A:1358:U:O2'	2.00	0.62
1:A:1031:G:H2'	1:A:1032:G:C8	2.34	0.62
1:A:1201:A:O2'	1:A:1202:G:OP2	2.18	0.62
4:D:105:VAL:HG21	4:D:126:ILE:CD1	2.30	0.62
7:G:32:ARG:O	7:G:33:ASP:HB2	1.99	0.62
1:A:1162:C:O2'	1:A:1163:C:H5'	2.00	0.62
9:I:33:PHE:CE2	9:I:47:LEU:HD11	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:102:LEU:HD12	9:I:102:LEU:H	1.65	0.62
14:N:22:THR:OG1	14:N:33:VAL:HG21	1.99	0.62
1:A:620:C:H6	1:A:620:C:H5'	1.65	0.61
1:A:985:C:H2'	1:A:986:A:C8	2.35	0.61
1:A:1276:G:C2'	1:A:1277:C:H5"	2.30	0.61
1:A:1327:C:O2'	1:A:1328:C:H5'	2.00	0.61
2:B:59:GLU:O	2:B:62:ALA:HB3	2.00	0.61
4:D:25:ARG:HH12	4:D:30:LYS:HD2	1.64	0.61
6:F:30:LEU:N	6:F:30:LEU:HD23	2.14	0.61
11:K:92:GLU:HA	11:K:95:ILE:HD13	1.82	0.61
12:L:55:VAL:HG12	12:L:56:ALA:N	2.10	0.61
1:A:6:G:N2	5:E:98:THR:HG23	2.15	0.61
1:A:750:G:H21	15:O:23:GLY:HA3	1.64	0.61
1:A:862:C:O2'	1:A:863:U:H5'	2.00	0.61
1:A:1208:C:H2'	1:A:1209:C:H6	1.64	0.61
4:D:199:ASN:HD21	4:D:201:GLN:CB	2.11	0.61
6:F:25:ILE:HG23	6:F:28:ARG:HD2	1.82	0.61
1:A:243:A:H4'	1:A:244:U:C5'	2.19	0.61
1:A:1114:C:H2'	1:A:1115:C:O5'	2.00	0.61
7:G:65:ALA:HB1	7:G:127:ALA:HB3	1.81	0.61
7:G:92:SER:HB2	7:G:93:PRO:HD2	1.82	0.61
1:A:1457:G:O2'	1:A:1458:G:H5'	2.00	0.61
2:B:91:PRO:HG3	2:B:154:LEU:CB	2.20	0.61
4:D:29:PRO:O	4:D:30:LYS:HG3	2.00	0.61
8:H:16:ALA:O	8:H:21:LYS:HG2	2.00	0.61
11:K:34:ASP:OD2	11:K:38:ASN:HB2	2.00	0.61
16:P:28:ARG:HG2	16:P:29:ASP:OD1	2.00	0.61
17:Q:59:ILE:HG23	17:Q:71:PHE:HB3	1.83	0.61
1:A:954:G:H21	1:A:1227:A:H62	1.48	0.61
1:A:1010:G:H2'	1:A:1011:G:C8	2.34	0.61
1:A:1301:U:O2	1:A:1301:U:H2'	2.00	0.61
1:A:1444:C:H2'	1:A:1445:C:H6	1.65	0.61
2:B:9:GLU:CD	2:B:10:LEU:H	2.03	0.61
3:C:91:LEU:CD2	3:C:99:VAL:H	2.14	0.61
7:G:65:ALA:O	7:G:69:VAL:HG23	2.00	0.61
9:I:65:VAL:HG21	9:I:73:GLN:HB3	1.81	0.61
14:N:26:ARG:CG	14:N:27:CYS:H	2.12	0.61
16:P:43:LYS:HG3	16:P:48:TRP:CD2	2.35	0.61
20:T:50:GLU:CA	20:T:100:ILE:HD11	2.17	0.61
5:E:101:ILE:HD13	5:E:119:LEU:HA	1.83	0.61
9:I:4:TYR:CE1	9:I:88:TYR:HA	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:17:ASP:O	10:J:21:GLN:HB2	2.00	0.61
1:A:1510:U:H2'	1:A:1511:G:C8	2.35	0.61
2:B:137:ARG:NH1	2:B:137:ARG:HB2	2.15	0.61
3:C:103:VAL:HG12	3:C:104:GLN:H	1.66	0.61
7:G:76:ARG:HH11	7:G:76:ARG:HG3	1.65	0.61
7:G:153:HIS:C	7:G:155:ARG:H	2.04	0.61
15:O:87:ILE:O	15:O:88:ARG:HB2	2.01	0.61
10:J:78:ASN:HB2	10:J:81:THR:OG1	2.00	0.61
10:J:81:THR:O	10:J:83:GLU:N	2.34	0.61
1:A:1157:A:O4'	1:A:1158:C:N3	2.34	0.61
12:L:50:SER:O	12:L:51:ALA:HB2	2.01	0.61
15:O:74:ASP:CB	15:O:77:ARG:HD3	2.31	0.61
20:T:56:MET:HG3	20:T:84:LEU:HD11	1.81	0.61
1:A:1152:A:O2'	1:A:1153:C:H5'	2.01	0.61
9:I:7:THR:H	9:I:83:ARG:HD3	1.66	0.61
12:L:117:ARG:HG3	12:L:122:THR:HB	1.82	0.61
19:S:4:SER:C	19:S:5:LEU:HD12	2.22	0.61
1:A:1053:G:H4'	1:A:1054:C:H5'	1.82	0.60
1:A:1103:C:H2'	1:A:1104:G:C5'	2.31	0.60
1:A:1208:C:H2'	1:A:1209:C:C6	2.36	0.60
2:B:91:PRO:HA	2:B:154:LEU:HD12	1.83	0.60
15:O:33:THR:HG21	15:O:85:LEU:HD22	1.81	0.60
15:O:41:GLU:OE1	15:O:44:LYS:HE2	2.01	0.60
16:P:81:ARG:HH11	16:P:81:ARG:HB2	1.65	0.60
18:R:26:LEU:CD1	18:R:27:GLY:H	2.13	0.60
1:A:1030(C):G:H2'	1:A:1030(D):A:C8	2.36	0.60
1:A:1157:A:C6	1:A:1180:A:C6	2.89	0.60
1:A:1239:A:H62	1:A:1299:A:N6	1.99	0.60
12:L:93:LEU:HD23	12:L:93:LEU:N	2.15	0.60
1:A:180:U:H2'	1:A:181:G:H5'	1.82	0.60
1:A:386:C:C2'	1:A:387:U:H5'	2.31	0.60
1:A:1096:C:O2'	1:A:1097:C:H5'	2.01	0.60
11:K:52:GLY:O	11:K:55:LYS:HG3	2.01	0.60
17:Q:34:LYS:HG3	17:Q:34:LYS:O	2.01	0.60
17:Q:68:ARG:O	17:Q:68:ARG:CG	2.49	0.60
1:A:1114:C:C2	1:A:1115:C:C6	2.89	0.60
1:A:510:A:H5'	1:A:511:C:OP2	2.02	0.60
1:A:1481:U:O2'	1:A:1482:G:H5'	2.01	0.60
8:H:80:ILE:HD12	8:H:80:ILE:H	1.65	0.60
23:Z:30:G:C2	23:Z:41:C:C5	2.90	0.60
1:A:411:A:H62	1:A:413:G:H21	1.49	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:84:ILE:O	3:C:84:ILE:HG12	2.02	0.60
3:C:91:LEU:HD23	3:C:92:ALA:N	2.16	0.60
9:I:97:LYS:HB3	9:I:98:PRO:HD3	1.82	0.60
10:J:94:VAL:CG1	10:J:95:GLU:N	2.65	0.60
1:A:900:A:H2'	1:A:901:A:C8	2.37	0.60
1:A:1157:A:C4'	1:A:1158:C:C2	2.85	0.60
1:A:1263:C:H2'	1:A:1264:C:H6	1.62	0.60
6:F:4:TYR:HE1	6:F:92:LYS:HG2	1.66	0.60
7:G:52:GLU:C	7:G:54:THR:H	2.04	0.60
9:I:127:LYS:HD2	9:I:127:LYS:N	2.08	0.60
1:A:189(C):C:H2'	1:A:189(D):C:O4'	2.02	0.60
1:A:619:U:H2'	1:A:620:C:H5"	1.83	0.60
4:D:108:LEU:HB3	4:D:110:PHE:CE1	2.37	0.60
10:J:19:SER:OG	10:J:91:PRO:HG3	2.02	0.60
15:O:81:LEU:O	15:O:85:LEU:HB2	2.02	0.60
1:A:329:A:C5	1:A:332:G:N1	2.69	0.60
1:A:1114:C:N3	1:A:1115:C:C5	2.70	0.60
1:A:1442(A):G:O5'	1:A:1442(B):A:H5'	2.01	0.60
2:B:213:LEU:O	2:B:217:ARG:HG2	2.02	0.60
3:C:43:LEU:HD21	3:C:47:LEU:HD22	1.83	0.60
3:C:49:SER:O	3:C:72:LYS:HD3	2.01	0.60
5:E:59:GLY:O	5:E:62:ALA:HB3	2.02	0.60
5:E:122:GLU:CD	5:E:131:ILE:HD13	2.22	0.60
12:L:25:PRO:C	12:L:27:LEU:H	2.05	0.60
21:V:2:GLY:C	21:V:4:GLY:H	2.03	0.60
1:A:1014:A:H2'	1:A:1015:A:C8	2.37	0.60
1:A:1133:G:H2'	1:A:1134:G:C8	2.35	0.60
1:A:1368:G:O2'	1:A:1369:C:H5'	2.01	0.60
3:C:60:ALA:O	3:C:61:ALA:CB	2.49	0.60
4:D:24:GLU:O	4:D:25:ARG:CB	2.50	0.60
13:M:88:ARG:CG	13:M:98:VAL:HG22	2.31	0.60
1:A:1016:A:H2'	1:A:1017:G:O4'	2.01	0.59
3:C:68:VAL:HG12	3:C:70:VAL:HG13	1.84	0.59
10:J:79:ARG:HH12	10:J:82:ILE:HD12	1.67	0.59
12:L:43:VAL:HG12	12:L:44:THR:N	2.16	0.59
16:P:63:GLY:O	16:P:64:ALA:C	2.39	0.59
1:A:192:U:H1'	20:T:103:GLY:HA2	1.84	0.59
1:A:1010:G:N2	1:A:1020:U:H1'	2.17	0.59
2:B:69:LEU:HB3	2:B:162:ILE:HD13	1.85	0.59
4:D:35:ARG:O	4:D:36:ARG:HG3	2.02	0.59
5:E:131:ILE:O	5:E:135:THR:HG23	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:155:ARG:O	7:G:156:TRP:CB	2.50	0.59
10:J:38:ILE:CG1	10:J:71:LEU:HB3	2.31	0.59
23:Z:36:A:H2'	23:Z:37:A:C8	2.37	0.59
1:A:309:G:O2'	1:A:310:G:H5'	2.02	0.59
2:B:117:GLU:O	2:B:121:LEU:HD13	2.01	0.59
2:B:206:ASP:O	2:B:207:ALA:HB3	2.02	0.59
3:C:64:VAL:HG23	3:C:99:VAL:HG11	1.84	0.59
3:C:179:ARG:CG	3:C:180:ALA:N	2.64	0.59
4:D:158:ILE:HD12	4:D:158:ILE:N	2.16	0.59
8:H:120:THR:HG23	8:H:123:GLU:OE2	2.03	0.59
11:K:126:ARG:HG3	11:K:127:LYS:H	1.67	0.59
17:Q:48:GLU:O	17:Q:49:GLU:C	2.40	0.59
19:S:5:LEU:O	19:S:6:LYS:HG3	2.03	0.59
20:T:45:GLN:HA	20:T:91:LEU:HD22	1.84	0.59
1:A:1181:G:H2'	1:A:1181:G:N3	2.17	0.59
1:A:1279:A:H5'	10:J:9:ARG:NH2	2.16	0.59
2:B:118:LEU:HD12	2:B:142:LEU:CD2	2.32	0.59
1:A:718:G:C5'	11:K:117:ASN:ND2	2.64	0.59
1:A:1041:A:H2'	1:A:1042:G:C8	2.38	0.59
1:A:1248:A:H5'	1:A:1248:A:H8	1.68	0.59
1:A:1391:U:H2'	1:A:1392:G:H8	1.67	0.59
3:C:58:GLU:H	3:C:65:ALA:HB3	1.67	0.59
3:C:157:ILE:HG21	3:C:164:ARG:NH2	2.12	0.59
3:C:158:GLY:O	3:C:160:ALA:N	2.36	0.59
4:D:8:VAL:C	4:D:10:ARG:H	2.05	0.59
7:G:62:PHE:HA	7:G:124:LEU:HD22	1.83	0.59
8:H:20:TYR:CE1	8:H:76:PRO:HG2	2.37	0.59
16:P:26:ARG:HD3	16:P:31:LYS:O	2.02	0.59
17:Q:29:HIS:HB2	17:Q:36:ILE:HD12	1.84	0.59
1:A:1276:G:C3'	1:A:1277:C:H5"	2.32	0.59
1:A:1532:U:H2'	1:A:1533:C:C5	2.38	0.59
2:B:44:LEU:HA	2:B:47:THR:OG1	2.01	0.59
4:D:3:ARG:NE	4:D:71:SER:H	2.00	0.59
4:D:31:CYS:O	4:D:32:ALA:HB3	2.02	0.59
17:Q:26:GLN:O	17:Q:27:PHE:HB3	2.02	0.59
1:A:189(I):G:O2'	1:A:189(J):G:H5'	2.02	0.59
1:A:342:C:H3'	1:A:343:U:C5'	2.33	0.59
1:A:1182:G:H4'	1:A:1183:A:H5'	1.83	0.59
12:L:15:ARG:HG3	12:L:15:ARG:HH11	1.66	0.59
1:A:376:G:OP1	16:P:67:THR:HG21	2.03	0.59
1:A:1320:C:N3	19:S:36:ARG:HD3	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:37:ASN:O	2:B:39:ILE:N	2.36	0.59
3:C:100:ALA:O	3:C:101:LEU:HB2	2.03	0.59
10:J:6:ILE:CD1	10:J:73:ASP:H	2.15	0.59
7:G:148:ASN:C	7:G:150:ALA:H	2.04	0.59
8:H:19:VAL:HB	8:H:21:LYS:HD3	1.84	0.59
12:L:83:VAL:HG21	12:L:100:ILE:CG2	2.32	0.59
1:A:134:A:H61	16:P:25:ARG:NH1	2.00	0.59
1:A:650:G:O2'	1:A:651:C:H5'	2.03	0.59
1:A:1442(A):G:C4'	1:A:1442(B):A:H5'	2.33	0.59
4:D:187:ARG:HE	4:D:187:ARG:HA	1.67	0.59
12:L:40:VAL:O	12:L:40:VAL:HG12	2.03	0.59
23:Z:38:A:C4	23:Z:39:U:H1'	2.38	0.59
1:A:522:C:H41	12:L:53:ARG:NH2	2.01	0.58
1:A:1195:C:H5'	1:A:1196:U:OP2	2.02	0.58
1:A:1305:G:H4'	21:V:4:GLY:O	2.02	0.58
1:A:1363(A):A:H1'	1:A:1365:G:N7	2.18	0.58
2:B:163:PHE:HD1	2:B:185:ILE:HB	1.68	0.58
3:C:47:LEU:H	3:C:47:LEU:CD1	2.16	0.58
5:E:79:GLU:HG2	5:E:92:LYS:HG2	1.85	0.58
10:J:6:ILE:HD11	10:J:73:ASP:N	2.16	0.58
12:L:110:VAL:HG22	12:L:120:TYR:HB3	1.84	0.58
21:V:2:GLY:O	21:V:4:GLY:N	2.35	0.58
4:D:199:ASN:ND2	4:D:201:GLN:HB2	2.13	0.58
5:E:57:LYS:HG2	5:E:61:TYR:HE2	1.68	0.58
6:F:4:TYR:CE2	6:F:72:VAL:HG21	2.38	0.58
14:N:32:SER:O	14:N:33:VAL:C	2.41	0.58
1:A:179:A:O2'	1:A:180:U:H5'	2.03	0.58
1:A:974:A:OP2	14:N:41:ARG:NH1	2.36	0.58
1:A:1360:A:H2'	1:A:1361:G:O4'	2.04	0.58
1:A:1493:A:H5"	1:A:1494:G:OP2	2.03	0.58
2:B:55:PHE:HA	2:B:58:ILE:HD11	1.85	0.58
2:B:61:LEU:HD13	2:B:64:ARG:NH1	2.18	0.58
3:C:91:LEU:HD21	3:C:99:VAL:N	2.18	0.58
8:H:3:THR:HG23	8:H:4:ASP:N	2.18	0.58
10:J:49:VAL:HG11	14:N:41:ARG:O	2.03	0.58
10:J:69:ASN:O	10:J:70:ARG:HD3	2.03	0.58
11:K:101:SER:C	11:K:103:LEU:H	2.06	0.58
1:A:314:C:O2'	1:A:315:A:H5'	2.03	0.58
1:A:858:G:O2'	1:A:859:A:H5"	2.04	0.58
2:B:48:MET:HA	2:B:51:LEU:HD12	1.86	0.58
2:B:115:LEU:CD2	2:B:153:ARG:HH21	2.16	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:14:ILE:CG2	3:C:15:THR:H	2.10	0.58
4:D:3:ARG:CZ	4:D:70:ILE:HG13	2.33	0.58
5:E:13:ILE:HG13	5:E:13:ILE:O	2.02	0.58
10:J:28:ARG:HG2	10:J:28:ARG:HH11	1.68	0.58
14:N:34:TYR:O	14:N:36:PHE:N	2.36	0.58
1:A:820:U:H4'	1:A:821:G:OP2	2.03	0.58
2:B:178:ARG:HB3	2:B:178:ARG:NH1	2.19	0.58
5:E:41:VAL:HG13	5:E:113:ALA:HA	1.86	0.58
3:C:46:GLU:O	3:C:48:TYR:N	2.37	0.58
5:E:79:GLU:CD	5:E:79:GLU:H	2.06	0.58
7:G:71:PRO:HD3	7:G:103:TRP:HZ3	1.67	0.58
2:B:184:VAL:HG12	2:B:197:VAL:HG13	1.85	0.58
3:C:47:LEU:HD12	3:C:47:LEU:N	2.18	0.58
8:H:111:ILE:O	8:H:134:ILE:HB	2.03	0.58
15:O:78:TYR:OH	15:O:88:ARG:HD2	2.03	0.58
1:A:134:A:H61	16:P:25:ARG:HH12	1.51	0.58
4:D:105:VAL:CG2	4:D:126:ILE:HD13	2.32	0.58
9:I:114:TYR:CD1	9:I:114:TYR:N	2.68	0.58
11:K:48:ILE:HD12	11:K:63:LEU:HB3	1.86	0.58
11:K:54:ARG:HH11	11:K:54:ARG:CB	2.12	0.58
18:R:53:ARG:C	18:R:55:ARG:H	2.07	0.58
1:A:386:C:H2'	1:A:387:U:H5'	1.85	0.58
1:A:424:G:O2'	1:A:425:G:H5'	2.03	0.58
1:A:1053:G:C4'	1:A:1054:C:H5'	2.34	0.58
1:A:1406:U:C5	1:A:1407:C:C5	2.91	0.58
1:A:1442(A):G:H5'	1:A:1442(A):G:C8	2.38	0.58
4:D:146:ILE:N	4:D:146:ILE:HD12	2.18	0.58
8:H:118:VAL:C	8:H:119:LEU:HD23	2.24	0.58
10:J:30:SER:HB3	10:J:80:LYS:C	2.24	0.58
10:J:90:LEU:H	10:J:91:PRO:HD2	1.68	0.58
1:A:444:C:H2'	1:A:445:G:C8	2.39	0.58
1:A:1311:G:N7	19:S:2:PRO:HA	2.18	0.58
1:A:1399:C:H4'	1:A:1400:C:C5'	2.34	0.58
1:A:1514:C:O2'	1:A:1515:C:H5'	2.03	0.58
2:B:223:ILE:HD13	2:B:226:ARG:HE	1.69	0.58
4:D:5:ILE:HG22	4:D:5:ILE:O	2.04	0.58
6:F:94:GLN:HE21	18:R:32:ARG:HD3	1.68	0.58
19:S:19:VAL:HG13	19:S:20:LEU:N	2.19	0.58
1:A:1216:G:H5"	14:N:5:ALA:HB1	1.85	0.57
3:C:44:GLU:HG2	3:C:52:LEU:HD22	1.86	0.57
5:E:32:VAL:HG22	5:E:58:ALA:HB1	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:39:PRO:HB3	10:J:70:ARG:NH1	2.19	0.57
1:A:103:C:P	20:T:17:ARG:HH11	2.28	0.57
1:A:882:C:O2'	1:A:883:C:H5'	2.04	0.57
1:A:922:G:N3	1:A:1398:A:H2	2.02	0.57
3:C:83:ARG:HA	3:C:86:VAL:CG2	2.28	0.57
6:F:4:TYR:CE1	6:F:92:LYS:HG2	2.39	0.57
10:J:38:ILE:HD11	10:J:71:LEU:HD12	1.85	0.57
11:K:108:ILE:O	11:K:109:VAL:HG23	2.03	0.57
12:L:113:ARG:NH2	12:L:120:TYR:HE2	2.02	0.57
18:R:53:ARG:HA	18:R:63:GLN:OE1	2.04	0.57
1:A:344:A:C3'	1:A:345:C:H5"	2.33	0.57
1:A:375:U:H4'	16:P:17:TYR:CE2	2.39	0.57
6:F:38:GLU:O	6:F:39:LYS:C	2.41	0.57
8:H:120:THR:OG1	8:H:123:GLU:HG3	2.04	0.57
13:M:107:ALA:O	13:M:111:LYS:HB2	2.04	0.57
16:P:75:ARG:C	16:P:77:ALA:H	2.08	0.57
1:A:21:G:H2'	1:A:22:G:H8	1.65	0.57
1:A:1230:C:H2'	1:A:1231:G:H8	1.69	0.57
2:B:21:ARG:HA	2:B:39:ILE:HA	1.87	0.57
7:G:113:GLU:O	7:G:119:ARG:HD3	2.04	0.57
10:J:36:GLY:O	10:J:72:VAL:HA	2.05	0.57
10:J:56:HIS:C	10:J:58:ASP:H	2.08	0.57
16:P:21:VAL:HG11	16:P:59:TRP:CD2	2.39	0.57
1:A:989:C:N4	1:A:1216:G:H1	2.00	0.57
1:A:1301:U:H3'	1:A:1302:U:C5'	2.32	0.57
1:A:1342:C:O2'	1:A:1343:G:H5'	2.04	0.57
12:L:27:LEU:HG	12:L:28:LYS:N	2.18	0.57
12:L:28:LYS:O	12:L:30:ALA:N	2.37	0.57
14:N:11:LYS:C	14:N:13:THR:H	2.06	0.57
20:T:48:LYS:O	20:T:52:ALA:HB2	2.05	0.57
3:C:32:LEU:O	3:C:36:ASP:HB2	2.03	0.57
3:C:139:GLN:CA	3:C:139:GLN:HE21	2.16	0.57
4:D:62:GLN:HE22	4:D:65:ARG:HH11	1.52	0.57
12:L:85:ILE:CD1	12:L:100:ILE:HD13	2.35	0.57
15:O:5:LYS:HD2	15:O:5:LYS:N	2.19	0.57
1:A:883:C:O2'	1:A:884:U:H5'	2.05	0.57
1:A:1239:A:H62	1:A:1299:A:H62	1.52	0.57
5:E:71:LEU:O	5:E:72:GLN:HG2	2.04	0.57
7:G:68:ASN:O	7:G:135:VAL:HG12	2.03	0.57
8:H:119:LEU:HD12	8:H:124:ALA:CB	2.35	0.57
10:J:4:ILE:N	10:J:4:ILE:CD1	2.66	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:C:H2'	1:A:166:G:C8	2.39	0.57
1:A:1001:A:H2'	1:A:1001:A:N3	2.19	0.57
1:A:1309:G:C2'	1:A:1310:G:H5'	2.35	0.57
4:D:207:TYR:C	4:D:209:ARG:H	2.08	0.57
13:M:49:THR:HB	13:M:52:GLU:HG3	1.87	0.57
1:A:1412:C:H2'	1:A:1413:A:C8	2.39	0.57
3:C:91:LEU:HD21	3:C:99:VAL:HG22	1.87	0.57
3:C:120:VAL:HG21	3:C:134:ILE:HD13	1.87	0.57
8:H:28:ALA:HB3	8:H:57:PRO:HB2	1.87	0.57
13:M:58:GLU:O	13:M:62:ASN:HB2	2.04	0.57
15:O:10:LYS:HE2	15:O:14:GLU:HB2	1.87	0.57
1:A:555:C:H2'	1:A:556:C:H6	1.68	0.57
5:E:122:GLU:OE2	5:E:131:ILE:HD13	2.05	0.57
9:I:17:VAL:HG22	9:I:63:ILE:CD1	2.30	0.57
10:J:87:THR:O	10:J:88:LEU:HG	2.04	0.57
16:P:67:THR:HG23	16:P:70:ALA:HB2	1.85	0.57
1:A:769:G:H4'	1:A:1513:A:H4'	1.87	0.56
1:A:1442(A):G:H4'	1:A:1442(B):A:H5'	1.86	0.56
2:B:115:LEU:HD12	2:B:145:LEU:HB3	1.86	0.56
3:C:157:ILE:CG2	3:C:164:ARG:HH21	2.14	0.56
8:H:116:LYS:HD3	8:H:127:LEU:HD12	1.87	0.56
11:K:27:ASN:HB2	11:K:55:LYS:HE2	1.87	0.56
16:P:6:LEU:HD12	16:P:6:LEU:N	2.20	0.56
17:Q:97:SER:HB3	17:Q:103:GLY:HA3	1.87	0.56
9:I:66:ARG:HB3	9:I:66:ARG:HH11	1.70	0.56
10:J:8:LEU:CD2	10:J:96:ILE:HG12	2.36	0.56
17:Q:81:ARG:HG3	17:Q:81:ARG:O	2.05	0.56
1:A:279:A:H5"	1:A:280:C:H3'	1.85	0.56
1:A:344:A:H5"	1:A:345:C:C6	2.41	0.56
1:A:530:G:O6	22:W:3:C:H1'	2.05	0.56
1:A:691:G:O6	11:K:55:LYS:NZ	2.38	0.56
1:A:949:A:N7	13:M:106:ASN:ND2	2.53	0.56
1:A:983:A:H5'	14:N:3:ARG:HH12	1.70	0.56
1:A:1027:C:H2'	1:A:1028:C:C6	2.39	0.56
2:B:25:ASN:ND2	2:B:27:LYS:H	2.02	0.56
2:B:102:LEU:N	2:B:102:LEU:CD1	2.68	0.56
2:B:112:VAL:CG1	2:B:153:ARG:HD3	2.35	0.56
4:D:3:ARG:NH2	4:D:74:GLN:HG3	2.12	0.56
4:D:187:ARG:HE	4:D:187:ARG:CA	2.18	0.56
8:H:91:ARG:HH11	8:H:91:ARG:HG2	1.69	0.56
10:J:21:GLN:O	10:J:25:GLU:HG2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:29:ARG:HH22	14:N:41:ARG:HH12	1.53	0.56
23:Z:39:U:C2'	23:Z:40:C:H5'	2.35	0.56
1:A:101:A:O2'	1:A:102:G:H5'	2.05	0.56
1:A:861:G:O2'	1:A:862:C:H5'	2.04	0.56
1:A:887:G:H1	1:A:910:C:H42	1.53	0.56
2:B:71:VAL:HG23	2:B:164:VAL:HA	1.87	0.56
2:B:98:LEU:H	2:B:98:LEU:CD2	2.12	0.56
3:C:107:GLN:H	3:C:107:GLN:NE2	2.04	0.56
4:D:61:LYS:HD2	4:D:61:LYS:C	2.25	0.56
6:F:33:TYR:CD2	6:F:75:LEU:HA	2.40	0.56
9:I:30:GLY:O	9:I:31:GLN:O	2.23	0.56
1:A:437:U:H5"	4:D:155:LEU:HD21	1.87	0.56
1:A:486:U:H2'	1:A:487:A:C8	2.40	0.56
1:A:628:G:O2'	1:A:629:G:H5'	2.05	0.56
1:A:1352:C:H2'	1:A:1353:G:C8	2.41	0.56
1:A:1446:U:HO2'	1:A:1447:A:H8	1.53	0.56
2:B:98:LEU:O	2:B:101:MET:HG3	2.06	0.56
3:C:70:VAL:HG21	3:C:76:VAL:HG21	1.88	0.56
6:F:43:LEU:HD22	6:F:43:LEU:N	2.20	0.56
17:Q:76:LEU:C	17:Q:76:LEU:HD23	2.26	0.56
2:B:222:ILE:O	2:B:226:ARG:HB2	2.06	0.56
10:J:12:ASP:HB3	10:J:15:THR:CG2	2.36	0.56
18:R:39:VAL:HG13	18:R:40:LEU:HD23	1.87	0.56
1:A:26:A:H2'	1:A:27:G:H5'	1.87	0.56
1:A:1148:U:H2'	1:A:1149:C:O4'	2.06	0.56
1:A:1399:C:C2	1:A:1502:A:N6	2.74	0.56
3:C:60:ALA:O	3:C:61:ALA:HB3	2.05	0.56
8:H:9:MET:O	8:H:13:ILE:HG12	2.05	0.56
1:A:329:A:H4'	1:A:330:C:OP2	2.06	0.56
2:B:107:THR:HG23	2:B:110:GLN:OE1	2.06	0.56
3:C:11:ARG:O	3:C:14:ILE:O	2.24	0.56
10:J:50:ILE:H	10:J:50:ILE:CD1	2.15	0.56
10:J:56:HIS:O	10:J:58:ASP:N	2.39	0.56
12:L:34:ARG:O	12:L:61:THR:HG23	2.06	0.56
1:A:192:U:C1'	20:T:103:GLY:HA2	2.35	0.56
1:A:1095:U:H5'	1:A:1095:U:C6	2.41	0.56
1:A:1115:C:O2	1:A:1115:C:H2'	2.04	0.56
1:A:1216:G:H5"	14:N:5:ALA:HB2	1.88	0.56
2:B:58:ILE:O	2:B:62:ALA:HB2	2.05	0.56
2:B:137:ARG:NH1	2:B:137:ARG:CB	2.69	0.56
2:B:154:LEU:N	2:B:154:LEU:HD23	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:170:GLU:O	2:B:173:ALA:HB3	2.06	0.56
2:B:219:VAL:HA	2:B:222:ILE:CD1	2.36	0.56
3:C:55:VAL:O	3:C:57:ILE:HG13	2.06	0.56
4:D:18:LYS:HG3	4:D:31:CYS:SG	2.46	0.56
9:I:28:VAL:HG22	9:I:63:ILE:HB	1.88	0.56
13:M:49:THR:HG22	13:M:51:ALA:N	2.21	0.56
15:O:27:VAL:CG1	15:O:31:LEU:HD22	2.35	0.56
19:S:30:LEU:HD11	19:S:50:ALA:CB	2.36	0.56
1:A:939:G:H2'	1:A:940:C:C6	2.41	0.56
2:B:12:GLU:HG3	2:B:213:LEU:HD11	1.86	0.56
8:H:17:THR:CG2	8:H:63:LEU:HD13	2.34	0.56
8:H:103:VAL:HG21	8:H:110:ALA:HB2	1.88	0.56
11:K:62:GLN:O	11:K:66:LEU:HG	2.06	0.56
1:A:80:G:H2'	1:A:81:U:H5"	1.86	0.55
1:A:344:A:H5"	1:A:345:C:C5	2.41	0.55
1:A:1366:C:C2	1:A:1367:C:C5	2.94	0.55
1:A:1376:U:O2'	1:A:1377:A:H5'	2.07	0.55
1:A:1392:G:O2'	1:A:1393:U:H5'	2.06	0.55
2:B:92:TYR:CD1	2:B:151:GLY:HA3	2.41	0.55
3:C:33:LEU:HD21	14:N:53:LEU:CD2	2.36	0.55
5:E:9:LYS:HE3	5:E:112:LEU:HD21	1.89	0.55
11:K:126:ARG:O	11:K:128:ALA:N	2.39	0.55
13:M:88:ARG:HG2	13:M:98:VAL:HG22	1.87	0.55
17:Q:63:ARG:HG2	17:Q:64:PRO:CD	2.35	0.55
1:A:619:U:C2'	1:A:620:C:H5"	2.36	0.55
1:A:1153:C:H2'	1:A:1154:G:C8	2.41	0.55
1:A:1527:C:O2'	1:A:1528:U:H5'	2.05	0.55
2:B:23:ARG:HH12	2:B:191:ASP:HA	1.71	0.55
2:B:92:TYR:CE1	2:B:151:GLY:HA3	2.41	0.55
3:C:79:ARG:HD3	3:C:79:ARG:N	2.02	0.55
4:D:17:VAL:O	4:D:19:LEU:HD12	2.06	0.55
5:E:63:ARG:HG2	5:E:63:ARG:HH11	1.70	0.55
7:G:64:GLN:HA	7:G:64:GLN:NE2	2.22	0.55
9:I:100:GLY:O	9:I:102:LEU:N	2.40	0.55
10:J:30:SER:HB3	10:J:81:THR:HA	1.88	0.55
17:Q:9:VAL:HG21	17:Q:84:LEU:HD13	1.88	0.55
19:S:20:LEU:HD12	19:S:21:GLU:HG3	1.88	0.55
1:A:329:A:C5	1:A:332:G:C5	2.94	0.55
1:A:616:G:O2'	1:A:617:G:H5'	2.06	0.55
1:A:1176:A:O2'	1:A:1177:G:H5'	2.06	0.55
1:A:1237:C:H4'	1:A:1334:G:N2	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:142:LEU:HD22	2:B:146:GLN:HE22	1.69	0.55
3:C:92:ALA:HA	3:C:95:THR:O	2.07	0.55
3:C:116:VAL:O	3:C:119:ARG:HB3	2.06	0.55
4:D:107:ARG:HH12	4:D:114:ARG:NH2	2.04	0.55
9:I:48:GLU:N	9:I:49:PRO:CD	2.69	0.55
10:J:12:ASP:HB3	10:J:15:THR:HG22	1.88	0.55
13:M:105:THR:HG22	13:M:106:ASN:H	1.71	0.55
14:N:26:ARG:HH11	14:N:47:LEU:HD11	1.72	0.55
15:O:74:ASP:HB3	15:O:77:ARG:HD3	1.87	0.55
1:A:666:G:H5'	1:A:726:C:H1'	1.88	0.55
1:A:673:G:H5"	6:F:87:ARG:NH1	2.21	0.55
1:A:1103:C:C5'	2:B:98:LEU:HD12	2.36	0.55
3:C:204:LEU:HD12	3:C:204:LEU:N	2.21	0.55
4:D:62:GLN:HE22	4:D:65:ARG:NH1	2.03	0.55
13:M:88:ARG:CZ	19:S:3:ARG:HH21	2.20	0.55
1:A:329:A:C4	1:A:332:G:C5	2.94	0.55
2:B:82:ARG:HB3	2:B:94:ASN:HD22	1.70	0.55
2:B:118:LEU:HB3	2:B:142:LEU:HD21	1.87	0.55
2:B:165:VAL:O	2:B:187:LEU:O	2.24	0.55
2:B:223:ILE:HD13	2:B:226:ARG:HD2	1.89	0.55
4:D:3:ARG:HH11	4:D:3:ARG:HG3	1.72	0.55
4:D:121:VAL:O	4:D:134:ASP:HA	2.06	0.55
5:E:72:GLN:O	5:E:73:ASN:HB3	2.07	0.55
6:F:28:ARG:HH11	6:F:28:ARG:CB	2.04	0.55
11:K:33:THR:HG22	11:K:39:PRO:HA	1.88	0.55
15:O:87:ILE:CG2	15:O:88:ARG:N	2.69	0.55
1:A:1067:A:H4'	1:A:1068:G:OP1	2.05	0.55
1:A:1333:A:H2'	1:A:1334:G:O4'	2.05	0.55
3:C:47:LEU:CD2	3:C:68:VAL:HG11	2.37	0.55
3:C:87:LEU:C	3:C:89:GLU:H	2.08	0.55
6:F:76:ALA:O	6:F:80:ARG:HG3	2.05	0.55
12:L:119:LYS:O	12:L:120:TYR:HB2	2.07	0.55
18:R:74:ARG:HD3	18:R:81:PHE:CD1	2.42	0.55
19:S:51:VAL:HG21	19:S:71:LEU:HD22	1.88	0.55
1:A:587:G:H5'	1:A:587:G:C8	2.42	0.55
1:A:923:A:H8	1:A:923:A:O5'	1.90	0.55
1:A:1447:A:H4'	1:A:1452:C:OP2	2.04	0.55
2:B:25:ASN:HD22	2:B:25:ASN:C	2.09	0.55
3:C:87:LEU:HA	3:C:90:GLU:HG2	1.88	0.55
4:D:162:LEU:HD13	4:D:181:MET:CG	2.36	0.55
8:H:119:LEU:HD12	8:H:124:ALA:HA	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:112:LYS:HD3	9:I:118:LYS:HA	1.87	0.55
11:K:67:ASP:O	11:K:71:LYS:HG3	2.07	0.55
11:K:77:MET:O	11:K:78:GLN:HB2	2.07	0.55
18:R:17:SER:HA	18:R:19:LYS:HZ1	1.72	0.55
1:A:1323:G:H2'	1:A:1324:A:C8	2.41	0.55
1:A:1368:G:OP2	9:I:112:LYS:HG3	2.07	0.55
9:I:10:ARG:HG2	9:I:10:ARG:HH11	1.72	0.55
15:O:87:ILE:CG2	15:O:88:ARG:H	2.20	0.55
17:Q:36:ILE:HD13	17:Q:36:ILE:N	2.21	0.55
1:A:494:U:H2'	1:A:495:A:H5'	1.89	0.55
1:A:849:C:O2'	1:A:850:U:H5'	2.06	0.55
3:C:46:GLU:C	3:C:48:TYR:H	2.11	0.55
14:N:26:ARG:NH1	14:N:47:LEU:HD11	2.22	0.55
1:A:103:C:OP1	20:T:17:ARG:HD2	2.07	0.55
1:A:477:A:C3'	1:A:479:C:H5"	2.37	0.55
1:A:590:C:O2'	1:A:591:U:H5'	2.07	0.55
1:A:639:G:O2'	1:A:640:A:H5'	2.06	0.55
2:B:69:LEU:CD1	2:B:155:LEU:HD11	2.37	0.55
2:B:71:VAL:HG21	2:B:164:VAL:HG22	1.89	0.55
6:F:75:LEU:C	6:F:75:LEU:HD13	2.28	0.55
9:I:50:LEU:HD21	9:I:81:ILE:HG22	1.89	0.55
10:J:6:ILE:HG13	10:J:71:LEU:O	2.07	0.55
1:A:629:G:H2'	1:A:630:G:O4'	2.06	0.54
2:B:112:VAL:O	2:B:116:GLU:HG3	2.07	0.54
3:C:39:ILE:C	3:C:41:GLY:H	2.10	0.54
5:E:72:GLN:C	5:E:74:GLY:H	2.11	0.54
9:I:114:TYR:N	9:I:114:TYR:HD1	2.05	0.54
14:N:12:ARG:C	14:N:14:PRO:HD3	2.27	0.54
1:A:189(A):C:H2'	1:A:189(B):C:H6	1.72	0.54
1:A:418:C:O2'	1:A:540:G:H1'	2.07	0.54
1:A:663:A:O2'	1:A:664:G:H5'	2.07	0.54
1:A:1004:A:H4'	1:A:1004:A:OP2	2.06	0.54
1:A:1227:A:H5'	13:M:111:LYS:NZ	2.22	0.54
3:C:93:LYS:HA	3:C:93:LYS:CE	2.32	0.54
3:C:155:GLY:HA3	3:C:164:ARG:O	2.07	0.54
7:G:23:VAL:O	7:G:27:ILE:HG13	2.06	0.54
10:J:12:ASP:O	10:J:15:THR:HG22	2.07	0.54
18:R:74:ARG:HB3	18:R:81:PHE:CE1	2.42	0.54
20:T:87:LYS:O	20:T:91:LEU:HB2	2.06	0.54
1:A:1028:C:H2'	1:A:1029:C:C6	2.42	0.54
2:B:134:GLU:HG2	2:B:137:ARG:HH21	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:6:HIS:HD2	3:C:8:ILE:H	1.55	0.54
4:D:165:MET:O	4:D:166:LYS:C	2.45	0.54
6:F:87:ARG:HG3	6:F:87:ARG:NH1	2.23	0.54
10:J:34:VAL:HG22	10:J:74:ILE:HG23	1.87	0.54
10:J:51:ARG:HB3	10:J:59:SER:CB	2.37	0.54
15:O:3:ILE:HA	15:O:7:GLU:OE2	2.07	0.54
17:Q:24:GLU:HG2	17:Q:39:SER:HB3	1.90	0.54
19:S:5:LEU:O	19:S:6:LYS:CB	2.55	0.54
19:S:16:LEU:O	19:S:20:LEU:HG	2.07	0.54
2:B:100:GLY:C	2:B:108:ILE:HG13	2.28	0.54
5:E:76:ILE:CG2	5:E:77:PRO:HD2	2.36	0.54
6:F:8:ILE:HG23	6:F:85:VAL:HG13	1.88	0.54
13:M:36:LYS:HD2	13:M:59:TYR:OH	2.07	0.54
13:M:105:THR:HG22	13:M:106:ASN:N	2.23	0.54
17:Q:68:ARG:O	17:Q:68:ARG:HG3	2.08	0.54
21:V:6:ARG:NE	21:V:15:ARG:NH1	2.53	0.54
1:A:231:G:H2'	1:A:232:G:C5'	2.34	0.54
1:A:390:C:H4'	16:P:28:ARG:NH2	2.23	0.54
2:B:211:ILE:H	2:B:211:ILE:HD12	1.73	0.54
3:C:50:ALA:HA	3:C:72:LYS:HB2	1.90	0.54
3:C:113:ALA:HB2	3:C:202:ILE:HG13	1.88	0.54
3:C:188:LEU:O	3:C:189:ALA:HB2	2.08	0.54
4:D:50:ARG:HB3	4:D:50:ARG:CZ	2.37	0.54
13:M:40:ASN:ND2	13:M:41:PRO:HD2	2.23	0.54
17:Q:95:TYR:HA	17:Q:98:LEU:HD13	1.90	0.54
18:R:39:VAL:HG13	18:R:40:LEU:N	2.22	0.54
1:A:533:A:O2'	1:A:535:A:OP2	2.26	0.54
1:A:570:G:H2'	1:A:571:U:C6	2.42	0.54
1:A:838:G:C2'	1:A:839:U:H5"	2.34	0.54
1:A:1120:G:O2'	1:A:1121:U:H5'	2.07	0.54
3:C:54:ARG:NH1	3:C:56:ASP:OD1	2.40	0.54
3:C:83:ARG:O	3:C:85:ARG:N	2.40	0.54
15:O:74:ASP:OD1	15:O:76:GLU:HB3	2.07	0.54
1:A:448:A:O2'	1:A:449:C:H5'	2.08	0.54
1:A:864:A:H2'	1:A:865:A:C8	2.43	0.54
1:A:1026:G:H2'	1:A:1026:G:N3	2.22	0.54
1:A:1277:C:C5'	1:A:1277:C:H6	2.21	0.54
2:B:69:LEU:HD12	2:B:155:LEU:CD1	2.36	0.54
5:E:102:ALA:HB1	5:E:120:THR:HG21	1.90	0.54
9:I:9:ARG:HA	9:I:13:ALA:O	2.07	0.54
10:J:46:ARG:HG2	10:J:46:ARG:HH11	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Z:31:A:H2'	23:Z:32:U:O4'	2.06	0.54
1:A:149:A:H2'	1:A:150:C:C6	2.43	0.54
1:A:323:U:H2'	1:A:324:G:O4'	2.07	0.54
1:A:953:G:H1'	13:M:125:ARG:HA	1.89	0.54
5:E:150:ARG:CG	5:E:150:ARG:NH1	2.68	0.54
7:G:137:LYS:O	7:G:141:VAL:HG23	2.08	0.54
18:R:36:ASN:O	18:R:40:LEU:HG	2.07	0.54
18:R:62:GLU:C	18:R:64:ARG:H	2.11	0.54
1:A:577:G:O2'	1:A:816:A:H2'	2.08	0.54
2:B:16:HIS:O	2:B:18:GLY:N	2.41	0.54
2:B:137:ARG:CB	2:B:137:ARG:HH11	2.21	0.54
3:C:13:GLY:O	3:C:14:ILE:HD13	2.07	0.54
8:H:119:LEU:HD23	8:H:119:LEU:N	2.23	0.54
15:O:75:PRO:O	15:O:78:TYR:HB3	2.07	0.54
17:Q:101:ARG:HA	17:Q:101:ARG:NE	2.20	0.54
1:A:223:U:C3'	1:A:224:C:H5"	2.38	0.54
1:A:998:G:H3'	1:A:999:C:C5'	2.30	0.54
1:A:1197:G:C2'	1:A:1198:G:H5"	2.38	0.54
2:B:24:TRP:HB3	2:B:40:HIS:CE1	2.44	0.54
2:B:24:TRP:CG	2:B:25:ASN:N	2.74	0.54
2:B:73:THR:HB	2:B:170:GLU:OE1	2.08	0.54
2:B:114:ARG:NH1	2:B:118:LEU:HG	2.22	0.54
5:E:18:ARG:HG2	5:E:19:MET:N	2.23	0.54
12:L:11:VAL:HG21	17:Q:34:LYS:HG2	1.90	0.54
12:L:41:ARG:HG2	12:L:41:ARG:NH1	2.22	0.54
13:M:3:ARG:O	13:M:3:ARG:HG3	2.07	0.54
18:R:25:THR:HG22	18:R:42:ARG:HH11	1.73	0.54
18:R:86:VAL:HG12	18:R:87:ARG:HG3	1.88	0.54
1:A:1004:A:N7	1:A:1026:G:C5	2.76	0.53
2:B:111:ARG:HB3	2:B:149:LEU:CD1	2.37	0.53
7:G:6:ARG:HG2	7:G:6:ARG:O	2.07	0.53
8:H:11:THR:HG22	8:H:15:ASN:ND2	2.23	0.53
10:J:10:GLY:H	10:J:16:LEU:HD11	1.73	0.53
11:K:48:ILE:HG21	11:K:63:LEU:HD12	1.89	0.53
14:N:9:LYS:C	14:N:11:LYS:H	2.12	0.53
19:S:3:ARG:HG2	19:S:3:ARG:NH1	2.22	0.53
19:S:22:LEU:HD13	19:S:28:LYS:CG	2.38	0.53
21:V:6:ARG:HB3	21:V:15:ARG:HH11	1.73	0.53
1:A:22:G:H2'	1:A:23:C:C6	2.44	0.53
1:A:251:G:H4'	1:A:252:U:O5'	2.08	0.53
3:C:189:ALA:O	3:C:191:THR:HG22	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:132:ARG:HB3	4:D:132:ARG:CZ	2.38	0.53
5:E:96:PRO:HA	5:E:117:ASP:OD2	2.09	0.53
13:M:8:GLU:O	13:M:10:PRO:CD	2.57	0.53
13:M:122:LYS:O	13:M:123:ALA:HB3	2.08	0.53
14:N:29:ARG:HG2	14:N:29:ARG:NH1	2.23	0.53
23:Z:36:A:H2'	23:Z:37:A:H8	1.73	0.53
1:A:320:C:H5'	1:A:321:A:OP2	2.09	0.53
1:A:692:U:OP1	11:K:124:LYS:CE	2.57	0.53
2:B:69:LEU:HD21	2:B:93:VAL:HG23	1.89	0.53
3:C:108:ASN:ND2	3:C:144:SER:HB2	2.17	0.53
6:F:62:TRP:CG	18:R:35:ARG:NH1	2.77	0.53
8:H:11:THR:HA	8:H:14:ARG:NH1	2.22	0.53
10:J:50:ILE:HD13	14:N:41:ARG:CD	2.38	0.53
14:N:53:LEU:HB3	14:N:56:VAL:HG21	1.89	0.53
1:A:250:A:H5'	1:A:251:G:OP1	2.08	0.53
1:A:501:C:H2'	1:A:502:G:C8	2.43	0.53
5:E:74:GLY:HA3	5:E:116:THR:HG22	1.91	0.53
18:R:53:ARG:NE	18:R:58:LEU:O	2.42	0.53
1:A:162:A:H2'	1:A:163:C:H5'	1.89	0.53
1:A:738:C:OP1	6:F:92:LYS:HD3	2.09	0.53
1:A:1124:G:HO2'	1:A:1145:C:N4	2.07	0.53
1:A:1258:G:O2'	1:A:1259:C:H5'	2.08	0.53
2:B:21:ARG:CD	2:B:21:ARG:H	2.22	0.53
2:B:158:LEU:H	2:B:158:LEU:HD22	1.73	0.53
3:C:154:SER:O	3:C:165:THR:HA	2.08	0.53
4:D:110:PHE:HD2	4:D:148:VAL:CG2	2.20	0.53
9:I:113:LYS:HD3	9:I:119:ALA:HA	1.90	0.53
15:O:65:ARG:O	15:O:68:ARG:HB3	2.09	0.53
2:B:140:HIS:HA	2:B:143:GLU:CG	2.38	0.53
2:B:168:THR:OG1	2:B:191:ASP:O	2.26	0.53
3:C:58:GLU:O	3:C:59:ARG:HG3	2.08	0.53
4:D:110:PHE:N	4:D:110:PHE:CD1	2.76	0.53
18:R:46:GLU:CD	18:R:46:GLU:N	2.62	0.53
1:A:866:C:C2'	1:A:867:G:H5'	2.39	0.53
1:A:972:C:C4'	10:J:57:LYS:HG2	2.20	0.53
1:A:1007:C:H2'	1:A:1008:C:C6	2.44	0.53
1:A:1237:C:C4'	1:A:1334:G:N2	2.71	0.53
2:B:91:PRO:CG	2:B:154:LEU:HB2	2.21	0.53
3:C:39:ILE:HG22	3:C:40:ARG:N	2.24	0.53
4:D:18:LYS:HE3	4:D:20:TYR:CE2	2.43	0.53
5:E:71:LEU:C	5:E:72:GLN:HG2	2.29	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:20:LEU:CD1	19:S:21:GLU:HG3	2.39	0.53
1:A:224:C:H6	1:A:224:C:H5'	1.74	0.53
1:A:1060:C:O2'	1:A:1061:G:H5'	2.09	0.53
1:A:1153:C:H2'	1:A:1154:G:H8	1.72	0.53
1:A:1206:G:C6	1:A:1207:G:C5	2.97	0.53
2:B:22:LYS:HA	2:B:40:HIS:HE1	1.73	0.53
2:B:91:PRO:HB3	2:B:151:GLY:O	2.09	0.53
3:C:83:ARG:C	3:C:85:ARG:N	2.60	0.53
3:C:111:LEU:HD21	3:C:144:SER:O	2.08	0.53
7:G:16:LEU:N	7:G:16:LEU:HD12	2.24	0.53
9:I:88:TYR:O	9:I:89:ASN:HB2	2.09	0.53
12:L:115:LYS:O	12:L:117:ARG:N	2.38	0.53
1:A:1144:G:N2	1:A:1146:A:H62	1.98	0.53
2:B:113:HIS:HD2	2:B:116:GLU:OE1	1.92	0.53
12:L:53:ARG:HG2	12:L:53:ARG:HH11	1.74	0.53
1:A:192:U:H2'	1:A:193:C:C6	2.43	0.53
1:A:224:C:H6	1:A:224:C:C5'	2.22	0.53
1:A:339:C:H2'	1:A:340:U:C6	2.42	0.53
1:A:577:G:H1'	1:A:816:A:C4	2.44	0.53
1:A:706:A:H1'	11:K:29:ILE:HD11	1.91	0.53
1:A:857:C:H2'	1:A:858:G:O4'	2.09	0.53
1:A:939:G:H2'	1:A:940:C:H6	1.74	0.53
1:A:1001:A:H4'	1:A:1001(A):G:OP1	2.08	0.53
1:A:1002:G:C2	1:A:1003:G:N7	2.77	0.53
1:A:1222:G:O2'	1:A:1223:C:H5'	2.08	0.53
1:A:1310:G:N7	19:S:2:PRO:HG3	2.24	0.53
2:B:15:VAL:HG21	2:B:209:ARG:HG3	1.91	0.53
3:C:64:VAL:N	3:C:99:VAL:HG11	2.24	0.53
3:C:167:TRP:O	3:C:168:ALA:HB3	2.09	0.53
1:A:866:C:H2'	1:A:867:G:C5'	2.36	0.52
1:A:1347:G:H22	1:A:1373:G:H2'	1.72	0.52
2:B:20:GLU:O	2:B:39:ILE:HG23	2.08	0.52
5:E:144:THR:N	5:E:147:ASP:OD1	2.38	0.52
6:F:80:ARG:HG2	6:F:80:ARG:HH11	1.73	0.52
8:H:20:TYR:CE2	8:H:75:ARG:HD2	2.36	0.52
9:I:7:THR:HB	9:I:83:ARG:NH1	2.23	0.52
10:J:10:GLY:N	10:J:16:LEU:HD11	2.25	0.52
11:K:108:ILE:HG22	11:K:109:VAL:N	2.23	0.52
14:N:3:ARG:HD3	14:N:6:LEU:HD12	1.90	0.52
14:N:57:ARG:HG2	14:N:58:LYS:N	2.25	0.52
1:A:427:U:C3'	1:A:428:G:H5"	2.37	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:471:G:H21	16:P:82:GLN:NE2	2.06	0.52
1:A:627:G:O2'	1:A:628:G:H5'	2.09	0.52
1:A:750:G:N2	15:O:23:GLY:HA3	2.23	0.52
1:A:781:A:H2	1:A:1514:C:O4'	1.92	0.52
1:A:877:C:H1'	8:H:3:THR:HG21	1.91	0.52
1:A:1297:C:O2	1:A:1297:C:C2'	2.57	0.52
1:A:1366:C:H2'	1:A:1367:C:C6	2.44	0.52
2:B:16:HIS:C	2:B:18:GLY:H	2.12	0.52
2:B:91:PRO:CA	2:B:154:LEU:HD12	2.39	0.52
3:C:35:GLU:O	3:C:39:ILE:HD13	2.10	0.52
12:L:86:ARG:HD3	12:L:101:VAL:HG22	1.92	0.52
16:P:39:TYR:HB2	16:P:49:LEU:HD13	1.90	0.52
17:Q:10:VAL:HG13	17:Q:19:VAL:HB	1.91	0.52
1:A:232:G:H5'	1:A:232:G:C8	2.36	0.52
1:A:833:U:H2'	1:A:834:C:C6	2.44	0.52
1:A:1103:C:C3'	1:A:1104:G:H5"	2.40	0.52
1:A:1197:G:H2'	1:A:1198:G:H5"	1.91	0.52
2:B:55:PHE:O	2:B:58:ILE:HG13	2.09	0.52
3:C:123:GLN:NE2	3:C:140:ARG:HH22	2.07	0.52
4:D:36:ARG:H	4:D:37:PRO:HD3	1.73	0.52
5:E:99:GLY:O	5:E:117:ASP:HA	2.09	0.52
6:F:10:LEU:HD12	6:F:59:TYR:HB3	1.92	0.52
7:G:26:PHE:O	7:G:30:ILE:HG13	2.08	0.52
8:H:11:THR:HG23	8:H:14:ARG:NH1	2.24	0.52
11:K:91:ARG:NH1	18:R:88:LYS:NZ	2.57	0.52
12:L:59:ARG:HD3	12:L:65:GLU:HG3	1.91	0.52
13:M:71:ARG:HG2	13:M:71:ARG:HH11	1.74	0.52
18:R:59:SER:HB3	18:R:62:GLU:CG	2.36	0.52
1:A:749:C:O2'	1:A:750:G:H8	1.92	0.52
1:A:974:A:OP1	14:N:31:ARG:HD3	2.09	0.52
1:A:1223:C:P	19:S:78:ARG:HH12	2.32	0.52
1:A:1281:U:H3'	1:A:1281:U:H6	1.74	0.52
1:A:1406:U:O2'	1:A:1407:C:H5'	2.09	0.52
2:B:112:VAL:HG11	2:B:153:ARG:HA	1.92	0.52
3:C:19:GLU:HG2	3:C:54:ARG:HH12	1.71	0.52
4:D:61:LYS:HG2	4:D:203:VAL:HG13	1.91	0.52
6:F:40:VAL:HG22	6:F:41:GLU:H	1.73	0.52
7:G:15:ASP:OD1	7:G:17:VAL:N	2.42	0.52
7:G:17:VAL:HG12	7:G:18:TYR:CD1	2.45	0.52
15:O:5:LYS:O	15:O:9:GLN:HG2	2.08	0.52
18:R:25:THR:O	18:R:25:THR:HG22	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:5:LEU:O	19:S:6:LYS:CG	2.57	0.52
1:A:757:U:H2'	1:A:758:G:O4'	2.09	0.52
1:A:908:A:O2'	1:A:909:A:H5'	2.10	0.52
1:A:1019:C:O2'	1:A:1020:U:H5'	2.08	0.52
1:A:1201:A:H4'	1:A:1202:G:C5'	2.40	0.52
2:B:7:VAL:HG12	2:B:8:LYS:N	2.13	0.52
2:B:111:ARG:CB	2:B:149:LEU:HD11	2.37	0.52
2:B:181:PHE:CD2	8:H:70:GLN:HB3	2.44	0.52
13:M:4:ILE:HG22	13:M:5:ALA:N	2.24	0.52
13:M:125:ARG:HD2	13:M:125:ARG:C	2.30	0.52
16:P:4:ILE:HA	16:P:20:VAL:O	2.08	0.52
16:P:59:TRP:HB3	16:P:64:ALA:HB2	1.92	0.52
18:R:53:ARG:HB2	18:R:63:GLN:HG2	1.91	0.52
1:A:404:U:H5'	4:D:122:ARG:HD2	1.92	0.52
1:A:1141:C:H2'	1:A:1142:G:H8	1.75	0.52
2:B:158:LEU:H	2:B:158:LEU:CD2	2.22	0.52
4:D:60:GLU:HG2	4:D:202:LEU:HB2	1.91	0.52
9:I:3:GLN:NE2	9:I:20:ARG:HG2	2.24	0.52
11:K:66:LEU:CD2	11:K:97:ALA:HB1	2.39	0.52
14:N:23:ARG:HH12	14:N:30:ALA:HB2	1.72	0.52
18:R:88:LYS:C	18:R:88:LYS:HD3	2.30	0.52
19:S:41:VAL:O	19:S:44:MET:HG3	2.10	0.52
21:V:2:GLY:C	21:V:4:GLY:N	2.63	0.52
2:B:84:GLU:CG	2:B:216:SER:HA	2.39	0.52
3:C:173:VAL:O	3:C:175:LEU:HD23	2.09	0.52
3:C:190:ARG:CB	3:C:190:ARG:HH11	2.22	0.52
4:D:8:VAL:O	4:D:10:ARG:N	2.39	0.52
6:F:19:LEU:C	6:F:19:LEU:HD23	2.30	0.52
7:G:38:LEU:O	7:G:42:ILE:HG12	2.10	0.52
7:G:64:GLN:HA	7:G:64:GLN:HE21	1.74	0.52
9:I:100:GLY:C	9:I:102:LEU:H	2.12	0.52
10:J:50:ILE:HD13	14:N:41:ARG:HD3	1.92	0.52
13:M:71:ARG:HG2	13:M:71:ARG:NH1	2.24	0.52
1:A:349:A:O2'	1:A:350:G:H5'	2.09	0.52
1:A:1214:C:O2	1:A:1214:C:H2'	2.09	0.52
3:C:14:ILE:O	3:C:16:ARG:N	2.43	0.52
4:D:36:ARG:H	4:D:37:PRO:CD	2.23	0.52
9:I:97:LYS:O	9:I:100:GLY:N	2.40	0.52
11:K:114:VAL:O	11:K:114:VAL:HG13	2.10	0.52
12:L:26:ALA:HB2	12:L:98:TYR:CE2	2.45	0.52
14:N:8:GLU:O	14:N:11:LYS:HB2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:16:PHE:HB2	14:N:18:VAL:HG22	1.91	0.52
20:T:23:ARG:HG2	20:T:23:ARG:HH11	1.74	0.52
1:A:605:U:O2'	1:A:606:G:H5'	2.10	0.52
1:A:965:A:C2	1:A:969:A:C2	2.97	0.52
3:C:115:LEU:HD23	3:C:118:GLN:OE1	2.10	0.52
4:D:170:VAL:CG2	4:D:171:GLY:N	2.72	0.52
4:D:176:LEU:CG	4:D:177:ASP:H	2.18	0.52
9:I:8:GLY:HA2	9:I:79:LEU:HD13	1.92	0.52
10:J:24:VAL:O	10:J:24:VAL:HG22	2.09	0.52
13:M:17:VAL:O	13:M:20:THR:HB	2.10	0.52
19:S:80:TYR:O	19:S:81:ARG:C	2.48	0.52
23:Z:31:A:H61	23:Z:39:U:H3	1.56	0.52
1:A:1473:A:H2'	1:A:1474:G:O4'	2.10	0.52
2:B:25:ASN:ND2	2:B:25:ASN:C	2.63	0.52
2:B:173:ALA:O	2:B:176:GLU:HB2	2.10	0.52
5:E:20:GLN:O	5:E:21:ALA:C	2.48	0.52
7:G:93:PRO:HG2	7:G:94:ARG:H	1.76	0.52
14:N:37:PHE:C	14:N:39:LEU:H	2.14	0.52
17:Q:18:THR:HG22	17:Q:19:VAL:N	2.24	0.52
18:R:32:ARG:NH2	18:R:65:ILE:HD12	2.23	0.52
19:S:53:ASN:HD21	19:S:56:GLN:HB2	1.75	0.52
20:T:96:GLY:O	20:T:97:ALA:CB	2.58	0.52
1:A:1473:A:H2'	1:A:1474:G:C5'	2.37	0.51
4:D:209:ARG:HG2	4:D:209:ARG:NH1	2.25	0.51
7:G:110:GLN:OE1	7:G:110:GLN:HA	2.09	0.51
10:J:79:ARG:HH22	10:J:82:ILE:HD12	1.76	0.51
13:M:40:ASN:HB3	13:M:43:THR:HG23	1.92	0.51
13:M:124:PRO:C	13:M:126:LYS:H	2.13	0.51
14:N:26:ARG:HG3	14:N:27:CYS:N	2.19	0.51
16:P:21:VAL:HG11	16:P:59:TRP:CE3	2.45	0.51
19:S:17:GLU:HA	19:S:20:LEU:HD11	1.91	0.51
1:A:55:A:O2'	1:A:56:U:H5'	2.09	0.51
1:A:1055:A:C2	1:A:1056:U:H1'	2.45	0.51
1:A:1090:U:H2'	1:A:1091:U:H6	1.76	0.51
1:A:1237:C:H2'	1:A:1336:C:H5	1.76	0.51
2:B:206:ASP:O	2:B:207:ALA:CB	2.59	0.51
3:C:64:VAL:CG2	3:C:99:VAL:HG21	2.39	0.51
5:E:74:GLY:HA3	5:E:116:THR:CG2	2.40	0.51
6:F:33:TYR:HA	6:F:71:ARG:NH2	2.24	0.51
9:I:91:ASP:C	9:I:93:ARG:H	2.13	0.51
10:J:45:ARG:HH11	10:J:45:ARG:HB2	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:59:ARG:HG2	12:L:59:ARG:HH11	1.76	0.51
13:M:79:LYS:HG2	13:M:83:ASP:OD2	2.09	0.51
17:Q:45:HIS:O	17:Q:47:PRO:HD3	2.11	0.51
1:A:109:A:C8	1:A:326:G:H2'	2.45	0.51
1:A:474:G:O2'	1:A:475:G:H5'	2.11	0.51
1:A:1047:G:H5"	14:N:4:LYS:HD2	1.91	0.51
1:A:1309:G:O2'	1:A:1310:G:H5'	2.10	0.51
2:B:84:GLU:HB3	2:B:219:VAL:HG21	1.90	0.51
3:C:15:THR:O	3:C:16:ARG:HB2	2.10	0.51
7:G:50:ILE:HA	7:G:125:MET:HE3	1.92	0.51
9:I:8:GLY:N	9:I:83:ARG:HH11	2.09	0.51
16:P:21:VAL:HG21	16:P:59:TRP:CD1	2.45	0.51
17:Q:53:LEU:C	17:Q:53:LEU:HD23	2.29	0.51
19:S:15:LEU:O	19:S:19:VAL:HG12	2.10	0.51
19:S:63:THR:CG2	19:S:64:GLU:N	2.73	0.51
19:S:63:THR:CG2	19:S:64:GLU:H	2.19	0.51
1:A:376:G:H2'	1:A:377:G:C8	2.43	0.51
1:A:625:G:H4'	16:P:16:HIS:CD2	2.45	0.51
1:A:1442(A):G:O5'	1:A:1442(B):A:C5'	2.57	0.51
2:B:79:ASP:O	2:B:82:ARG:N	2.42	0.51
6:F:62:TRP:CB	18:R:35:ARG:HH12	2.23	0.51
10:J:30:SER:HB3	10:J:80:LYS:O	2.10	0.51
10:J:72:VAL:O	10:J:73:ASP:HB2	2.10	0.51
11:K:108:ILE:HG22	11:K:109:VAL:H	1.75	0.51
12:L:119:LYS:O	12:L:120:TYR:CB	2.58	0.51
16:P:45:THR:OG1	16:P:46:PRO:HD2	2.11	0.51
18:R:61:LYS:O	18:R:65:ILE:HG12	2.10	0.51
1:A:818:G:O2'	1:A:819:A:H5'	2.10	0.51
1:A:1112:C:H1'	3:C:179:ARG:HH21	1.74	0.51
1:A:1337:G:H5"	1:A:1338:G:OP1	2.10	0.51
3:C:43:LEU:HD21	3:C:68:VAL:CG2	2.41	0.51
11:K:19:ALA:HB2	11:K:80:VAL:HG21	1.93	0.51
15:O:86:GLY:O	15:O:87:ILE:HD13	2.11	0.51
16:P:43:LYS:HA	16:P:48:TRP:CB	2.41	0.51
1:A:329:A:N6	1:A:332:G:N2	2.57	0.51
1:A:542:G:H5'	4:D:41:GLY:HA3	1.91	0.51
1:A:865:A:H5'	1:A:1078:U:O4	2.11	0.51
1:A:1425:U:H2'	1:A:1426:C:C6	2.46	0.51
2:B:55:PHE:HA	2:B:58:ILE:CD1	2.41	0.51
8:H:5:PRO:O	8:H:8:ASP:HB3	2.11	0.51
8:H:6:ILE:O	8:H:10:LEU:HG	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:5:TYR:O	9:I:84:ALA:HA	2.11	0.51
1:A:250:A:H4'	1:A:251:G:O5'	2.11	0.51
2:B:55:PHE:HA	2:B:58:ILE:CG1	2.41	0.51
3:C:112:SER:OG	3:C:115:LEU:HD12	2.10	0.51
5:E:100:VAL:HG13	5:E:118:ILE:HG22	1.92	0.51
6:F:2:ARG:CD	6:F:69:GLU:HG2	2.40	0.51
7:G:143:ARG:HB3	7:G:143:ARG:NH1	2.26	0.51
14:N:57:ARG:HG2	14:N:58:LYS:H	1.76	0.51
16:P:26:ARG:HG2	16:P:26:ARG:HH11	1.76	0.51
1:A:1081:G:O2'	1:A:1082:G:H5'	2.11	0.51
1:A:1131:G:OP1	1:A:1131:G:H4'	2.11	0.51
1:A:1327:C:H5"	21:V:20:LYS:HE3	1.91	0.51
2:B:23:ARG:C	2:B:23:ARG:HD3	2.31	0.51
2:B:55:PHE:HA	2:B:58:ILE:HG13	1.93	0.51
2:B:108:ILE:O	2:B:108:ILE:HG22	2.09	0.51
3:C:51:GLY:O	3:C:115:LEU:HD21	2.11	0.51
8:H:134:ILE:O	8:H:135:CYS:HB3	2.10	0.51
1:A:313:A:H2'	1:A:314:C:C6	2.46	0.51
1:A:718:G:C5'	11:K:117:ASN:HD22	2.20	0.51
1:A:1340:A:O2'	1:A:1341:U:H5'	2.11	0.51
2:B:51:LEU:O	2:B:55:PHE:HD1	1.93	0.51
2:B:67:THR:HA	2:B:90:MET:CE	2.41	0.51
2:B:82:ARG:NH1	2:B:82:ARG:HB2	2.26	0.51
2:B:97:TRP:CZ2	2:B:102:LEU:HD13	2.43	0.51
4:D:158:ILE:HG23	4:D:162:LEU:HD12	1.93	0.51
15:O:11:VAL:HG21	15:O:34:LEU:HD22	1.92	0.51
1:A:491:G:O2'	1:A:492:G:H5'	2.11	0.51
1:A:1053:G:O2'	1:A:1199:U:H5	1.93	0.51
1:A:1244:C:C3'	1:A:1245:A:H5"	2.41	0.51
2:B:161:ALA:HB1	2:B:185:ILE:HD11	1.92	0.51
2:B:162:ILE:HG22	2:B:164:VAL:HG23	1.92	0.51
5:E:12:LEU:HD12	5:E:12:LEU:O	2.11	0.51
9:I:17:VAL:CG1	9:I:81:ILE:HD13	2.41	0.51
13:M:29:ARG:O	13:M:32:GLU:HB3	2.11	0.51
15:O:39:LEU:O	15:O:43:LEU:HG	2.11	0.51
16:P:6:LEU:HD23	16:P:17:TYR:CD2	2.46	0.51
1:A:721:G:OP2	18:R:63:GLN:HG2	2.11	0.50
1:A:840:C:O2	1:A:840:C:H2'	2.10	0.50
1:A:1152:A:H4'	10:J:13:HIS:HD2	1.75	0.50
1:A:1197:G:C3'	1:A:1198:G:C5'	2.89	0.50
1:A:1364:U:O2'	1:A:1365:G:H5'	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:78:GLN:NE2	2:B:96:ARG:NH1	2.58	0.50
2:B:95:GLN:O	2:B:96:ARG:HD2	2.11	0.50
2:B:137:ARG:HH11	2:B:137:ARG:HB3	1.75	0.50
7:G:119:ARG:HH11	7:G:119:ARG:HG3	1.76	0.50
8:H:81:HIS:O	8:H:82:HIS:HB2	2.10	0.50
10:J:8:LEU:HB2	10:J:70:ARG:HB2	1.92	0.50
20:T:45:GLN:CB	20:T:91:LEU:HD22	2.41	0.50
1:A:1004:A:H5"	1:A:1025:U:O2	2.11	0.50
1:A:1352:C:O2	1:A:1371:G:C2	2.64	0.50
1:A:1473:A:C3'	1:A:1474:G:H5"	2.41	0.50
3:C:155:GLY:O	3:C:156:ARG:CB	2.57	0.50
9:I:8:GLY:H	9:I:83:ARG:HH11	1.59	0.50
1:A:329:A:C4	1:A:332:G:C6	2.98	0.50
1:A:979:C:H2'	1:A:980:C:H5'	1.93	0.50
1:A:1128:C:H1'	1:A:1146:A:H61	1.75	0.50
1:A:1128:C:C5'	9:I:16:ARG:HH12	2.23	0.50
1:A:1355:G:O2'	1:A:1356:G:H5'	2.10	0.50
3:C:132:ARG:HA	3:C:135:LYS:CE	2.39	0.50
10:J:28:ARG:C	10:J:29:ARG:HD3	2.32	0.50
14:N:4:LYS:HA	14:N:7:ILE:HG13	1.92	0.50
18:R:66:LEU:HD11	18:R:70:ILE:HD11	1.92	0.50
20:T:43:LEU:HD13	20:T:51:GLU:HG3	1.92	0.50
1:A:248:C:O2'	1:A:249:U:H5'	2.11	0.50
1:A:1151:A:O2'	1:A:1152:A:H8	1.95	0.50
1:A:1206:G:C4	1:A:1207:G:C8	3.00	0.50
1:A:1495:U:H2'	1:A:1496:C:H6	1.76	0.50
2:B:79:ASP:O	2:B:80:ILE:C	2.48	0.50
2:B:216:SER:O	2:B:219:VAL:N	2.44	0.50
3:C:82:GLU:O	3:C:86:VAL:HG23	2.12	0.50
11:K:16:SER:O	11:K:35:PRO:HG3	2.12	0.50
12:L:27:LEU:O	12:L:29:GLY:N	2.45	0.50
12:L:36:VAL:HG22	12:L:82:VAL:HG12	1.93	0.50
1:A:500:G:H5"	12:L:124:LYS:HE2	1.93	0.50
1:A:1049:U:H4'	1:A:1050:G:H5"	1.94	0.50
2:B:84:GLU:HG3	2:B:219:VAL:HG21	1.94	0.50
3:C:129:ALA:HB3	3:C:132:ARG:HH12	1.73	0.50
4:D:67:ILE:HG22	4:D:68:TYR:CD1	2.46	0.50
5:E:79:GLU:HB3	5:E:92:LYS:HA	1.94	0.50
7:G:52:GLU:C	7:G:54:THR:N	2.64	0.50
7:G:148:ASN:C	7:G:150:ALA:N	2.64	0.50
16:P:75:ARG:HH11	16:P:75:ARG:HG3	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:A:H2'	1:A:180:U:C6	2.47	0.50
1:A:231:G:O2'	1:A:232:G:H5"	2.12	0.50
1:A:254:G:OP1	17:Q:67:LYS:O	2.28	0.50
1:A:275:G:OP1	17:Q:14:LYS:HD2	2.11	0.50
1:A:328:C:O2	1:A:328:C:C2'	2.59	0.50
1:A:443:C:O2'	1:A:444:C:H5'	2.10	0.50
1:A:538:G:OP2	12:L:115:LYS:HG3	2.12	0.50
1:A:976:G:N7	1:A:1358:U:C2	2.80	0.50
1:A:1330:U:OP1	13:M:23:TYR:O	2.29	0.50
1:A:1378:C:O2	1:A:1378:C:H2'	2.11	0.50
2:B:32:ILE:HD12	2:B:40:HIS:HB3	1.92	0.50
2:B:90:MET:HE2	2:B:90:MET:HA	1.94	0.50
4:D:19:LEU:O	4:D:21:LEU:HG	2.12	0.50
9:I:3:GLN:HA	9:I:3:GLN:NE2	2.14	0.50
14:N:23:ARG:NH1	14:N:28:GLY:O	2.45	0.50
14:N:36:PHE:O	14:N:36:PHE:CD1	2.65	0.50
1:A:180:U:O2'	1:A:181:G:H5'	2.12	0.50
1:A:232:G:H1'	1:A:262:A:N1	2.26	0.50
1:A:501:C:O3'	12:L:118:SER:HB2	2.12	0.50
1:A:1001(A):G:C2	1:A:1002:G:H1'	2.47	0.50
1:A:1194:U:H2'	1:A:1195:C:C6	2.46	0.50
3:C:150:LYS:HB2	3:C:169:ALA:HB2	1.94	0.50
5:E:55:VAL:O	5:E:58:ALA:HB3	2.11	0.50
9:I:4:TYR:CZ	9:I:88:TYR:HD1	2.30	0.50
10:J:81:THR:C	10:J:83:GLU:N	2.60	0.50
1:A:922:G:H5'	5:E:19:MET:O	2.12	0.50
1:A:978:A:N7	1:A:1361:G:N2	2.60	0.50
3:C:102:ASN:N	3:C:102:ASN:ND2	2.55	0.50
3:C:120:VAL:CG1	3:C:198:VAL:HG11	2.41	0.50
5:E:17:ALA:HA	5:E:26:PHE:HA	1.94	0.50
9:I:10:ARG:HD3	9:I:105:ASP:HB3	1.92	0.50
9:I:114:TYR:HD1	9:I:114:TYR:H	1.57	0.50
10:J:19:SER:O	10:J:23:ILE:HG12	2.11	0.50
10:J:68:HIS:N	10:J:68:HIS:CD2	2.78	0.50
15:O:36:ILE:HG12	15:O:59:MET:HE2	1.94	0.50
18:R:33:ASP:OD2	18:R:36:ASN:HB2	2.12	0.50
1:A:473:G:H5"	16:P:81:ARG:CZ	2.42	0.50
1:A:1054:C:N3	23:Z:34:G:O4'	2.45	0.50
1:A:1260:C:H4'	1:A:1283:G:O2'	2.11	0.50
1:A:1360:A:C2'	1:A:1361:G:H5'	2.42	0.50
1:A:1403:C:O5'	1:A:1403:C:H6	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1468:A:H2'	1:A:1469:G:O4'	2.12	0.50
7:G:21:VAL:HG23	7:G:22:LEU:N	2.26	0.50
11:K:109:VAL:HG22	18:R:86:VAL:HA	1.94	0.50
12:L:93:LEU:H	12:L:93:LEU:CD2	2.24	0.50
16:P:4:ILE:HG21	16:P:74:LEU:HD11	1.94	0.50
1:A:370:C:O2'	1:A:371:G:H5'	2.10	0.49
1:A:624:C:H2'	1:A:625:G:H8	1.75	0.49
1:A:673:G:H2'	1:A:674:G:C8	2.47	0.49
1:A:737:A:H1'	6:F:73:ASN:OD1	2.11	0.49
1:A:802:A:H2'	1:A:803:G:O4'	2.12	0.49
2:B:88:ALA:HB1	2:B:90:MET:HG2	1.93	0.49
5:E:79:GLU:HG3	5:E:93:PRO:CD	2.40	0.49
5:E:150:ARG:NH1	5:E:150:ARG:HG3	2.27	0.49
6:F:86:ARG:HH11	6:F:86:ARG:HG3	1.75	0.49
8:H:23:SER:O	8:H:24:THR:HB	2.11	0.49
13:M:3:ARG:HH11	13:M:3:ARG:HG2	1.77	0.49
20:T:10:LEU:O	20:T:12:ALA:N	2.45	0.49
1:A:262:A:C6	1:A:263:A:C6	2.99	0.49
1:A:555:C:H2'	1:A:556:C:C6	2.46	0.49
1:A:1030(A):G:N2	1:A:1030(C):G:H3'	2.26	0.49
2:B:84:GLU:CB	2:B:219:VAL:HG21	2.43	0.49
9:I:113:LYS:N	9:I:113:LYS:CD	2.75	0.49
13:M:5:ALA:HB3	13:M:8:GLU:HG3	1.93	0.49
13:M:120:LYS:HE2	13:M:122:LYS:O	2.12	0.49
17:Q:74:LEU:HD23	17:Q:74:LEU:C	2.33	0.49
1:A:409:G:OP1	4:D:24:GLU:O	2.31	0.49
1:A:905:U:H5'	1:A:906:G:OP2	2.11	0.49
3:C:139:GLN:NE2	3:C:139:GLN:CA	2.70	0.49
3:C:158:GLY:C	3:C:160:ALA:H	2.16	0.49
4:D:64:LEU:O	4:D:64:LEU:HD13	2.13	0.49
4:D:151:LYS:N	4:D:151:LYS:HD2	2.26	0.49
5:E:99:GLY:N	5:E:117:ASP:OD1	2.45	0.49
9:I:118:LYS:O	9:I:119:ALA:CB	2.60	0.49
10:J:83:GLU:O	10:J:85:LEU:N	2.44	0.49
1:A:485:G:C2'	1:A:486:U:OP2	2.60	0.49
1:A:576:G:C3'	1:A:577:G:C5'	2.89	0.49
1:A:777:A:H2'	1:A:778:G:H8	1.78	0.49
1:A:959:A:C2	1:A:1222:G:O4'	2.65	0.49
1:A:1226:C:C5	13:M:104:ARG:HB2	2.47	0.49
2:B:83:MET:CB	2:B:235:SER:OG	2.60	0.49
2:B:178:ARG:O	8:H:71:GLY:HA2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:3:ARG:HE	13:M:7:VAL:HA	1.76	0.49
18:R:18:ARG:HA	18:R:18:ARG:HE	1.78	0.49
23:Z:28:G:H2'	23:Z:29:G:N7	2.26	0.49
1:A:436:C:H5"	4:D:156:GLU:OE1	2.12	0.49
1:A:661:G:O2'	1:A:662:G:H5'	2.13	0.49
1:A:777:A:H2'	1:A:778:G:C8	2.47	0.49
1:A:832:C:O2'	1:A:833:U:H5'	2.12	0.49
1:A:1070:U:H2'	1:A:1071:C:H6	1.76	0.49
1:A:1115:C:H1'	14:N:61:TRP:CB	2.42	0.49
1:A:1329:A:C2'	1:A:1330:U:H5'	2.42	0.49
1:A:1329:A:O2'	1:A:1330:U:H5'	2.12	0.49
2:B:9:GLU:OE1	2:B:9:GLU:HA	2.12	0.49
3:C:67:THR:HG22	3:C:69:HIS:CD2	2.47	0.49
4:D:207:TYR:C	4:D:209:ARG:N	2.66	0.49
5:E:10:MET:HA	5:E:32:VAL:HG12	1.93	0.49
5:E:76:ILE:HG23	5:E:77:PRO:HD2	1.95	0.49
6:F:100:ASN:HB3	18:R:27:GLY:HA2	1.93	0.49
8:H:89:PRO:HA	8:H:92:ARG:NH1	2.28	0.49
10:J:8:LEU:CD1	10:J:20:ALA:HB2	2.29	0.49
10:J:37:PRO:CA	10:J:72:VAL:HG22	2.39	0.49
10:J:47:PHE:CZ	14:N:37:PHE:HE2	2.30	0.49
15:O:4:THR:O	15:O:7:GLU:HG2	2.12	0.49
16:P:33:ILE:O	16:P:34:GLU:HB2	2.13	0.49
1:A:129(A):G:O2'	1:A:189(F):U:C2'	2.57	0.49
1:A:975:A:H4'	1:A:976:G:O5'	2.11	0.49
1:A:1090:U:H2'	1:A:1091:U:C6	2.48	0.49
2:B:223:ILE:HD13	2:B:226:ARG:NE	2.27	0.49
6:F:21:LEU:O	6:F:25:ILE:HG13	2.12	0.49
9:I:53:VAL:CG2	9:I:85:LEU:HD21	2.38	0.49
9:I:63:ILE:HD11	9:I:81:ILE:HD11	1.94	0.49
9:I:93:ARG:O	9:I:95:LYS:N	2.46	0.49
15:O:36:ILE:HG23	15:O:56:LEU:HD11	1.95	0.49
19:S:49:ILE:O	19:S:60:VAL:HG12	2.13	0.49
1:A:394:G:H2'	1:A:395:C:C6	2.48	0.49
1:A:1047:G:O2'	1:A:1048:G:H5"	2.12	0.49
1:A:1203:C:O5'	1:A:1203:C:H6	1.94	0.49
3:C:193:TYR:HE1	3:C:196:LEU:HD11	1.77	0.49
4:D:110:PHE:CD2	4:D:148:VAL:CG2	2.96	0.49
5:E:80:ILE:HG22	8:H:104:ARG:NH1	2.27	0.49
7:G:76:ARG:HG3	7:G:76:ARG:NH1	2.28	0.49
16:P:4:ILE:CG1	16:P:64:ALA:HB1	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:A:H2'	1:A:198:G:O4'	2.13	0.49
1:A:421:U:C5	3:C:127:ARG:NH2	2.81	0.49
1:A:1057:G:H2'	1:A:1058:G:O4'	2.12	0.49
1:A:1191:A:P	3:C:3:ASN:ND2	2.85	0.49
1:A:1192:C:C5	1:A:1193:G:C8	3.00	0.49
2:B:91:PRO:O	2:B:92:TYR:HB3	2.13	0.49
2:B:211:ILE:HD12	2:B:211:ILE:N	2.28	0.49
4:D:3:ARG:NH1	4:D:70:ILE:HD12	2.28	0.49
7:G:12:LEU:HD12	7:G:12:LEU:N	2.28	0.49
14:N:25:VAL:HG12	14:N:39:LEU:CD2	2.43	0.49
1:A:1002:G:H2'	1:A:1003:G:H8	1.78	0.49
1:A:1255:G:H3'	1:A:1279:A:N6	2.26	0.49
2:B:17:PHE:O	2:B:41:ILE:HG23	2.13	0.49
2:B:87:ARG:HH21	2:B:219:VAL:HB	1.78	0.49
2:B:187:LEU:HA	2:B:201:ILE:HB	1.95	0.49
3:C:73:PRO:O	3:C:76:VAL:HB	2.12	0.49
4:D:3:ARG:O	4:D:5:ILE:HG13	2.12	0.49
4:D:61:LYS:HA	4:D:203:VAL:HG22	1.95	0.49
4:D:132:ARG:NH1	4:D:132:ARG:CB	2.76	0.49
9:I:82:ALA:HB1	9:I:96:LEU:HD21	1.94	0.49
1:A:59:A:H2'	1:A:59:A:N3	2.28	0.49
1:A:162:A:C2'	1:A:163:C:H5'	2.43	0.49
1:A:697:U:H2'	1:A:698:G:H5'	1.94	0.49
1:A:1061:G:O2'	1:A:1062:U:H5'	2.13	0.49
1:A:1124:G:N7	1:A:1145:C:H2'	2.28	0.49
1:A:1128:C:H5'	9:I:16:ARG:HH12	1.77	0.49
9:I:106:ALA:O	9:I:108:VAL:HG23	2.12	0.49
11:K:50:TYR:HB3	11:K:54:ARG:HB2	1.93	0.49
15:O:26:GLU:HA	15:O:81:LEU:HD11	1.95	0.49
1:A:175:C:H2'	1:A:176:C:H6	1.78	0.48
1:A:328:C:O2	1:A:328:C:H2'	2.13	0.48
1:A:1057:G:O2'	1:A:1058:G:H5'	2.13	0.48
1:A:1221:G:O3'	19:S:77:THR:HG21	2.12	0.48
1:A:1250:A:H2	1:A:1353:G:H21	1.61	0.48
4:D:8:VAL:HG21	4:D:115:ARG:HE	1.77	0.48
7:G:88:PRO:HB3	7:G:145:ALA:HB1	1.94	0.48
11:K:14:VAL:O	11:K:15:ALA:HB3	2.13	0.48
12:L:55:VAL:CG1	12:L:56:ALA:H	2.17	0.48
12:L:90:VAL:O	12:L:92:ASP:N	2.45	0.48
1:A:877:C:O2'	1:A:878:G:H5'	2.13	0.48
1:A:939:G:H5"	7:G:102:ARG:HH22	1.74	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1091:U:O2	1:A:1093:A:C8	2.66	0.48
1:A:1216:G:O2'	1:A:1217:C:H5'	2.13	0.48
1:A:1251:A:H4'	9:I:12:GLU:CD	2.33	0.48
1:A:1309:G:H2'	1:A:1310:G:H5'	1.95	0.48
3:C:37:GLN:NE2	14:N:52:GLN:OE1	2.39	0.48
3:C:58:GLU:HB2	3:C:65:ALA:CB	2.42	0.48
3:C:91:LEU:CD1	3:C:99:VAL:HG23	2.31	0.48
7:G:38:LEU:O	7:G:38:LEU:HD12	2.13	0.48
1:A:920:U:H2'	1:A:921:U:C6	2.48	0.48
1:A:1115:C:H1'	14:N:61:TRP:HB2	1.95	0.48
3:C:195:VAL:C	3:C:196:LEU:HD12	2.34	0.48
4:D:31:CYS:O	4:D:31:CYS:SG	2.71	0.48
6:F:3:ARG:HG2	6:F:3:ARG:HH11	1.79	0.48
6:F:43:LEU:HD22	6:F:43:LEU:H	1.78	0.48
7:G:107:ALA:O	7:G:110:GLN:HB2	2.13	0.48
8:H:68:ARG:HG2	8:H:68:ARG:HH11	1.77	0.48
9:I:5:TYR:OH	9:I:16:ARG:HG3	2.12	0.48
15:O:4:THR:H	15:O:7:GLU:CD	2.17	0.48
17:Q:95:TYR:N	17:Q:95:TYR:HD1	2.10	0.48
18:R:70:ILE:HG23	18:R:79:LEU:HD13	1.95	0.48
1:A:476:G:H2'	1:A:477:A:C8	2.46	0.48
1:A:1060:C:H5	3:C:2:GLY:HA3	1.72	0.48
2:B:77:ALA:CB	2:B:211:ILE:HG12	2.43	0.48
4:D:39:PRO:O	4:D:44:GLY:HA3	2.13	0.48
5:E:50:GLU:HG2	5:E:52:PRO:HD2	1.94	0.48
13:M:81:LEU:CD2	13:M:88:ARG:HH21	2.20	0.48
13:M:86:CYS:SG	13:M:87:TYR:N	2.86	0.48
1:A:250:A:H1'	1:A:252:U:C5	2.47	0.48
1:A:473:G:H5"	16:P:81:ARG:NH2	2.28	0.48
1:A:829:G:O2'	1:A:830:G:H5'	2.13	0.48
1:A:1077:G:H5'	1:A:1078:U:OP2	2.13	0.48
1:A:1273:G:C2	1:A:1274:G:H1'	2.49	0.48
1:A:1508:G:H2'	1:A:1509:C:H6	1.78	0.48
3:C:108:ASN:OD1	3:C:110:ASN:HB2	2.14	0.48
3:C:112:SER:O	3:C:115:LEU:HB2	2.13	0.48
4:D:133:VAL:HG11	4:D:138:TYR:CD2	2.48	0.48
7:G:148:ASN:O	7:G:150:ALA:N	2.46	0.48
11:K:69:ALA:HB1	11:K:103:LEU:HD12	1.95	0.48
20:T:57:ARG:NH1	20:T:102:GLY:CA	2.76	0.48
1:A:189(E):U:O2'	1:A:189(F):U:H5'	2.13	0.48
1:A:200:G:H2'	1:A:201:C:O4'	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:U:H1'	1:A:430:A:H5"	1.93	0.48
1:A:1118:C:H1'	1:A:1179:A:C4	2.49	0.48
1:A:1305:G:O2'	1:A:1332:A:N6	2.46	0.48
1:A:1420:C:N4	1:A:1480:G:H1	2.07	0.48
2:B:60:ASP:C	2:B:62:ALA:H	2.15	0.48
2:B:145:LEU:CD2	2:B:149:LEU:HD12	2.43	0.48
4:D:80:GLU:OE1	4:D:80:GLU:HA	2.13	0.48
4:D:149:ALA:HB3	4:D:152:SER:OG	2.14	0.48
5:E:79:GLU:HB3	5:E:91:LEU:O	2.13	0.48
6:F:32:ASN:N	6:F:32:ASN:HD22	2.11	0.48
7:G:122:HIS:O	7:G:126:ASP:HB2	2.14	0.48
9:I:27:THR:OG1	9:I:62:TYR:HD1	1.96	0.48
9:I:31:GLN:HB3	9:I:35:GLU:HB3	1.94	0.48
12:L:10:LEU:HD21	12:L:15:ARG:HE	1.78	0.48
15:O:70:LEU:CD2	15:O:81:LEU:HD12	2.43	0.48
1:A:1305:G:P	21:V:2:GLY:N	2.87	0.48
2:B:74:LYS:NZ	2:B:206:ASP:HB2	2.28	0.48
3:C:19:GLU:HB3	3:C:40:ARG:NH2	2.28	0.48
3:C:148:GLY:O	3:C:149:ALA:HB2	2.14	0.48
6:F:19:LEU:HD23	6:F:20:ALA:N	2.29	0.48
10:J:79:ARG:O	10:J:83:GLU:HB2	2.13	0.48
11:K:77:MET:O	11:K:78:GLN:CB	2.61	0.48
13:M:117:VAL:CG1	13:M:118:ALA:H	2.17	0.48
14:N:31:ARG:HH11	14:N:31:ARG:HG3	1.79	0.48
16:P:76:GLN:O	16:P:76:GLN:CG	2.61	0.48
17:Q:74:LEU:HD23	17:Q:74:LEU:O	2.14	0.48
20:T:57:ARG:NH1	20:T:102:GLY:HA2	2.28	0.48
1:A:755:G:OP2	15:O:65:ARG:HD2	2.14	0.48
1:A:858:G:O6	1:A:869:G:C8	2.67	0.48
1:A:1271:G:C3'	1:A:1272:G:H5"	2.41	0.48
3:C:10:PHE:CZ	3:C:178:LEU:HD13	2.49	0.48
3:C:87:LEU:C	3:C:89:GLU:N	2.66	0.48
19:S:60:VAL:HG13	19:S:60:VAL:O	2.14	0.48
20:T:10:LEU:O	20:T:11:SER:C	2.52	0.48
1:A:369:C:O2	1:A:369:C:C2'	2.62	0.48
1:A:1313:U:OP2	19:S:6:LYS:HA	2.14	0.48
3:C:149:ALA:HB1	3:C:201:TYR:O	2.14	0.48
11:K:105:VAL:HG11	11:K:108:ILE:HD11	1.95	0.48
12:L:27:LEU:C	12:L:29:GLY:H	2.17	0.48
12:L:33:ARG:HD3	12:L:62:SER:HB3	1.96	0.48
17:Q:95:TYR:N	17:Q:95:TYR:CD1	2.80	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:36:ASN:O	18:R:39:VAL:HG12	2.14	0.48
18:R:63:GLN:HG3	18:R:63:GLN:O	2.14	0.48
1:A:321:A:O2'	1:A:322:C:H5'	2.14	0.48
1:A:428:G:O2'	1:A:429:U:P	2.72	0.48
1:A:496:A:N3	1:A:496:A:H2'	2.29	0.48
1:A:965:A:C2	1:A:969:A:N1	2.81	0.48
1:A:1040:U:H2'	1:A:1041:A:H8	1.79	0.48
2:B:158:LEU:HD22	2:B:158:LEU:N	2.29	0.48
3:C:76:VAL:O	3:C:83:ARG:HB3	2.14	0.48
10:J:57:LYS:O	10:J:60:ARG:NH1	2.46	0.48
13:M:50:GLU:O	13:M:54:VAL:HG23	2.14	0.48
16:P:50:LYS:HD3	16:P:51:VAL:N	2.29	0.48
18:R:43:PHE:O	18:R:51:LEU:HD12	2.14	0.48
1:A:244:U:O4	1:A:906:G:H1'	2.14	0.47
1:A:855:G:C2'	1:A:856:C:H5'	2.44	0.47
1:A:1034:G:H2'	1:A:1034:G:N3	2.28	0.47
1:A:1115:C:N4	1:A:1186:G:C6	2.82	0.47
1:A:1196:U:O2	1:A:1196:U:H5"	2.14	0.47
1:A:1417:G:N2	1:A:1482:G:H2'	2.29	0.47
4:D:132:ARG:HB2	4:D:132:ARG:HH11	1.79	0.47
13:M:15:VAL:CG1	13:M:34:LEU:HD21	2.43	0.47
18:R:70:ILE:O	18:R:74:ARG:HG3	2.14	0.47
1:A:627:G:H2'	1:A:628:G:H8	1.78	0.47
1:A:707:C:O2'	1:A:708:C:H5'	2.14	0.47
1:A:1330:U:C2'	1:A:1331:G:H5'	2.43	0.47
2:B:132:LYS:HD3	2:B:135:GLN:NE2	2.29	0.47
3:C:134:ILE:HD11	3:C:153:VAL:CG2	2.44	0.47
4:D:3:ARG:CZ	4:D:70:ILE:HA	2.44	0.47
4:D:171:GLY:C	4:D:173:TRP:H	2.16	0.47
6:F:33:TYR:CE2	6:F:75:LEU:HA	2.49	0.47
7:G:121:ALA:O	7:G:125:MET:HG3	2.14	0.47
8:H:80:ILE:N	8:H:80:ILE:CD1	2.71	0.47
10:J:27:ALA:HB2	10:J:85:LEU:CD2	2.39	0.47
12:L:50:SER:O	12:L:51:ALA:CB	2.62	0.47
16:P:64:ALA:O	16:P:66:PRO:HD3	2.14	0.47
19:S:65:ASN:HD22	19:S:65:ASN:N	2.12	0.47
23:Z:28:G:H3'	23:Z:29:G:C8	2.49	0.47
1:A:386:C:O2'	1:A:387:U:H5'	2.14	0.47
1:A:1128:C:H4'	9:I:16:ARG:HH12	1.78	0.47
1:A:1144:G:H21	1:A:1146:A:N6	2.01	0.47
1:A:1157:A:C6	1:A:1180:A:C5	3.02	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1160:G:H2'	1:A:1160:G:N3	2.29	0.47
7:G:59:LEU:HD11	7:G:63:LYS:HE2	1.96	0.47
7:G:105:VAL:HG12	7:G:109:ASN:ND2	2.29	0.47
11:K:121:PRO:HG2	11:K:126:ARG:HB3	1.96	0.47
12:L:86:ARG:HH11	12:L:86:ARG:HG3	1.79	0.47
1:A:22:G:H2'	1:A:23:C:H6	1.78	0.47
1:A:226:G:O2'	1:A:227:G:H5'	2.15	0.47
1:A:248:C:C2'	1:A:249:U:H5'	2.44	0.47
1:A:329:A:N7	1:A:332:G:N1	2.62	0.47
1:A:663:A:C2'	1:A:664:G:H5'	2.43	0.47
4:D:130:GLY:O	4:D:131:ARG:O	2.31	0.47
5:E:84:PHE:HB3	5:E:134:ALA:HB2	1.96	0.47
8:H:91:ARG:HH11	8:H:91:ARG:CG	2.27	0.47
11:K:59:TYR:CZ	11:K:63:LEU:HD21	2.50	0.47
15:O:73:GLU:O	15:O:75:PRO:HD3	2.14	0.47
17:Q:27:PHE:O	17:Q:36:ILE:HD13	2.14	0.47
17:Q:53:LEU:HD23	17:Q:54:GLY:N	2.28	0.47
23:Z:38:A:H2'	23:Z:39:U:O4'	2.14	0.47
1:A:181:G:O2'	1:A:182:U:C6	2.67	0.47
1:A:625:G:H2'	1:A:626:U:C6	2.50	0.47
1:A:1219:U:OP1	14:N:19:ARG:NH2	2.43	0.47
2:B:84:GLU:HG3	2:B:219:VAL:CG2	2.45	0.47
3:C:152:ILE:O	3:C:152:ILE:HG22	2.13	0.47
4:D:25:ARG:HH11	4:D:25:ARG:HG3	1.79	0.47
8:H:79:VAL:HB	8:H:80:ILE:CD1	2.41	0.47
9:I:28:VAL:O	9:I:29:ASN:HB2	2.15	0.47
9:I:75:ASP:O	9:I:78:LYS:HB3	2.14	0.47
12:L:85:ILE:HG22	12:L:86:ARG:N	2.28	0.47
13:M:88:ARG:HG3	13:M:98:VAL:HG22	1.94	0.47
1:A:622:A:H2'	1:A:623:C:H5'	1.97	0.47
1:A:628:G:H2'	1:A:629:G:H8	1.79	0.47
1:A:1129:C:OP1	1:A:1130:A:H5"	2.15	0.47
1:A:1236:A:O2'	1:A:1304:G:H4'	2.14	0.47
7:G:28:ASN:OD1	7:G:36:LYS:HE2	2.15	0.47
7:G:116:ALA:HA	7:G:119:ARG:NH1	2.29	0.47
8:H:112:LEU:C	8:H:112:LEU:HD12	2.35	0.47
9:I:8:GLY:H	9:I:83:ARG:NH1	2.11	0.47
1:A:192:U:O2'	1:A:193:C:H5'	2.14	0.47
1:A:689:C:H2'	1:A:690:G:O4'	2.14	0.47
1:A:721:G:OP2	18:R:53:ARG:HB2	2.14	0.47
1:A:724:G:O2'	1:A:725:G:H5'	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:803:G:C6	1:A:804:U:C4	3.03	0.47
1:A:918:A:H2'	1:A:919:A:C8	2.49	0.47
1:A:1226:C:C4	13:M:104:ARG:HB2	2.49	0.47
1:A:1257:U:O2	1:A:1257:U:H2'	2.15	0.47
1:A:1279:A:H5'	10:J:9:ARG:HH22	1.79	0.47
1:A:1310:G:O2'	1:A:1311:G:H8	1.96	0.47
1:A:1496:C:H1'	1:A:1517:G:H22	1.80	0.47
2:B:21:ARG:H	2:B:21:ARG:HD3	1.79	0.47
2:B:70:PHE:CE2	2:B:215:LEU:HD21	2.49	0.47
2:B:112:VAL:C	2:B:114:ARG:H	2.18	0.47
4:D:60:GLU:OE2	4:D:199:ASN:HB3	2.15	0.47
4:D:110:PHE:CE2	4:D:148:VAL:HG23	2.50	0.47
4:D:180:GLY:O	4:D:181:MET:HB2	2.14	0.47
4:D:196:LEU:C	4:D:198:VAL:H	2.18	0.47
5:E:35:GLY:HA3	5:E:112:LEU:HB3	1.97	0.47
5:E:148:VAL:O	5:E:152:ARG:HG3	2.14	0.47
6:F:4:TYR:CZ	6:F:72:VAL:HG21	2.49	0.47
9:I:86:VAL:HG22	9:I:92:TYR:O	2.15	0.47
9:I:111:ARG:HD2	14:N:61:TRP:O	2.14	0.47
10:J:76:ASN:C	10:J:78:ASN:H	2.17	0.47
11:K:29:ILE:C	11:K:29:ILE:HD13	2.35	0.47
11:K:115:PRO:C	11:K:117:ASN:H	2.18	0.47
12:L:83:VAL:HG22	12:L:84:LEU:N	2.28	0.47
13:M:96:LEU:O	13:M:110:ARG:NH1	2.48	0.47
13:M:122:LYS:HD2	13:M:123:ALA:H	1.78	0.47
14:N:37:PHE:O	14:N:39:LEU:N	2.48	0.47
14:N:43:CYS:O	14:N:46:GLU:HB2	2.15	0.47
16:P:26:ARG:HG2	16:P:26:ARG:NH1	2.29	0.47
17:Q:43:LEU:O	17:Q:69:LYS:HG3	2.13	0.47
17:Q:51:TYR:CD1	17:Q:51:TYR:N	2.82	0.47
19:S:19:VAL:HG13	19:S:20:LEU:H	1.79	0.47
1:A:413:G:H2'	1:A:428:G:N2	2.30	0.47
1:A:1052:U:O2'	1:A:1055:A:OP2	2.32	0.47
2:B:18:GLY:CA	2:B:42:ILE:HG12	2.29	0.47
2:B:36:ARG:O	2:B:37:ASN:HB3	2.15	0.47
2:B:82:ARG:CA	2:B:92:TYR:HE2	2.26	0.47
7:G:6:ARG:O	7:G:7:ALA:C	2.52	0.47
11:K:103:LEU:HD23	11:K:104:GLN:H	1.80	0.47
12:L:87:GLY:HA2	12:L:98:TYR:HA	1.96	0.47
12:L:90:VAL:CG1	12:L:93:LEU:HD21	2.45	0.47
20:T:23:ARG:HG2	20:T:23:ARG:NH1	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:G:O2'	1:A:140:A:H5'	2.14	0.47
1:A:375:U:H4'	16:P:17:TYR:HE2	1.79	0.47
1:A:1186:G:N2	1:A:1187:G:H1'	2.29	0.47
1:A:1238:A:N7	1:A:1301:U:O4	2.48	0.47
1:A:1287:A:H2'	1:A:1288:A:C8	2.49	0.47
1:A:1305:G:OP1	21:V:2:GLY:N	2.48	0.47
3:C:6:HIS:CD2	3:C:8:ILE:H	2.33	0.47
8:H:65:TYR:N	8:H:65:TYR:CD1	2.83	0.47
11:K:27:ASN:OD1	11:K:45:GLY:HA3	2.14	0.47
11:K:128:ALA:O	11:K:129:SER:HB3	2.15	0.47
14:N:24:CYS:N	14:N:29:ARG:O	2.48	0.47
1:A:820:U:O4	26:A:3002:AM2:HA2	2.15	0.47
1:A:833:U:H2'	1:A:834:C:H6	1.80	0.47
1:A:1124:G:C2	1:A:1127:G:N2	2.83	0.47
1:A:1188:A:H2'	1:A:1189:C:H5'	1.97	0.47
1:A:1247:U:O2'	1:A:1248:A:H5"	2.15	0.47
1:A:1379:G:OP2	7:G:6:ARG:NE	2.48	0.47
3:C:6:HIS:NE2	3:C:8:ILE:HD12	2.30	0.47
3:C:180:ALA:O	3:C:181:ASN:CB	2.58	0.47
4:D:47:ARG:HG2	4:D:48:ALA:N	2.30	0.47
6:F:3:ARG:HG2	6:F:3:ARG:NH1	2.30	0.47
6:F:44:GLY:O	6:F:59:TYR:HA	2.14	0.47
10:J:13:HIS:HB3	10:J:68:HIS:CE1	2.50	0.47
14:N:25:VAL:HG13	14:N:26:ARG:N	2.29	0.47
15:O:59:MET:O	15:O:62:GLN:HB3	2.15	0.47
17:Q:59:ILE:HG22	17:Q:71:PHE:CD1	2.50	0.47
18:R:69:THR:HG22	18:R:70:ILE:N	2.30	0.47
19:S:51:VAL:CG2	19:S:71:LEU:HD22	2.45	0.47
23:Z:34:G:C6	23:Z:35:A:C6	3.03	0.47
1:A:1004:A:N7	1:A:1026:G:C6	2.83	0.46
1:A:1054:C:OP1	1:A:1197:G:OP2	2.32	0.46
1:A:1136:U:H5"	1:A:1137:C:OP2	2.15	0.46
1:A:1157:A:H4'	1:A:1158:C:C2	2.49	0.46
1:A:1157:A:C5'	1:A:1158:C:C2	2.98	0.46
1:A:1190:G:C5'	3:C:176:HIS:NE2	2.77	0.46
1:A:1307:U:H2'	1:A:1308:U:C6	2.50	0.46
2:B:137:ARG:HB2	2:B:137:ARG:CZ	2.45	0.46
3:C:116:VAL:HG11	3:C:141:VAL:HG21	1.97	0.46
3:C:136:GLN:O	3:C:139:GLN:N	2.48	0.46
5:E:68:GLU:O	5:E:70:PRO:HD3	2.15	0.46
8:H:20:TYR:HD1	8:H:65:TYR:CD2	2.32	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:100:GLY:C	9:I:102:LEU:N	2.69	0.46
10:J:9:ARG:HG2	10:J:9:ARG:HH11	1.79	0.46
17:Q:12:SER:HB3	17:Q:20:THR:HB	1.98	0.46
17:Q:90:ILE:HG23	17:Q:91:ARG:N	2.30	0.46
1:A:393:A:OP2	16:P:12:LYS:HE2	2.15	0.46
1:A:439:A:C6	1:A:496:A:H1'	2.50	0.46
1:A:1404:C:H2'	1:A:1405:G:C8	2.51	0.46
3:C:87:LEU:HA	3:C:90:GLU:CG	2.44	0.46
6:F:52:ILE:O	6:F:53:ALA:HB3	2.14	0.46
9:I:99:LEU:CB	9:I:101:PHE:HE1	2.25	0.46
15:O:10:LYS:NZ	15:O:14:GLU:HG3	2.30	0.46
1:A:229:U:O2'	16:P:23:ASP:HB2	2.16	0.46
1:A:274:A:O2'	1:A:275:G:C8	2.69	0.46
1:A:642:A:N3	8:H:113:SER:OG	2.49	0.46
1:A:942:G:C2	1:A:943:U:C6	3.03	0.46
1:A:1051:C:C2	1:A:1052:U:C5	3.03	0.46
1:A:1053:G:N7	1:A:1200:C:H5"	2.31	0.46
1:A:1125:U:H3	10:J:5:ARG:NH2	2.11	0.46
2:B:76:GLN:NE2	2:B:208:ILE:H	2.13	0.46
2:B:81:VAL:HG12	2:B:92:TYR:HD2	1.80	0.46
2:B:92:TYR:CE1	2:B:151:GLY:CA	2.98	0.46
3:C:37:GLN:O	3:C:39:ILE:N	2.49	0.46
5:E:89:ILE:HG12	5:E:135:THR:HG22	1.96	0.46
13:M:63:THR:HG23	13:M:64:TRP:CD2	2.50	0.46
1:A:299:G:H2'	1:A:300:A:C8	2.50	0.46
1:A:1066:C:C5	1:A:1067:A:N6	2.83	0.46
1:A:1126:U:N3	1:A:1127:G:N2	2.63	0.46
1:A:1226:C:H42	13:M:104:ARG:HD2	1.79	0.46
1:A:1392:G:H21	1:A:1502:A:H8	1.63	0.46
3:C:23:TYR:CG	3:C:24:ALA:N	2.84	0.46
5:E:150:ARG:HH11	5:E:150:ARG:HG3	1.80	0.46
7:G:18:TYR:CD2	7:G:59:LEU:HB2	2.51	0.46
9:I:58:ARG:HB3	9:I:58:ARG:NH1	2.30	0.46
12:L:120:TYR:N	12:L:120:TYR:CD1	2.81	0.46
15:O:45:VAL:O	15:O:46:HIS:C	2.53	0.46
17:Q:61:GLU:HA	17:Q:71:PHE:CE1	2.50	0.46
19:S:5:LEU:O	19:S:6:LYS:HB2	2.15	0.46
19:S:78:ARG:HG2	19:S:78:ARG:HH11	1.79	0.46
20:T:59:ALA:O	20:T:63:ILE:HG13	2.16	0.46
1:A:438:G:O2'	1:A:494:U:O4	2.34	0.46
1:A:667:G:H2'	1:A:668:G:H8	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:760:G:H1	17:Q:105:ALA:CB	2.28	0.46
1:A:1147:C:C3'	1:A:1148:U:H5"	2.44	0.46
1:A:1272:G:H5'	1:A:1272:G:H8	1.80	0.46
1:A:1521:G:H2'	1:A:1522:U:C6	2.51	0.46
2:B:36:ARG:O	2:B:36:ARG:HG3	2.16	0.46
2:B:82:ARG:HB2	2:B:82:ARG:CZ	2.46	0.46
5:E:8:GLU:HA	5:E:33:VAL:O	2.15	0.46
5:E:110:LEU:HD21	5:E:139:LEU:HD21	1.97	0.46
6:F:1:MET:SD	6:F:1:MET:N	2.86	0.46
8:H:19:VAL:HG23	8:H:21:LYS:HG2	1.97	0.46
16:P:28:ARG:HG2	16:P:28:ARG:HH11	1.81	0.46
1:A:308:C:H2'	1:A:309:G:H8	1.79	0.46
1:A:539:A:H2'	1:A:540:G:H8	1.78	0.46
1:A:956:U:O2	1:A:1225:A:C2	2.69	0.46
1:A:1256:A:N1	1:A:1278:U:O2	2.48	0.46
1:A:1318:A:O2'	19:S:37:ARG:HD2	2.15	0.46
2:B:10:LEU:HD23	2:B:11:LEU:N	2.30	0.46
2:B:47:THR:HA	2:B:202:PRO:HG2	1.96	0.46
2:B:156:LYS:O	2:B:156:LYS:HD2	2.16	0.46
2:B:223:ILE:HD13	2:B:226:ARG:CD	2.45	0.46
5:E:64:ARG:H	5:E:64:ARG:HD2	1.81	0.46
6:F:62:TRP:CH2	6:F:64:GLN:HB2	2.50	0.46
13:M:91:ARG:HH22	13:M:103:THR:HG21	1.81	0.46
14:N:4:LYS:CA	14:N:7:ILE:HG13	2.46	0.46
17:Q:68:ARG:H	17:Q:70:ARG:NH1	2.12	0.46
22:W:3:C:H2'	22:W:4:A:O4'	2.16	0.46
1:A:177:C:O2'	1:A:178:C:H5'	2.16	0.46
1:A:1286:A:C8	1:A:1287:A:H4'	2.51	0.46
1:A:1379:G:OP2	7:G:6:ARG:CZ	2.64	0.46
1:A:1426:C:O2'	1:A:1427:U:H5'	2.15	0.46
2:B:87:ARG:HD3	2:B:234:PRO:HD2	1.98	0.46
3:C:121:ALA:HB1	3:C:188:LEU:O	2.15	0.46
5:E:110:LEU:O	5:E:111:GLU:C	2.54	0.46
7:G:119:ARG:HG3	7:G:119:ARG:NH1	2.31	0.46
11:K:12:ARG:HG2	11:K:12:ARG:O	2.15	0.46
12:L:41:ARG:HG3	12:L:42:THR:O	2.15	0.46
13:M:11:ARG:HG3	13:M:12:ASN:HB2	1.97	0.46
16:P:39:TYR:CD2	16:P:73:LEU:HD11	2.51	0.46
19:S:19:VAL:O	19:S:22:LEU:N	2.45	0.46
1:A:414:A:H2'	1:A:415:A:O4'	2.16	0.46
1:A:488:C:O5'	1:A:488:C:H6	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1191:A:P	3:C:3:ASN:HD22	2.38	0.46
1:A:1229:A:O2'	13:M:125:ARG:NE	2.47	0.46
1:A:1249:C:H4'	9:I:36:TYR:OH	2.15	0.46
2:B:44:LEU:O	2:B:45:GLN:C	2.54	0.46
2:B:46:LYS:O	2:B:49:GLU:HB2	2.16	0.46
2:B:101:MET:HG2	2:B:108:ILE:HG21	1.98	0.46
4:D:8:VAL:HG21	4:D:115:ARG:NE	2.31	0.46
9:I:11:LYS:O	9:I:11:LYS:HG2	2.16	0.46
10:J:85:LEU:O	10:J:87:THR:N	2.49	0.46
12:L:75:HIS:HD2	12:L:77:LEU:HB2	1.81	0.46
14:N:32:SER:O	14:N:34:TYR:N	2.49	0.46
16:P:5:ARG:C	16:P:6:LEU:HD12	2.36	0.46
18:R:58:LEU:HB3	18:R:62:GLU:HB2	1.98	0.46
19:S:7:LYS:HG2	19:S:7:LYS:O	2.15	0.46
20:T:53:LEU:CD1	20:T:104:LEU:HD12	2.42	0.46
1:A:411:A:N6	1:A:413:G:H21	2.14	0.46
1:A:750:G:H21	15:O:23:GLY:CA	2.29	0.46
1:A:928:G:O2'	1:A:929:G:H5'	2.16	0.46
1:A:1418:A:H2'	1:A:1419:G:H5'	1.98	0.46
1:A:1497:G:C2'	1:A:1498:U:H5'	2.46	0.46
1:A:1530:G:H4'	1:A:1530:G:OP1	2.15	0.46
2:B:17:PHE:CD1	2:B:17:PHE:C	2.89	0.46
2:B:71:VAL:CG2	2:B:164:VAL:HG22	2.45	0.46
3:C:107:GLN:NE2	3:C:107:GLN:N	2.64	0.46
5:E:43:LEU:HD11	5:E:132:ALA:CB	2.39	0.46
5:E:60:TYR:O	5:E:64:ARG:NE	2.48	0.46
7:G:41:ARG:O	7:G:42:ILE:C	2.53	0.46
10:J:47:PHE:N	10:J:63:PHE:O	2.45	0.46
15:O:38:ARG:HG3	15:O:38:ARG:NH1	2.31	0.46
17:Q:83:ASP:O	17:Q:86:GLU:HB2	2.15	0.46
19:S:13:ASP:HA	19:S:16:LEU:CB	2.45	0.46
1:A:982:U:OP1	1:A:982:U:H6	1.99	0.46
1:A:1288:A:H2'	1:A:1289:A:O4'	2.16	0.46
2:B:167:PRO:O	2:B:168:THR:C	2.53	0.46
4:D:19:LEU:HB3	4:D:21:LEU:HD21	1.98	0.46
4:D:91:SER:O	4:D:94:LEU:HB2	2.16	0.46
5:E:36:ASP:OD1	5:E:40:ARG:HB2	2.15	0.46
7:G:6:ARG:O	7:G:7:ALA:O	2.33	0.46
11:K:95:ILE:HD12	11:K:95:ILE:N	2.29	0.46
13:M:52:GLU:HG2	13:M:55:ARG:NH2	2.26	0.46
15:O:31:LEU:HD12	15:O:31:LEU:HA	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:56:ALA:C	16:P:58:TYR:H	2.20	0.46
20:T:64:ASP:O	20:T:67:ALA:HB3	2.15	0.46
1:A:677:U:H3	1:A:713:G:H22	1.63	0.45
1:A:1070:U:P	5:E:25:ARG:HH12	2.39	0.45
3:C:31:HIS:C	3:C:33:LEU:H	2.19	0.45
9:I:42:ARG:NH2	9:I:71:SER:HB2	2.27	0.45
10:J:75:ILE:O	10:J:76:ASN:HB2	2.16	0.45
13:M:7:VAL:HG23	13:M:7:VAL:O	2.16	0.45
13:M:8:GLU:O	13:M:10:PRO:HD3	2.16	0.45
15:O:38:ARG:HG3	15:O:38:ARG:HH11	1.81	0.45
17:Q:60:ILE:C	17:Q:71:PHE:HD1	2.18	0.45
17:Q:60:ILE:O	17:Q:71:PHE:HD1	1.98	0.45
20:T:8:ARG:O	20:T:9:ASN:HB2	2.16	0.45
20:T:43:LEU:CD1	20:T:51:GLU:HG3	2.45	0.45
1:A:538:G:O2'	1:A:539:A:H5'	2.17	0.45
1:A:1157:A:OP2	1:A:1157:A:H3'	2.16	0.45
1:A:1279:A:H2'	1:A:1279:A:N3	2.31	0.45
1:A:1362:C:H2'	1:A:1363:C:H5"	1.97	0.45
4:D:61:LYS:HE3	4:D:62:GLN:NE2	2.31	0.45
10:J:4:ILE:HD11	10:J:74:ILE:HB	1.98	0.45
11:K:58:PRO:O	11:K:61:ALA:HB3	2.17	0.45
11:K:82:VAL:HG23	11:K:105:VAL:HG13	1.99	0.45
11:K:128:ALA:O	11:K:129:SER:CB	2.63	0.45
23:Z:29:G:H2'	23:Z:30:G:C5	2.51	0.45
1:A:26:A:C2'	1:A:27:G:H5'	2.46	0.45
1:A:794:A:H2'	1:A:795:C:C6	2.52	0.45
1:A:972:C:H4'	10:J:57:LYS:CG	2.23	0.45
1:A:1049:U:H4'	1:A:1050:G:C5'	2.46	0.45
1:A:1277:C:H6	1:A:1277:C:H5'	1.81	0.45
1:A:1343:G:H2'	1:A:1344:C:C6	2.52	0.45
4:D:19:LEU:O	4:D:21:LEU:N	2.49	0.45
4:D:64:LEU:HB2	4:D:198:VAL:HG11	1.99	0.45
5:E:15:ARG:HD2	5:E:15:ARG:O	2.16	0.45
5:E:99:GLY:HA2	5:E:116:THR:O	2.16	0.45
9:I:16:ARG:NH2	9:I:64:THR:HG21	2.31	0.45
10:J:47:PHE:HB2	10:J:63:PHE:HB2	1.97	0.45
14:N:11:LYS:O	14:N:12:ARG:HB2	2.17	0.45
15:O:88:ARG:HH11	15:O:88:ARG:HG2	1.81	0.45
17:Q:97:SER:C	17:Q:98:LEU:HD12	2.37	0.45
18:R:53:ARG:O	18:R:55:ARG:N	2.48	0.45
1:A:620:C:H2'	1:A:621:A:O4'	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1047:G:C3'	1:A:1048:G:H5"	2.44	0.45
1:A:1121:U:O2'	1:A:1122:U:H6	2.00	0.45
1:A:1250:A:H4'	9:I:68:GLY:CA	2.45	0.45
1:A:1309:G:H5'	13:M:78:ILE:HD11	1.97	0.45
1:A:1371:G:C6	1:A:1372:U:C4	3.05	0.45
2:B:28:PHE:CZ	2:B:189:ASP:HA	2.51	0.45
4:D:8:VAL:C	4:D:10:ARG:N	2.69	0.45
5:E:107:ARG:O	5:E:110:LEU:N	2.47	0.45
6:F:40:VAL:CG2	6:F:41:GLU:N	2.79	0.45
14:N:24:CYS:HB3	14:N:28:GLY:N	2.31	0.45
15:O:5:LYS:H	15:O:5:LYS:CD	2.27	0.45
17:Q:95:TYR:HA	17:Q:98:LEU:CD1	2.46	0.45
20:T:45:GLN:CA	20:T:91:LEU:HD22	2.46	0.45
1:A:16:A:C2	1:A:920:U:O2	2.70	0.45
1:A:67:C:O2'	1:A:171:A:H1'	2.16	0.45
1:A:242:C:H2'	1:A:243:A:H5'	1.97	0.45
1:A:279:A:C5'	1:A:280:C:H3'	2.46	0.45
1:A:1060:C:C2	1:A:1198:G:C2	3.05	0.45
1:A:1103:C:H4'	2:B:98:LEU:HD12	1.98	0.45
1:A:1508:G:H2'	1:A:1509:C:C6	2.51	0.45
3:C:91:LEU:HD23	3:C:91:LEU:C	2.37	0.45
6:F:9:VAL:HG22	6:F:60:PHE:CD2	2.51	0.45
9:I:5:TYR:CD1	9:I:6:GLY:N	2.84	0.45
9:I:27:THR:OG1	9:I:62:TYR:HA	2.17	0.45
10:J:42:THR:HG23	10:J:67:THR:C	2.37	0.45
11:K:104:GLN:NE2	11:K:106:LYS:HE2	2.31	0.45
12:L:78:GLN:HB3	12:L:79:GLU:H	1.46	0.45
1:A:135:C:C2	16:P:1:MET:HB2	2.46	0.45
1:A:192:U:O4'	20:T:103:GLY:HA2	2.17	0.45
1:A:343:U:H6	1:A:343:U:C5'	2.28	0.45
1:A:599:C:O2'	1:A:600:C:H5'	2.17	0.45
1:A:792:A:H1'	1:A:794:A:N7	2.31	0.45
1:A:1397:C:O2'	22:W:5:A:N6	2.49	0.45
2:B:73:THR:HG22	2:B:169:LYS:HZ1	1.82	0.45
2:B:163:PHE:HA	2:B:185:ILE:O	2.17	0.45
3:C:108:ASN:C	3:C:110:ASN:H	2.20	0.45
3:C:132:ARG:NH1	3:C:132:ARG:HB3	2.32	0.45
3:C:188:LEU:HB3	3:C:189:ALA:H	1.55	0.45
3:C:195:VAL:HG23	3:C:196:LEU:N	2.30	0.45
4:D:29:PRO:HA	4:D:34:GLU:HG2	1.99	0.45
7:G:50:ILE:HD11	7:G:121:ALA:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:34:ASP:C	11:K:36:ASP:H	2.19	0.45
13:M:5:ALA:O	13:M:6:GLY:C	2.55	0.45
13:M:8:GLU:O	13:M:10:PRO:HD2	2.17	0.45
13:M:21:TYR:N	13:M:21:TYR:CD1	2.84	0.45
20:T:73:HIS:O	20:T:74:LYS:CG	2.60	0.45
1:A:90:U:O5'	1:A:90:U:H6	1.99	0.45
1:A:622:A:C8	1:A:623:C:C6	3.05	0.45
1:A:865:A:O5'	1:A:865:A:H8	1.99	0.45
1:A:987:G:H2'	1:A:988:G:C8	2.52	0.45
1:A:1298:C:N4	7:G:114:ARG:HG2	2.32	0.45
2:B:25:ASN:HD22	2:B:26:PRO:CD	2.29	0.45
2:B:197:VAL:HB	2:B:200:ILE:HG12	1.98	0.45
4:D:60:GLU:OE1	4:D:60:GLU:HA	2.16	0.45
4:D:119:GLN:HG3	4:D:123:HIS:CD2	2.51	0.45
5:E:72:GLN:O	5:E:73:ASN:CB	2.65	0.45
5:E:110:LEU:O	5:E:113:ALA:N	2.47	0.45
13:M:108:ARG:NE	13:M:108:ARG:HA	2.32	0.45
14:N:3:ARG:O	14:N:5:ALA:N	2.49	0.45
1:A:374:A:C6	1:A:375:U:C4	3.05	0.45
1:A:609:A:H2'	1:A:610:G:H5'	1.98	0.45
1:A:1197:G:H3'	1:A:1198:G:H5'	1.99	0.45
1:A:1214:C:O2	1:A:1214:C:C2'	2.65	0.45
1:A:1238:A:N7	1:A:1303:C:H1'	2.32	0.45
2:B:23:ARG:NH1	2:B:191:ASP:HA	2.31	0.45
2:B:69:LEU:HD23	2:B:69:LEU:C	2.36	0.45
3:C:165:THR:O	3:C:165:THR:HG22	2.15	0.45
4:D:170:VAL:HG22	4:D:171:GLY:H	1.78	0.45
8:H:51:VAL:HG11	8:H:60:ARG:NE	2.32	0.45
9:I:9:ARG:HG2	9:I:14:VAL:CG1	2.34	0.45
9:I:35:GLU:OE1	9:I:35:GLU:HA	2.16	0.45
12:L:54:LYS:N	12:L:54:LYS:HD2	2.31	0.45
13:M:82:MET:CE	13:M:93:ARG:HB2	2.46	0.45
18:R:47:THR:HG23	18:R:83:GLU:H	1.81	0.45
1:A:10:A:OP2	5:E:126:ARG:NH1	2.50	0.45
1:A:129:U:H5"	1:A:129(A):G:H5'	1.99	0.45
1:A:855:G:O2'	1:A:856:C:H5'	2.17	0.45
1:A:1103:C:H5'	2:B:98:LEU:HD12	1.99	0.45
1:A:1113:C:C3'	1:A:1114:C:H5'	2.38	0.45
1:A:1273:G:H2'	1:A:1274:G:O4'	2.16	0.45
1:A:1286:A:H2'	1:A:1287:A:H4'	1.98	0.45
1:A:1410:G:H1	1:A:1490:C:H42	1.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1506:U:O2'	1:A:1507:A:H5'	2.17	0.45
2:B:88:ALA:C	2:B:90:MET:H	2.19	0.45
4:D:3:ARG:HG3	4:D:3:ARG:NH1	2.31	0.45
4:D:111:ALA:HB2	4:D:120:LEU:CD1	2.47	0.45
4:D:199:ASN:ND2	4:D:199:ASN:C	2.69	0.45
5:E:101:ILE:CD1	5:E:119:LEU:HA	2.47	0.45
7:G:67:GLU:HA	7:G:67:GLU:OE1	2.17	0.45
7:G:118:VAL:O	7:G:121:ALA:HB3	2.17	0.45
15:O:2:PRO:HB2	15:O:3:ILE:H	1.65	0.45
16:P:14:ASN:N	16:P:15:PRO:CD	2.80	0.45
19:S:41:VAL:HB	19:S:43:GLU:OE2	2.17	0.45
20:T:79:ARG:HD2	20:T:83:ARG:NH2	2.32	0.45
1:A:476:G:O2'	1:A:477:A:H5'	2.17	0.45
1:A:1141:C:O2'	1:A:1142:G:H5'	2.16	0.45
2:B:78:GLN:CG	2:B:94:ASN:OD1	2.65	0.45
2:B:97:TRP:CZ2	2:B:101:MET:HB2	2.51	0.45
2:B:142:LEU:HD22	2:B:146:GLN:NE2	2.31	0.45
2:B:223:ILE:HG22	2:B:224:GLN:N	2.32	0.45
4:D:12:CYS:SG	4:D:19:LEU:O	2.75	0.45
9:I:49:PRO:O	9:I:52:ALA:HB3	2.17	0.45
11:K:101:SER:C	11:K:103:LEU:N	2.70	0.45
12:L:27:LEU:C	12:L:29:GLY:N	2.70	0.45
13:M:115:LYS:O	13:M:116:THR:C	2.54	0.45
20:T:94:ALA:O	20:T:95:ALA:HB3	2.16	0.45
1:A:52:G:O2'	1:A:53:A:H5'	2.17	0.44
1:A:922:G:H2'	1:A:923:A:C8	2.52	0.44
1:A:981:U:C3'	1:A:982:U:H5"	2.44	0.44
1:A:1232:U:H5"	9:I:124:GLN:O	2.16	0.44
1:A:1291:G:H2'	1:A:1292:U:C6	2.51	0.44
1:A:1305:G:N2	1:A:1331:G:H1'	2.31	0.44
2:B:211:ILE:HG23	2:B:215:LEU:HD12	1.98	0.44
3:C:190:ARG:HB3	3:C:190:ARG:NH1	2.32	0.44
4:D:170:VAL:CG2	4:D:171:GLY:H	2.30	0.44
4:D:196:LEU:HA	4:D:197:PRO:HD2	1.85	0.44
5:E:76:ILE:CG1	5:E:118:ILE:HD12	2.47	0.44
1:A:1176:A:H2'	1:A:1177:G:O4'	2.18	0.44
1:A:1366:C:O2'	10:J:60:ARG:NH2	2.50	0.44
1:A:1424:C:O2'	1:A:1425:U:H5'	2.18	0.44
2:B:25:ASN:HD22	2:B:26:PRO:N	2.15	0.44
2:B:64:ARG:NH1	2:B:64:ARG:CB	2.81	0.44
2:B:82:ARG:HB3	2:B:94:ASN:ND2	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:101:MET:C	2:B:102:LEU:HD12	2.37	0.44
3:C:39:ILE:C	3:C:41:GLY:N	2.70	0.44
3:C:173:VAL:HG12	3:C:175:LEU:CD2	2.47	0.44
8:H:125:ARG:HE	8:H:125:ARG:HB2	1.63	0.44
9:I:6:GLY:CA	9:I:83:ARG:HB2	2.44	0.44
18:R:26:LEU:HD22	18:R:26:LEU:HA	1.85	0.44
19:S:65:ASN:ND2	19:S:65:ASN:N	2.65	0.44
1:A:640:A:C2'	1:A:641:U:H5'	2.47	0.44
1:A:1477:C:H2'	1:A:1478:C:C6	2.52	0.44
6:F:48:LEU:HD13	6:F:52:ILE:CD1	2.47	0.44
15:O:76:GLU:O	15:O:77:ARG:C	2.55	0.44
18:R:48:GLY:O	18:R:74:ARG:NH2	2.50	0.44
18:R:62:GLU:C	18:R:64:ARG:N	2.70	0.44
20:T:54:LYS:HB3	20:T:54:LYS:HE2	1.87	0.44
21:V:5:ASP:C	21:V:7:ARG:H	2.21	0.44
23:Z:29:G:H22	23:Z:42:C:N4	2.15	0.44
1:A:373:A:C2	1:A:482:A:C6	3.06	0.44
1:A:997:U:H6	1:A:997:U:H5'	1.83	0.44
1:A:1100:C:O2'	1:A:1101:A:H5'	2.17	0.44
1:A:1112:C:H1'	3:C:179:ARG:NH2	2.32	0.44
1:A:1157:A:H5'	1:A:1158:C:C4	2.53	0.44
2:B:178:ARG:HH11	2:B:178:ARG:CB	2.29	0.44
3:C:20:SER:O	14:N:54:PRO:HB3	2.17	0.44
5:E:31:LEU:HD23	5:E:31:LEU:HA	1.87	0.44
11:K:29:ILE:HD13	11:K:29:ILE:O	2.17	0.44
13:M:63:THR:HG23	13:M:64:TRP:CG	2.52	0.44
20:T:24:LEU:HD12	20:T:24:LEU:HA	1.82	0.44
1:A:451:A:N6	1:A:480:U:H2'	2.32	0.44
1:A:644:G:C5	1:A:645:C:C5	3.05	0.44
1:A:940:C:H2'	1:A:941:G:C8	2.53	0.44
1:A:986:A:H2'	1:A:987:G:C8	2.53	0.44
1:A:1030:C:C1'	1:A:1032:G:H22	2.31	0.44
1:A:1463:C:O2'	1:A:1464:G:H5'	2.17	0.44
2:B:224:GLN:O	2:B:225:ALA:HB2	2.18	0.44
3:C:5:ILE:CD1	3:C:5:ILE:H	2.31	0.44
3:C:54:ARG:O	3:C:55:VAL:HG23	2.18	0.44
3:C:134:ILE:HG22	3:C:168:ALA:HB3	1.97	0.44
4:D:59:ARG:NH2	4:D:66:ARG:HH12	2.15	0.44
4:D:153:ARG:HG2	4:D:181:MET:SD	2.57	0.44
5:E:31:LEU:HD22	5:E:43:LEU:CD2	2.47	0.44
5:E:79:GLU:CG	5:E:93:PRO:HD2	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:17:THR:HB	8:H:78:GLN:OE1	2.18	0.44
9:I:18:PHE:HD2	9:I:62:TYR:CD2	2.36	0.44
10:J:63:PHE:HE2	14:N:45:ARG:HA	1.82	0.44
13:M:42:ALA:O	13:M:43:THR:C	2.55	0.44
15:O:75:PRO:O	15:O:79:ARG:HG3	2.18	0.44
17:Q:59:ILE:CG2	17:Q:71:PHE:HB3	2.48	0.44
1:A:385:C:H2'	1:A:386:C:C6	2.40	0.44
1:A:545:C:O2'	1:A:546:G:H5'	2.17	0.44
1:A:1352:C:N3	1:A:1371:G:C6	2.86	0.44
2:B:216:SER:OG	2:B:217:ARG:N	2.51	0.44
2:B:237:ALA:C	2:B:239:VAL:H	2.20	0.44
3:C:14:ILE:HG22	3:C:15:THR:HG23	2.00	0.44
3:C:23:TYR:CD1	3:C:23:TYR:C	2.91	0.44
4:D:150:GLU:HG2	4:D:153:ARG:HH22	1.76	0.44
6:F:32:ASN:N	6:F:32:ASN:ND2	2.66	0.44
8:H:51:VAL:HG12	8:H:60:ARG:HB2	1.99	0.44
8:H:103:VAL:CG2	8:H:110:ALA:HB2	2.47	0.44
9:I:99:LEU:CB	9:I:101:PHE:CE1	2.97	0.44
10:J:48:THR:OG1	10:J:62:HIS:CD2	2.71	0.44
10:J:63:PHE:HA	14:N:57:ARG:O	2.17	0.44
12:L:48:PRO:O	12:L:49:ASN:ND2	2.45	0.44
18:R:50:ILE:CD1	18:R:70:ILE:HG21	2.47	0.44
1:A:81:U:H6	1:A:81:U:H5'	1.82	0.44
1:A:419:C:O2	1:A:419:C:H2'	2.18	0.44
1:A:750:G:N3	15:O:23:GLY:HA3	2.32	0.44
1:A:930:C:C2'	1:A:931:C:H5'	2.48	0.44
1:A:1182:G:O2'	1:A:1183:A:P	2.76	0.44
3:C:180:ALA:HB1	3:C:203:PHE:HE1	1.83	0.44
5:E:96:PRO:HA	5:E:117:ASP:CG	2.38	0.44
9:I:108:VAL:HG12	9:I:109:VAL:N	2.33	0.44
1:A:8:A:N7	4:D:208:SER:O	2.50	0.44
1:A:46:G:O2'	1:A:365:U:H1'	2.17	0.44
1:A:1402:C:H2'	1:A:1403:C:O4'	2.18	0.44
1:A:1496:C:H2'	1:A:1497:G:C8	2.52	0.44
2:B:78:GLN:HG2	2:B:94:ASN:OD1	2.17	0.44
3:C:10:PHE:CE2	3:C:178:LEU:HD13	2.53	0.44
3:C:29:TYR:OH	14:N:54:PRO:HG2	2.18	0.44
3:C:79:ARG:HE	3:C:82:GLU:CG	2.22	0.44
4:D:150:GLU:CA	4:D:153:ARG:HH21	2.27	0.44
5:E:81:GLU:CG	5:E:88:LYS:HE2	2.48	0.44
10:J:25:GLU:C	10:J:27:ALA:H	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:34:VAL:C	10:J:36:GLY:H	2.21	0.44
11:K:13:GLN:HA	11:K:75:TYR:O	2.18	0.44
16:P:6:LEU:N	16:P:6:LEU:CD1	2.80	0.44
1:A:38:G:C2	1:A:397:A:C2	3.06	0.44
1:A:107:G:H5'	1:A:108:G:OP2	2.18	0.44
1:A:329:A:C6	1:A:332:G:N1	2.85	0.44
1:A:1402:C:O2	1:A:1500:A:N1	2.51	0.44
2:B:75:LYS:HD2	2:B:78:GLN:OE1	2.18	0.44
2:B:95:GLN:OE1	2:B:95:GLN:HA	2.18	0.44
3:C:16:ARG:HD2	3:C:16:ARG:HA	1.88	0.44
4:D:194:LEU:HD22	4:D:194:LEU:N	2.33	0.44
6:F:16:GLN:NE2	6:F:16:GLN:O	2.51	0.44
7:G:16:LEU:O	7:G:17:VAL:HG23	2.18	0.44
10:J:62:HIS:O	14:N:59:ALA:N	2.44	0.44
15:O:25:THR:HG21	15:O:70:LEU:HB2	1.99	0.44
1:A:160:A:H2'	1:A:161:A:O4'	2.18	0.43
1:A:428:G:H1'	1:A:430:A:N7	2.33	0.43
1:A:520:A:H61	1:A:529:G:H1'	1.83	0.43
1:A:714:G:H2'	1:A:715:A:C8	2.52	0.43
1:A:840:C:O2'	1:A:848:C:N3	2.50	0.43
1:A:985:C:H2'	1:A:986:A:H8	1.82	0.43
7:G:95:ARG:HA	7:G:98:SER:OG	2.17	0.43
9:I:18:PHE:HD2	9:I:62:TYR:HD2	1.64	0.43
11:K:38:ASN:HA	11:K:39:PRO:HD3	1.62	0.43
11:K:43:SER:HB3	11:K:68:ALA:HB2	2.00	0.43
11:K:78:GLN:O	11:K:104:GLN:N	2.39	0.43
20:T:85:MET:CE	20:T:103:GLY:O	2.66	0.43
1:A:99:U:O2'	1:A:100:C:H5'	2.18	0.43
1:A:128:G:O2'	17:Q:3:LYS:HE3	2.18	0.43
1:A:380:G:C2	1:A:384:G:C6	3.06	0.43
1:A:716:A:N3	11:K:117:ASN:O	2.52	0.43
1:A:933:G:OP1	7:G:4:ARG:HB2	2.19	0.43
1:A:1460:A:H2'	1:A:1461:G:O4'	2.18	0.43
2:B:118:LEU:HD12	2:B:142:LEU:CG	2.48	0.43
2:B:137:ARG:O	2:B:141:GLU:HB2	2.18	0.43
2:B:222:ILE:HG22	2:B:226:ARG:NH2	2.33	0.43
3:C:39:ILE:HG21	3:C:57:ILE:HD11	2.00	0.43
3:C:115:LEU:O	3:C:117:ALA:N	2.51	0.43
6:F:94:GLN:NE2	18:R:32:ARG:CZ	2.81	0.43
9:I:16:ARG:HD2	9:I:18:PHE:CZ	2.53	0.43
10:J:34:VAL:H	10:J:75:ILE:HG22	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:120:ARG:HG3	11:K:120:ARG:NH1	2.33	0.43
12:L:82:VAL:HG23	12:L:105:TYR:HB3	1.99	0.43
14:N:25:VAL:CG1	14:N:26:ARG:N	2.81	0.43
17:Q:27:PHE:C	17:Q:35:VAL:HG23	2.39	0.43
18:R:23:LYS:HG2	18:R:23:LYS:O	2.19	0.43
20:T:10:LEU:O	20:T:10:LEU:HD13	2.18	0.43
20:T:103:GLY:O	20:T:104:LEU:HG	2.17	0.43
1:A:167:G:O2'	1:A:168:G:H5'	2.17	0.43
1:A:196:A:C3'	1:A:197:A:H5"	2.49	0.43
1:A:682:G:C6	1:A:709:G:C6	3.06	0.43
1:A:839:U:O2	1:A:839:U:C2'	2.65	0.43
1:A:1014:A:H2	1:A:1219:U:H1'	1.78	0.43
3:C:175:LEU:HD23	3:C:175:LEU:N	2.33	0.43
4:D:3:ARG:NE	4:D:71:SER:N	2.66	0.43
4:D:115:ARG:NH1	4:D:115:ARG:HG2	2.33	0.43
5:E:26:PHE:O	5:E:27:ARG:HB2	2.17	0.43
9:I:63:ILE:HD11	9:I:81:ILE:CD1	2.47	0.43
10:J:76:ASN:HB2	10:J:78:ASN:ND2	2.32	0.43
12:L:55:VAL:O	12:L:56:ALA:HB2	2.18	0.43
14:N:26:ARG:CG	14:N:27:CYS:N	2.79	0.43
1:A:329:A:H2'	1:A:332:G:N7	2.34	0.43
1:A:457:C:H2'	1:A:458:C:H6	1.82	0.43
1:A:802:A:H2'	1:A:803:G:H5'	2.00	0.43
1:A:940:C:H2'	1:A:941:G:H8	1.84	0.43
1:A:1043:C:H2'	1:A:1044:A:C8	2.53	0.43
1:A:1347:G:N7	9:I:10:ARG:NH2	2.64	0.43
2:B:213:LEU:HD23	2:B:213:LEU:C	2.39	0.43
4:D:15:GLU:C	4:D:17:VAL:H	2.22	0.43
7:G:50:ILE:HA	7:G:125:MET:CE	2.49	0.43
12:L:9:GLN:O	12:L:13:LYS:N	2.36	0.43
20:T:74:LYS:HE2	20:T:74:LYS:HB3	1.73	0.43
1:A:499:A:N1	1:A:546:G:O2'	2.43	0.43
1:A:684:A:O4'	11:K:38:ASN:ND2	2.52	0.43
1:A:1030:C:C2	1:A:1032:G:N1	2.85	0.43
1:A:1418:A:C2'	1:A:1419:G:H5'	2.48	0.43
10:J:19:SER:C	10:J:21:GLN:H	2.21	0.43
10:J:51:ARG:O	14:N:45:ARG:CZ	2.67	0.43
11:K:104:GLN:HE21	11:K:104:GLN:HB3	1.61	0.43
16:P:74:LEU:HB3	16:P:79:VAL:HG21	1.99	0.43
20:T:100:ILE:O	20:T:102:GLY:N	2.46	0.43
1:A:153:C:O2'	1:A:154:C:H5'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:U:H2'	1:A:254:G:C8	2.53	0.43
1:A:1107:C:C4	1:A:1108:G:C8	3.06	0.43
2:B:61:LEU:HD22	2:B:61:LEU:N	2.33	0.43
3:C:5:ILE:H	3:C:5:ILE:HD13	1.82	0.43
3:C:31:HIS:O	3:C:33:LEU:N	2.51	0.43
4:D:100:ARG:HB3	4:D:102:ASP:OD1	2.19	0.43
4:D:150:GLU:CG	4:D:153:ARG:HH21	2.28	0.43
4:D:175:SER:OG	4:D:186:LEU:HD21	2.19	0.43
5:E:57:LYS:O	5:E:61:TYR:CD2	2.71	0.43
5:E:63:ARG:HG2	5:E:63:ARG:NH1	2.33	0.43
6:F:19:LEU:C	6:F:21:LEU:H	2.21	0.43
6:F:67:MET:HB2	6:F:68:PRO:HD2	2.01	0.43
8:H:11:THR:O	8:H:12:ARG:C	2.55	0.43
8:H:63:LEU:N	8:H:63:LEU:HD23	2.32	0.43
10:J:20:ALA:HB1	10:J:72:VAL:HG21	1.99	0.43
10:J:45:ARG:HD3	10:J:47:PHE:CZ	2.53	0.43
10:J:76:ASN:O	10:J:78:ASN:N	2.45	0.43
13:M:21:TYR:HD1	13:M:21:TYR:H	1.67	0.43
13:M:23:TYR:HB3	13:M:67:GLU:H	1.84	0.43
14:N:44:LEU:C	14:N:44:LEU:HD12	2.38	0.43
19:S:78:ARG:H	19:S:78:ARG:HG3	1.65	0.43
20:T:58:LYS:O	20:T:58:LYS:HG2	2.18	0.43
23:Z:30:G:N1	23:Z:41:C:N4	2.65	0.43
23:Z:37:A:H3'	23:Z:38:A:H8	1.82	0.43
1:A:494:U:C2'	1:A:495:A:H5'	2.48	0.43
1:A:1032:G:H2'	1:A:1033:G:H8	1.83	0.43
1:A:1210:C:H2'	1:A:1211:U:O4'	2.18	0.43
2:B:64:ARG:NH1	2:B:64:ARG:HB2	2.34	0.43
2:B:98:LEU:HD23	2:B:98:LEU:N	2.16	0.43
2:B:157:ARG:HB2	2:B:157:ARG:HH11	1.83	0.43
3:C:119:ARG:O	3:C:122:GLU:HB3	2.18	0.43
4:D:77:ASN:HD22	4:D:77:ASN:N	2.15	0.43
4:D:187:ARG:NE	4:D:187:ARG:HA	2.34	0.43
6:F:11:ASN:HD21	6:F:13:ASN:HB2	1.84	0.43
7:G:140:ASP:O	7:G:144:MET:HB2	2.18	0.43
11:K:111:ASP:OD1	18:R:84:LYS:HE3	2.18	0.43
12:L:53:ARG:HG2	12:L:53:ARG:NH1	2.33	0.43
19:S:39:THR:CG2	19:S:40:ILE:N	2.63	0.43
19:S:51:VAL:O	19:S:57:HIS:HA	2.19	0.43
21:V:6:ARG:HB3	21:V:15:ARG:NH1	2.33	0.43
1:A:39:G:O2'	1:A:40:C:H5'	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:C:H2'	1:A:391:G:C8	2.54	0.43
1:A:792:A:H4'	1:A:793:U:C5'	2.48	0.43
1:A:1126:U:H3	1:A:1127:G:N2	2.17	0.43
1:A:1492:A:OP1	12:L:47:LYS:N	2.51	0.43
2:B:58:ILE:O	2:B:62:ALA:N	2.52	0.43
2:B:120:ALA:C	2:B:122:PHE:H	2.22	0.43
2:B:148:TYR:O	2:B:149:LEU:HD23	2.19	0.43
3:C:19:GLU:CB	3:C:40:ARG:HH22	2.30	0.43
3:C:22:TRP:CE3	3:C:22:TRP:O	2.71	0.43
4:D:30:LYS:C	4:D:32:ALA:H	2.22	0.43
5:E:82:VAL:HG12	5:E:89:ILE:CG2	2.48	0.43
10:J:45:ARG:HH11	10:J:45:ARG:CB	2.32	0.43
14:N:4:LYS:O	14:N:7:ILE:HG13	2.19	0.43
1:A:13:U:O4'	1:A:914:A:H5"	2.19	0.43
1:A:187:C:H5"	20:T:86:ARG:NH1	2.34	0.43
1:A:294:U:H2'	1:A:295:C:H6	1.83	0.43
1:A:581:G:O6	1:A:758:G:C8	2.72	0.43
1:A:969:A:C2'	1:A:970:C:H5'	2.48	0.43
1:A:1175:G:O2'	1:A:1176:A:H5'	2.19	0.43
1:A:1266:G:N2	1:A:1270:C:N3	2.66	0.43
2:B:18:GLY:HA2	2:B:42:ILE:H	1.84	0.43
3:C:173:VAL:HG12	3:C:175:LEU:HD21	2.00	0.43
4:D:31:CYS:O	4:D:32:ALA:CB	2.67	0.43
4:D:64:LEU:HD13	4:D:64:LEU:C	2.38	0.43
4:D:158:ILE:CG2	4:D:162:LEU:HD12	2.48	0.43
5:E:88:LYS:HB3	5:E:123:LEU:HB2	2.01	0.43
5:E:137:GLU:OE2	5:E:140:ARG:HD2	2.18	0.43
5:E:138:ALA:O	5:E:139:LEU:C	2.57	0.43
10:J:28:ARG:HG2	10:J:28:ARG:NH1	2.33	0.43
10:J:35:SER:HB3	10:J:72:VAL:O	2.19	0.43
10:J:44:VAL:HG22	10:J:66:ARG:HB3	2.00	0.43
10:J:72:VAL:HG12	10:J:73:ASP:N	2.33	0.43
16:P:26:ARG:CD	16:P:31:LYS:O	2.65	0.43
20:T:100:ILE:HD13	20:T:100:ILE:N	2.33	0.43
23:Z:38:A:C5	23:Z:39:U:H1'	2.54	0.43
1:A:1158:C:O2	1:A:1158:C:C4'	2.67	0.43
1:A:1249:C:O2'	9:I:73:GLN:NE2	2.52	0.43
1:A:1405:G:O4'	1:A:1519:A:H4'	2.19	0.43
26:A:3005:AM2:HC6	26:A:3005:AM2:HA1	1.89	0.43
2:B:64:ARG:HH11	2:B:64:ARG:HB3	1.84	0.43
2:B:83:MET:HB3	2:B:235:SER:OG	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:77:ILE:O	3:C:83:ARG:N	2.52	0.43
4:D:58:LEU:O	4:D:62:GLN:HG2	2.19	0.43
4:D:150:GLU:CB	4:D:153:ARG:HH21	2.32	0.43
6:F:25:ILE:O	6:F:28:ARG:HB3	2.18	0.43
7:G:138:LYS:HG2	7:G:139:GLU:N	2.34	0.43
8:H:11:THR:HG23	8:H:14:ARG:HH12	1.84	0.43
10:J:21:GLN:HA	10:J:24:VAL:HG12	2.01	0.43
12:L:58:VAL:O	12:L:65:GLU:HA	2.19	0.43
12:L:90:VAL:O	12:L:91:LYS:C	2.57	0.43
14:N:56:VAL:HG12	14:N:57:ARG:N	2.33	0.43
16:P:56:ALA:C	16:P:58:TYR:N	2.72	0.43
16:P:56:ALA:O	16:P:58:TYR:N	2.52	0.43
16:P:60:LEU:HD23	16:P:60:LEU:HA	1.88	0.43
17:Q:97:SER:CB	17:Q:103:GLY:HA3	2.48	0.43
19:S:29:ARG:HH11	19:S:29:ARG:HG3	1.84	0.43
20:T:50:GLU:O	20:T:100:ILE:CG1	2.59	0.43
20:T:51:GLU:HA	20:T:54:LYS:HB3	2.01	0.43
1:A:162:A:H2'	1:A:163:C:C5'	2.48	0.42
1:A:263:A:P	20:T:79:ARG:HH12	2.42	0.42
1:A:479:C:C5'	1:A:479:C:C6	2.91	0.42
1:A:969:A:H61	13:M:126:LYS:HB2	1.84	0.42
1:A:1030(A):G:H22	1:A:1030(C):G:H3'	1.83	0.42
1:A:1114:C:N3	1:A:1115:C:H5	2.16	0.42
2:B:132:LYS:CA	2:B:135:GLN:HB2	2.46	0.42
4:D:18:LYS:HE3	4:D:20:TYR:CZ	2.54	0.42
5:E:82:VAL:HG12	5:E:89:ILE:HG22	2.02	0.42
6:F:7:ASN:O	6:F:88:VAL:HA	2.17	0.42
7:G:72:ARG:HG3	7:G:72:ARG:HH11	1.84	0.42
7:G:80:VAL:HG12	7:G:81:GLY:N	2.34	0.42
8:H:41:ARG:HG2	8:H:41:ARG:O	2.18	0.42
9:I:3:GLN:HE21	9:I:3:GLN:CA	2.09	0.42
10:J:64:GLU:N	14:N:59:ALA:HB2	2.34	0.42
11:K:126:ARG:C	11:K:128:ALA:N	2.73	0.42
12:L:117:ARG:CG	12:L:122:THR:HB	2.47	0.42
18:R:47:THR:HG22	18:R:48:GLY:N	2.34	0.42
19:S:30:LEU:C	19:S:31:ILE:HG13	2.39	0.42
1:A:17:U:H2'	1:A:18:C:C6	2.54	0.42
1:A:429:U:H4'	1:A:430:A:O5'	2.19	0.42
1:A:1093:A:C5	1:A:1095:U:O4'	2.72	0.42
1:A:1479:C:O2'	1:A:1480:G:H5'	2.19	0.42
2:B:16:HIS:C	2:B:18:GLY:N	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:204:ASN:HB3	2:B:206:ASP:O	2.19	0.42
3:C:5:ILE:HD13	3:C:5:ILE:O	2.19	0.42
3:C:29:TYR:O	3:C:29:TYR:HD1	2.02	0.42
5:E:102:ALA:CB	5:E:120:THR:HB	2.45	0.42
7:G:78:ARG:HD3	7:G:156:TRP:CE3	2.54	0.42
8:H:90:GLY:O	8:H:91:ARG:HB2	2.19	0.42
8:H:114:THR:HG21	8:H:129:VAL:HG23	2.01	0.42
13:M:98:VAL:O	13:M:98:VAL:HG13	2.19	0.42
17:Q:48:GLU:O	17:Q:50:LYS:N	2.51	0.42
17:Q:93:GLN:HE21	17:Q:93:GLN:HB3	1.49	0.42
1:A:219:C:C4	1:A:220:G:C8	3.07	0.42
1:A:335:C:H2'	1:A:336:C:C6	2.54	0.42
1:A:620:C:C1'	4:D:135:LEU:HD13	2.50	0.42
1:A:1055:A:C8	1:A:1206:G:C2	3.08	0.42
1:A:1191:A:OP1	3:C:3:ASN:ND2	2.52	0.42
1:A:1309:G:C6	1:A:1329:A:C2	3.06	0.42
1:A:1347:G:C8	9:I:107:ARG:HB3	2.54	0.42
2:B:178:ARG:NH1	8:H:71:GLY:O	2.51	0.42
4:D:3:ARG:HH22	4:D:70:ILE:HG13	1.83	0.42
4:D:133:VAL:HG11	4:D:138:TYR:HD2	1.84	0.42
5:E:41:VAL:CG1	5:E:113:ALA:HA	2.48	0.42
5:E:95:ALA:O	5:E:98:THR:OG1	2.36	0.42
6:F:26:ILE:HG21	6:F:63:TYR:HE2	1.78	0.42
6:F:48:LEU:CD1	6:F:52:ILE:HD12	2.47	0.42
6:F:95:GLU:O	6:F:97:PHE:N	2.52	0.42
7:G:31:MET:CG	7:G:32:ARG:N	2.81	0.42
7:G:88:PRO:CB	7:G:145:ALA:HB1	2.49	0.42
9:I:58:ARG:NH1	9:I:58:ARG:CB	2.82	0.42
12:L:15:ARG:HG3	12:L:15:ARG:NH1	2.34	0.42
12:L:117:ARG:HG2	12:L:122:THR:O	2.20	0.42
13:M:62:ASN:HD22	13:M:62:ASN:HA	1.71	0.42
18:R:51:LEU:HA	18:R:52:PRO:HD3	1.91	0.42
19:S:7:LYS:HE2	19:S:7:LYS:HB3	1.94	0.42
19:S:16:LEU:O	19:S:19:VAL:HG12	2.19	0.42
20:T:11:SER:N	20:T:13:LEU:CD1	2.83	0.42
23:Z:30:G:N2	23:Z:41:C:C5	2.87	0.42
23:Z:37:A:H3'	23:Z:38:A:C8	2.55	0.42
1:A:100:C:H2'	1:A:101:A:C8	2.54	0.42
1:A:1169:A:H2'	1:A:1170:A:C8	2.54	0.42
1:A:1368:G:H5"	9:I:112:LYS:CG	2.49	0.42
2:B:142:LEU:CD2	2:B:146:GLN:HE22	2.30	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:13:GLY:HA3	14:N:57:ARG:HH21	1.85	0.42
4:D:9:CYS:SG	4:D:31:CYS:O	2.78	0.42
4:D:54:TYR:O	4:D:55:ALA:C	2.57	0.42
5:E:76:ILE:HG23	5:E:142:LEU:CD1	2.49	0.42
7:G:31:MET:HA	7:G:39:ALA:HB2	2.02	0.42
13:M:59:TYR:O	13:M:59:TYR:CG	2.71	0.42
14:N:27:CYS:SG	14:N:29:ARG:HB2	2.59	0.42
15:O:6:GLU:CD	15:O:6:GLU:N	2.67	0.42
1:A:244:U:O2'	26:A:3005:AM2:OB3	2.32	0.42
1:A:976:G:C8	1:A:1358:U:H2'	2.55	0.42
1:A:993:G:H2'	1:A:993:G:N3	2.34	0.42
1:A:1201:A:H4'	1:A:1202:G:H5"	2.01	0.42
1:A:1202:G:H2'	1:A:1203:C:C5'	2.49	0.42
1:A:1404:C:O4'	1:A:1499:A:C2	2.72	0.42
2:B:23:ARG:CZ	2:B:23:ARG:O	2.67	0.42
3:C:72:LYS:C	3:C:74:GLY:N	2.72	0.42
4:D:60:GLU:HG2	4:D:202:LEU:HD12	2.00	0.42
6:F:19:LEU:C	6:F:21:LEU:N	2.73	0.42
12:L:70:ILE:HD13	12:L:77:LEU:HD12	2.01	0.42
17:Q:5:VAL:O	17:Q:6:LEU:HD23	2.20	0.42
1:A:175:C:O2'	1:A:176:C:H5'	2.19	0.42
1:A:1223:C:H3'	1:A:1224:G:H5"	2.02	0.42
1:A:1225:A:H2'	1:A:1225:A:N3	2.34	0.42
1:A:1237:C:C4'	1:A:1334:G:H21	2.33	0.42
1:A:1314:C:OP2	19:S:6:LYS:CD	2.52	0.42
1:A:1442(A):G:C3'	1:A:1442(B):A:H5'	2.50	0.42
2:B:23:ARG:NH1	2:B:24:TRP:O	2.53	0.42
3:C:131:ARG:HD3	5:E:50:GLU:OE2	2.20	0.42
4:D:137:SER:O	4:D:138:TYR:C	2.58	0.42
6:F:33:TYR:HD2	6:F:75:LEU:CD2	2.32	0.42
8:H:89:PRO:HA	8:H:92:ARG:HH11	1.83	0.42
10:J:54:PHE:O	10:J:55:LYS:HG2	2.20	0.42
11:K:82:VAL:HG12	11:K:83:ILE:N	2.35	0.42
19:S:4:SER:O	19:S:5:LEU:HD12	2.19	0.42
1:A:603:U:H2'	1:A:604:G:H8	1.85	0.42
1:A:1050:G:N2	1:A:1209:C:H1'	2.35	0.42
1:A:1126:U:HO2'	1:A:1127:G:C5'	2.33	0.42
1:A:1190:G:H5'	3:C:176:HIS:NE2	2.34	0.42
1:A:1356:G:H2'	1:A:1357:A:H8	1.82	0.42
2:B:178:ARG:HD3	2:B:184:VAL:HG21	2.02	0.42
3:C:22:TRP:CZ3	3:C:32:LEU:HB3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:28:GLN:O	3:C:30:ARG:N	2.53	0.42
3:C:43:LEU:O	3:C:47:LEU:HD13	2.20	0.42
5:E:75:THR:HG23	5:E:76:ILE:N	2.35	0.42
5:E:80:ILE:CD1	5:E:138:ALA:HB1	2.50	0.42
6:F:75:LEU:HD13	6:F:75:LEU:O	2.19	0.42
7:G:155:ARG:O	7:G:156:TRP:HB3	2.20	0.42
11:K:101:SER:O	11:K:103:LEU:N	2.53	0.42
17:Q:60:ILE:HG12	17:Q:61:GLU:N	2.34	0.42
18:R:39:VAL:CG1	18:R:40:LEU:N	2.83	0.42
1:A:646:U:O2'	1:A:647:C:H5'	2.19	0.42
1:A:718:G:C4'	11:K:117:ASN:HD22	2.33	0.42
1:A:797:C:OP1	11:K:124:LYS:HD2	2.19	0.42
1:A:948:C:OP1	13:M:109:THR:N	2.52	0.42
1:A:986:A:N3	19:S:52:TYR:OH	2.43	0.42
1:A:1023:G:H2'	1:A:1024:G:H5'	2.01	0.42
1:A:1140:C:H6	1:A:1140:C:H5'	1.85	0.42
1:A:1230:C:H1'	13:M:126:LYS:HA	2.02	0.42
1:A:1459:C:O2'	1:A:1460:A:H5'	2.19	0.42
2:B:16:HIS:HA	2:B:204:ASN:CG	2.38	0.42
2:B:97:TRP:HH2	2:B:176:GLU:CD	2.22	0.42
2:B:216:SER:C	2:B:218:ALA:N	2.73	0.42
4:D:3:ARG:NH1	4:D:70:ILE:HA	2.35	0.42
4:D:4:TYR:CG	4:D:5:ILE:N	2.88	0.42
4:D:134:ASP:O	4:D:136:PRO:HD3	2.20	0.42
6:F:21:LEU:HD12	6:F:24:GLU:OE1	2.19	0.42
6:F:62:TRP:HB2	18:R:35:ARG:NH1	2.34	0.42
7:G:16:LEU:HD21	9:I:42:ARG:HG3	2.02	0.42
7:G:54:THR:CG2	7:G:56:GLN:HB2	2.50	0.42
10:J:76:ASN:CB	10:J:78:ASN:ND2	2.83	0.42
12:L:30:ALA:O	12:L:31:PRO:C	2.57	0.42
13:M:14:ARG:HE	13:M:42:ALA:HA	1.84	0.42
15:O:55:GLY:HA2	15:O:58:MET:CE	2.50	0.42
16:P:67:THR:HG23	16:P:70:ALA:CB	2.50	0.42
18:R:23:LYS:HD2	18:R:58:LEU:HD23	2.01	0.42
18:R:37:VAL:O	18:R:41:LYS:HG2	2.20	0.42
18:R:44:LEU:HD12	18:R:44:LEU:N	2.35	0.42
19:S:22:LEU:O	19:S:27:GLU:HA	2.19	0.42
20:T:49:ALA:O	20:T:100:ILE:HG12	2.20	0.42
1:A:30:U:O2	1:A:30:U:H2'	2.20	0.42
1:A:77:G:O2'	1:A:78:G:H5'	2.20	0.42
1:A:321:A:C2	1:A:333:G:C2	3.08	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:C:H2'	1:A:387:U:C5'	2.50	0.42
1:A:389:A:H2'	1:A:390:C:C5'	2.47	0.42
1:A:618:C:H5"	1:A:619:U:H5"	2.02	0.42
1:A:1054:C:O5'	1:A:1197:G:OP2	2.37	0.42
1:A:1197:G:O5'	1:A:1198:G:OP2	2.38	0.42
1:A:1272:G:O2'	1:A:1273:G:H5'	2.20	0.42
2:B:140:HIS:CA	2:B:143:GLU:HG2	2.42	0.42
3:C:103:VAL:CG1	3:C:104:GLN:H	2.32	0.42
3:C:103:VAL:CG1	3:C:104:GLN:N	2.81	0.42
3:C:156:ARG:O	3:C:157:ILE:C	2.57	0.42
6:F:8:ILE:HD13	6:F:26:ILE:HD12	2.01	0.42
7:G:143:ARG:CB	7:G:143:ARG:HH11	2.33	0.42
9:I:65:VAL:CG2	9:I:73:GLN:HB3	2.46	0.42
10:J:12:ASP:OD1	10:J:13:HIS:N	2.53	0.42
11:K:52:GLY:C	11:K:54:ARG:N	2.73	0.42
14:N:23:ARG:CZ	14:N:30:ALA:HB2	2.50	0.42
17:Q:9:VAL:O	17:Q:11:VAL:HG13	2.20	0.42
17:Q:27:PHE:CE1	17:Q:36:ILE:HD11	2.55	0.42
17:Q:27:PHE:HD1	17:Q:28:PRO:O	2.02	0.42
18:R:40:LEU:C	18:R:42:ARG:N	2.72	0.42
1:A:455:C:H42	1:A:476:G:H1	1.67	0.42
1:A:802:A:C2'	1:A:803:G:H5'	2.50	0.42
1:A:949:A:C2	1:A:1233:G:N3	2.88	0.42
1:A:1051:C:H2'	1:A:1052:U:C6	2.49	0.42
1:A:1095:U:H2'	1:A:1096:C:C6	2.54	0.42
1:A:1158:C:C6	1:A:1160:G:C8	3.08	0.42
1:A:1193:G:HO2'	1:A:1194:U:H5'	1.85	0.42
1:A:1311:G:O6	19:S:2:PRO:HB3	2.20	0.42
1:A:1360:A:H8	1:A:1360:A:O5'	2.02	0.42
2:B:28:PHE:CD2	2:B:190:THR:HA	2.55	0.42
2:B:211:ILE:H	2:B:211:ILE:CD1	2.32	0.42
3:C:79:ARG:O	3:C:81:GLY:N	2.52	0.42
3:C:83:ARG:CA	3:C:86:VAL:HG23	2.33	0.42
6:F:86:ARG:HG3	6:F:86:ARG:NH1	2.35	0.42
8:H:44:PHE:O	8:H:80:ILE:HD11	2.19	0.42
12:L:25:PRO:C	12:L:27:LEU:N	2.71	0.42
12:L:126:LYS:HD2	12:L:126:LYS:C	2.40	0.42
13:M:23:TYR:O	13:M:25:ILE:N	2.53	0.42
14:N:54:PRO:C	14:N:56:VAL:H	2.23	0.42
16:P:71:ARG:NH1	16:P:71:ARG:HB2	2.35	0.42
20:T:86:ARG:O	20:T:90:GLN:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:C:H2'	1:A:90:U:O4'	2.20	0.41
1:A:947:G:P	13:M:108:ARG:HG2	2.60	0.41
1:A:1051:C:N3	1:A:1052:U:C5	2.88	0.41
1:A:1103:C:H2'	1:A:1104:G:O4'	2.20	0.41
2:B:23:ARG:HH11	2:B:24:TRP:HA	1.85	0.41
2:B:219:VAL:HA	2:B:222:ILE:CG1	2.50	0.41
4:D:18:LYS:HD2	4:D:31:CYS:CB	2.50	0.41
4:D:47:ARG:HH12	4:D:49:ARG:HG2	1.85	0.41
4:D:107:ARG:HH12	4:D:114:ARG:HH22	1.68	0.41
7:G:141:VAL:HA	7:G:144:MET:HB2	2.02	0.41
12:L:43:VAL:HG12	12:L:44:THR:H	1.83	0.41
14:N:37:PHE:C	14:N:39:LEU:N	2.73	0.41
15:O:36:ILE:CG1	15:O:59:MET:HE2	2.49	0.41
18:R:40:LEU:O	18:R:43:PHE:N	2.31	0.41
20:T:33:ILE:HD13	20:T:63:ILE:HA	2.02	0.41
20:T:49:ALA:HB3	20:T:99:LEU:HG	2.02	0.41
1:A:439:A:H2'	1:A:441:A:H5'	2.02	0.41
1:A:519:C:O2'	1:A:520:A:H5'	2.21	0.41
1:A:601:C:H2'	1:A:602:A:C8	2.56	0.41
1:A:667:G:H2'	1:A:668:G:C8	2.54	0.41
1:A:909:A:H2'	1:A:910:C:O4'	2.20	0.41
1:A:959:A:H5"	1:A:960:U:OP2	2.20	0.41
1:A:1172:C:H2'	1:A:1173:G:H8	1.84	0.41
1:A:1203:C:O2'	1:A:1204:A:H5'	2.21	0.41
1:A:1227:A:H8	1:A:1227:A:H3'	1.85	0.41
1:A:1297:C:HO2'	1:A:1298:C:H6	1.64	0.41
2:B:84:GLU:HG3	2:B:216:SER:HA	2.02	0.41
3:C:85:ARG:HH11	3:C:85:ARG:HG3	1.85	0.41
3:C:191:THR:OG1	3:C:192:THR:N	2.51	0.41
4:D:35:ARG:O	4:D:36:ARG:CB	2.67	0.41
4:D:119:GLN:CG	4:D:123:HIS:HD2	2.33	0.41
6:F:23:LYS:NZ	6:F:42:GLU:OE1	2.53	0.41
8:H:51:VAL:HG21	8:H:60:ARG:CZ	2.49	0.41
11:K:120:ARG:HG3	11:K:120:ARG:HH11	1.86	0.41
12:L:104:VAL:O	12:L:105:TYR:HB2	2.20	0.41
3:C:37:GLN:O	3:C:38:ARG:C	2.59	0.41
3:C:44:GLU:HG2	3:C:52:LEU:CD2	2.50	0.41
3:C:135:LYS:NZ	5:E:52:PRO:HG3	2.35	0.41
8:H:109:ILE:HG12	8:H:137:VAL:HB	2.01	0.41
10:J:45:ARG:HB2	10:J:45:ARG:NH1	2.34	0.41
12:L:93:LEU:HD12	12:L:96:VAL:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:66:LEU:O	13:M:67:GLU:C	2.59	0.41
13:M:66:LEU:O	13:M:67:GLU:O	2.38	0.41
15:O:17:ARG:HG3	15:O:17:ARG:NH1	2.31	0.41
16:P:8:ARG:HH11	16:P:8:ARG:HG3	1.85	0.41
1:A:52:G:H2'	1:A:53:A:H8	1.85	0.41
1:A:189(G):G:H4'	1:A:189(H):G:OP2	2.21	0.41
1:A:244:U:HO2'	26:A:3005:AM2:H6	1.60	0.41
1:A:485:G:H2'	1:A:486:U:OP2	2.21	0.41
1:A:515:G:H8	1:A:515:G:O5'	2.03	0.41
1:A:662:G:O2'	1:A:836:G:C5'	2.68	0.41
1:A:721:G:H8	1:A:721:G:OP1	2.03	0.41
1:A:999:C:OP1	1:A:999:C:H4'	2.20	0.41
1:A:1288:A:H1'	1:A:1352:C:O2'	2.19	0.41
1:A:1385:G:C2'	1:A:1386:G:H5"	2.47	0.41
1:A:1466:C:H2'	1:A:1467:G:O4'	2.20	0.41
2:B:142:LEU:O	2:B:143:GLU:C	2.58	0.41
3:C:31:HIS:C	3:C:33:LEU:N	2.74	0.41
3:C:52:LEU:HA	3:C:70:VAL:HG12	2.02	0.41
4:D:4:TYR:O	4:D:5:ILE:CB	2.66	0.41
6:F:23:LYS:HB3	6:F:23:LYS:HE2	1.89	0.41
6:F:44:GLY:HA3	6:F:59:TYR:CE1	2.54	0.41
10:J:92:THR:C	10:J:94:VAL:H	2.24	0.41
11:K:70:LYS:HE3	11:K:70:LYS:HB2	1.64	0.41
12:L:75:HIS:HD2	12:L:77:LEU:H	1.67	0.41
13:M:87:TYR:O	13:M:90:LEU:N	2.53	0.41
14:N:23:ARG:HH11	14:N:23:ARG:HB3	1.85	0.41
15:O:45:VAL:O	15:O:47:LYS:N	2.54	0.41
19:S:60:VAL:HG21	19:S:74:PHE:CB	2.48	0.41
20:T:26:ASN:O	20:T:27:LYS:C	2.58	0.41
20:T:65:LYS:O	20:T:68:LYS:HB2	2.21	0.41
1:A:596:C:O2'	1:A:597:G:H5'	2.20	0.41
1:A:840:C:O2	1:A:840:C:C2'	2.67	0.41
1:A:930:C:O2'	1:A:931:C:H5'	2.19	0.41
1:A:950:U:C5	13:M:102:ARG:CZ	3.04	0.41
1:A:1075:C:O2'	1:A:1076:C:H5'	2.20	0.41
1:A:1247:U:H2'	1:A:1248:A:C5'	2.38	0.41
1:A:1266:G:H5'	1:A:1267:C:OP2	2.21	0.41
1:A:1376:U:P	7:G:94:ARG:HH22	2.43	0.41
1:A:1442:G:N3	1:A:1442:G:H3'	2.36	0.41
2:B:54:THR:O	2:B:57:PHE:HB3	2.21	0.41
2:B:187:LEU:C	2:B:187:LEU:HD13	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:195:ASP:O	8:H:74:PRO:HG3	2.20	0.41
4:D:132:ARG:NH1	4:D:132:ARG:HB2	2.35	0.41
4:D:158:ILE:O	4:D:162:LEU:HB2	2.19	0.41
5:E:29:GLY:HA2	5:E:47:LYS:HB3	2.01	0.41
5:E:144:THR:O	5:E:145:LYS:C	2.58	0.41
7:G:80:VAL:O	7:G:82:GLY:N	2.46	0.41
8:H:104:ARG:O	8:H:105:ARG:C	2.59	0.41
10:J:56:HIS:C	10:J:58:ASP:N	2.72	0.41
10:J:99:LYS:O	10:J:100:THR:HB	2.20	0.41
11:K:126:ARG:O	11:K:127:LYS:C	2.58	0.41
12:L:28:LYS:HE2	12:L:33:ARG:HH22	1.85	0.41
13:M:108:ARG:HH11	13:M:114:ARG:NH1	2.17	0.41
17:Q:18:THR:HG23	17:Q:69:LYS:HE3	2.01	0.41
17:Q:93:GLN:O	17:Q:96:GLN:HB2	2.21	0.41
19:S:3:ARG:H	19:S:3:ARG:HD2	1.86	0.41
1:A:6:G:O2'	1:A:7:G:H5'	2.21	0.41
1:A:90:U:H2'	1:A:91:C:C6	2.55	0.41
1:A:129:U:O3'	1:A:129(A):G:H4'	2.20	0.41
1:A:1152:A:O3'	10:J:13:HIS:CD2	2.73	0.41
1:A:1372:U:O2'	1:A:1373:G:H5'	2.21	0.41
1:A:1477:C:H2'	1:A:1478:C:H6	1.86	0.41
2:B:187:LEU:O	2:B:187:LEU:HD13	2.21	0.41
2:B:231:GLU:CB	2:B:232:PRO:CD	2.99	0.41
3:C:46:GLU:C	3:C:48:TYR:N	2.73	0.41
5:E:147:ASP:OD1	5:E:147:ASP:N	2.53	0.41
8:H:83:ILE:O	8:H:83:ILE:HG23	2.20	0.41
10:J:29:ARG:HD3	10:J:29:ARG:N	2.36	0.41
11:K:59:TYR:CE2	11:K:63:LEU:HD11	2.55	0.41
14:N:56:VAL:O	14:N:57:ARG:HB2	2.20	0.41
17:Q:50:LYS:HD2	17:Q:51:TYR:CE1	2.56	0.41
18:R:37:VAL:O	18:R:39:VAL:N	2.53	0.41
23:Z:37:A:H2'	23:Z:38:A:O4'	2.20	0.41
1:A:76:C:O2'	1:A:77:G:H5'	2.20	0.41
1:A:162:A:H2'	1:A:163:C:C4'	2.50	0.41
1:A:749:C:HO2'	1:A:750:G:H8	1.68	0.41
1:A:762:C:H5'	17:Q:104:LYS:HZ2	1.86	0.41
1:A:1194:U:H2'	1:A:1195:C:H6	1.86	0.41
1:A:1196:U:C5	3:C:162:GLN:NE2	2.89	0.41
1:A:1370:G:C2	1:A:1371:G:C8	3.09	0.41
2:B:136:VAL:O	2:B:140:HIS:CB	2.61	0.41
3:C:107:GLN:CD	3:C:107:GLN:N	2.70	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:76:ILE:HG23	5:E:142:LEU:HD13	2.02	0.41
7:G:129:GLU:HG3	7:G:131:LYS:NZ	2.35	0.41
7:G:144:MET:HA	7:G:144:MET:CE	2.50	0.41
8:H:84:ARG:HG3	8:H:84:ARG:NH1	2.31	0.41
10:J:79:ARG:NH1	10:J:82:ILE:HD12	2.33	0.41
13:M:53:VAL:HG12	13:M:57:ARG:HH21	1.85	0.41
13:M:96:LEU:O	13:M:97:PRO:O	2.39	0.41
14:N:14:PRO:O	14:N:15:LYS:CB	2.65	0.41
17:Q:95:TYR:HD1	17:Q:95:TYR:H	1.68	0.41
1:A:198:G:H2'	1:A:199:G:H8	1.85	0.41
1:A:229:U:H4'	16:P:33:ILE:CD1	2.51	0.41
1:A:552:U:O2	12:L:31:PRO:HB3	2.21	0.41
1:A:629:G:H8	1:A:629:G:O5'	2.03	0.41
1:A:760:G:H1	17:Q:105:ALA:HA	1.86	0.41
1:A:1051:C:C2	1:A:1052:U:C6	3.08	0.41
1:A:1173:G:H2'	1:A:1174:G:O4'	2.21	0.41
1:A:1397:C:C2	22:W:6:A:C2	3.09	0.41
2:B:64:ARG:CB	2:B:64:ARG:HH11	2.34	0.41
2:B:221:LEU:O	2:B:221:LEU:HD13	2.20	0.41
3:C:120:VAL:HG11	3:C:198:VAL:HG11	2.02	0.41
4:D:31:CYS:C	4:D:33:MET:H	2.24	0.41
4:D:91:SER:O	4:D:94:LEU:N	2.54	0.41
4:D:200:GLU:HG2	4:D:201:GLN:N	2.35	0.41
5:E:127:ASN:HD22	5:E:130:ASN:HD22	1.61	0.41
7:G:72:ARG:CZ	7:G:142:GLU:OE2	2.69	0.41
7:G:126:ASP:O	7:G:129:GLU:HB2	2.21	0.41
8:H:11:THR:HG22	8:H:15:ASN:HD21	1.84	0.41
9:I:33:PHE:CE1	9:I:37:PHE:CD2	3.09	0.41
10:J:30:SER:CB	10:J:81:THR:HA	2.50	0.41
10:J:48:THR:HG1	10:J:62:HIS:CD2	2.39	0.41
10:J:90:LEU:HB2	10:J:91:PRO:CD	2.51	0.41
12:L:59:ARG:HG2	12:L:59:ARG:NH1	2.36	0.41
13:M:73:GLU:O	13:M:77:ASN:HB2	2.20	0.41
13:M:87:TYR:C	13:M:89:GLY:N	2.72	0.41
19:S:67:VAL:O	19:S:67:VAL:HG23	2.20	0.41
1:A:342:C:H2'	1:A:343:U:H5"	2.03	0.41
1:A:410:G:OP2	4:D:25:ARG:HD2	2.21	0.41
1:A:456:C:H2'	1:A:457:C:C6	2.56	0.41
1:A:818:G:C6	26:A:3002:AM2:HB61	2.56	0.41
1:A:973:G:C6	1:A:974:A:N6	2.89	0.41
1:A:1048:G:C8	1:A:1048:G:H3'	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1095:U:H2'	1:A:1096:C:O4'	2.20	0.41
1:A:1190:G:H5"	3:C:176:HIS:NE2	2.36	0.41
1:A:1227:A:H3'	1:A:1227:A:C8	2.55	0.41
1:A:1406:U:C2'	1:A:1407:C:H5'	2.51	0.41
1:A:1482:G:HO2'	1:A:1483:A:H8	1.65	0.41
2:B:9:GLU:CD	2:B:10:LEU:N	2.72	0.41
4:D:175:SER:HB3	4:D:186:LEU:HD11	2.03	0.41
5:E:150:ARG:HB3	5:E:150:ARG:NH1	2.28	0.41
6:F:2:ARG:CZ	6:F:69:GLU:HG2	2.51	0.41
6:F:27:GLN:H	6:F:27:GLN:HG2	1.59	0.41
6:F:67:MET:HB2	6:F:68:PRO:CD	2.51	0.41
7:G:94:ARG:HH12	7:G:98:SER:HB3	1.86	0.41
8:H:68:ARG:HG2	8:H:68:ARG:NH1	2.34	0.41
9:I:8:GLY:HA3	9:I:79:LEU:HB3	2.03	0.41
9:I:88:TYR:O	9:I:88:TYR:CG	2.73	0.41
10:J:4:ILE:O	10:J:73:ASP:OD1	2.39	0.41
11:K:105:VAL:HG11	11:K:108:ILE:CD1	2.50	0.41
11:K:109:VAL:CG2	18:R:86:VAL:HA	2.51	0.41
12:L:27:LEU:HB2	12:L:62:SER:HB2	2.02	0.41
12:L:105:TYR:C	12:L:107:ALA:H	2.24	0.41
13:M:15:VAL:HG11	13:M:34:LEU:HD21	2.02	0.41
14:N:11:LYS:C	14:N:13:THR:N	2.74	0.41
16:P:38:TYR:CD1	16:P:38:TYR:O	2.74	0.41
18:R:50:ILE:HD12	18:R:70:ILE:HD12	2.03	0.41
18:R:86:VAL:O	18:R:87:ARG:HB2	2.21	0.41
20:T:22:ARG:O	20:T:23:ARG:C	2.58	0.41
20:T:92:LEU:HD23	20:T:92:LEU:HA	1.94	0.41
23:Z:38:A:H2'	23:Z:39:U:C4'	2.51	0.41
1:A:198:G:H2'	1:A:199:G:C8	2.56	0.41
1:A:382:A:H2'	1:A:383:A:C8	2.55	0.41
1:A:520:A:N6	1:A:529:G:H1'	2.36	0.41
1:A:536:C:H2'	1:A:537:G:C8	2.56	0.41
1:A:1358:U:OP2	1:A:1359:C:H5	2.04	0.41
1:A:1429:C:O2'	1:A:1430:C:H5'	2.20	0.41
1:A:1502:A:H5'	1:A:1504:G:N7	2.35	0.41
2:B:97:TRP:CH2	2:B:176:GLU:HG3	2.56	0.41
2:B:184:VAL:N	2:B:198:ASP:OD2	2.45	0.41
3:C:14:ILE:O	3:C:15:THR:C	2.59	0.41
3:C:115:LEU:O	3:C:116:VAL:C	2.58	0.41
3:C:151:VAL:HG12	3:C:152:ILE:N	2.36	0.41
5:E:122:GLU:O	5:E:123:LEU:HD23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:79:LYS:HA	13:M:82:MET:HG2	2.03	0.41
19:S:43:GLU:CD	19:S:43:GLU:H	2.24	0.41
20:T:57:ARG:HH22	20:T:100:ILE:CG2	2.32	0.41
1:A:325:A:N6	1:A:326:G:N1	2.69	0.40
1:A:573:A:H3'	1:A:573:A:OP2	2.21	0.40
1:A:739:C:O2'	15:O:42:HIS:ND1	2.52	0.40
1:A:840:C:OP1	1:A:840:C:C4'	2.69	0.40
1:A:1008:C:O2'	1:A:1009:G:H5'	2.21	0.40
1:A:1158:C:O2	1:A:1158:C:H5"	2.20	0.40
1:A:1226:C:N4	13:M:104:ARG:HB2	2.37	0.40
1:A:1281:U:H3'	1:A:1281:U:C6	2.55	0.40
1:A:1298:C:H4'	1:A:1299:A:O4'	2.21	0.40
2:B:100:GLY:O	2:B:108:ILE:HG13	2.21	0.40
3:C:55:VAL:O	3:C:56:ASP:C	2.58	0.40
6:F:34:GLY:O	6:F:67:MET:HB3	2.21	0.40
6:F:43:LEU:H	6:F:43:LEU:CD2	2.34	0.40
7:G:70:LYS:HA	7:G:71:PRO:HD2	1.97	0.40
9:I:55:ALA:O	9:I:56:LEU:CB	2.68	0.40
9:I:114:TYR:HE2	10:J:60:ARG:O	2.03	0.40
9:I:118:LYS:HG3	9:I:121:ARG:HB3	2.02	0.40
10:J:50:ILE:O	10:J:52:GLY:N	2.54	0.40
15:O:10:LYS:O	15:O:14:GLU:HB2	2.21	0.40
18:R:40:LEU:O	18:R:42:ARG:N	2.54	0.40
18:R:47:THR:C	18:R:49:LYS:H	2.24	0.40
1:A:404:U:H2'	1:A:405:U:H6	1.86	0.40
1:A:541:G:H2'	1:A:542:G:H8	1.86	0.40
1:A:620:C:C6	4:D:135:LEU:CD1	3.05	0.40
1:A:937:A:C2	1:A:1379:G:C6	3.09	0.40
1:A:1058:G:C6	1:A:1059:C:N3	2.90	0.40
1:A:1115:C:O2	1:A:1115:C:C2'	2.70	0.40
1:A:1158:C:C4	1:A:1160:G:N7	2.89	0.40
2:B:239:VAL:O	2:B:239:VAL:HG12	2.21	0.40
3:C:120:VAL:O	3:C:124:ILE:HG12	2.21	0.40
3:C:167:TRP:O	3:C:168:ALA:CB	2.69	0.40
4:D:29:PRO:O	4:D:30:LYS:CB	2.68	0.40
4:D:119:GLN:HG2	4:D:123:HIS:HD2	1.86	0.40
4:D:153:ARG:HD3	4:D:180:GLY:O	2.21	0.40
7:G:65:ALA:HB2	7:G:124:LEU:O	2.21	0.40
8:H:39:LEU:HD22	8:H:111:ILE:HD11	2.03	0.40
11:K:34:ASP:HB2	11:K:35:PRO:HD2	2.02	0.40
12:L:29:GLY:O	12:L:30:ALA:C	2.59	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:82:ILE:HG22	15:O:83:GLU:N	2.35	0.40
18:R:66:LEU:O	18:R:69:THR:HB	2.21	0.40
19:S:52:TYR:CD1	19:S:56:GLN:O	2.74	0.40
1:A:342:C:C2'	1:A:343:U:H5"	2.51	0.40
1:A:662:G:O2'	1:A:836:G:H5"	2.22	0.40
1:A:888:G:C3'	1:A:889:A:H5"	2.43	0.40
1:A:946:A:O2'	1:A:1333:A:N3	2.49	0.40
1:A:998:G:H2'	1:A:999:C:C4'	2.52	0.40
1:A:1350:A:C6	1:A:1351:U:N3	2.89	0.40
3:C:173:VAL:O	3:C:173:VAL:HG12	2.21	0.40
5:E:44:GLY:HA3	5:E:62:ALA:HB2	2.03	0.40
6:F:27:GLN:HE21	6:F:27:GLN:HB3	1.66	0.40
9:I:32:ASP:O	9:I:33:PHE:C	2.58	0.40
9:I:58:ARG:CB	9:I:58:ARG:HH11	2.34	0.40
9:I:102:LEU:N	9:I:102:LEU:CD1	2.73	0.40
10:J:17:ASP:O	10:J:21:GLN:CB	2.68	0.40
11:K:80:VAL:HG12	11:K:104:GLN:O	2.21	0.40
11:K:122:LYS:HB2	11:K:122:LYS:NZ	2.36	0.40
12:L:101:VAL:HG12	12:L:104:VAL:HG23	2.03	0.40
16:P:20:VAL:HG12	16:P:35:LYS:HA	2.03	0.40
18:R:53:ARG:C	18:R:55:ARG:N	2.74	0.40
19:S:12:ASP:H	19:S:38:SER:CB	2.29	0.40
20:T:57:ARG:NH1	20:T:102:GLY:HA3	2.37	0.40
1:A:59:A:H3'	1:A:331:G:H22	1.87	0.40
1:A:116:A:O2'	1:A:117:G:H5'	2.22	0.40
1:A:229:U:C5'	16:P:33:ILE:HD13	2.48	0.40
1:A:233:C:H2'	1:A:234:C:H6	1.85	0.40
1:A:404:U:O2'	1:A:405:U:H5'	2.21	0.40
1:A:658:G:C2	1:A:749:C:N3	2.89	0.40
1:A:716:A:O2'	1:A:717:C:H5'	2.21	0.40
1:A:726:C:O2'	1:A:727:G:H5'	2.21	0.40
1:A:1120:G:C2	1:A:1154:G:C2	3.09	0.40
1:A:1129:C:N4	1:A:1135:U:H3	2.20	0.40
1:A:1238:A:C8	1:A:1303:C:H1'	2.56	0.40
1:A:1281:U:H4'	1:A:1282:C:OP2	2.22	0.40
1:A:1371:G:OP1	9:I:11:LYS:O	2.39	0.40
2:B:19:HIS:CB	2:B:204:ASN:HA	2.51	0.40
2:B:22:LYS:HA	2:B:40:HIS:CE1	2.53	0.40
2:B:59:GLU:CB	2:B:221:LEU:HD11	2.46	0.40
2:B:142:LEU:CB	2:B:146:GLN:HE22	2.34	0.40
3:C:91:LEU:CD2	3:C:92:ALA:N	2.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:132:ARG:CZ	4:D:132:ARG:CB	3.00	0.40
5:E:17:ALA:HB2	5:E:26:PHE:CD1	2.55	0.40
5:E:24:ARG:NH2	22:W:6:A:N7	2.69	0.40
7:G:94:ARG:NH1	7:G:98:SER:HB3	2.36	0.40
7:G:111:ARG:NH2	7:G:122:HIS:HB3	2.36	0.40
13:M:13:LYS:O	13:M:45:VAL:HG12	2.21	0.40
16:P:63:GLY:O	16:P:65:GLN:N	2.55	0.40
18:R:88:LYS:C	18:R:88:LYS:CD	2.90	0.40
20:T:101:GLY:O	20:T:102:GLY:O	2.39	0.40
1:A:803:G:C5	1:A:804:U:C4	3.09	0.40
1:A:878:G:OP1	8:H:89:PRO:O	2.39	0.40
3:C:118:GLN:H	3:C:118:GLN:HG2	1.72	0.40
4:D:88:VAL:O	4:D:92:VAL:HG23	2.22	0.40
6:F:14:LEU:HD21	6:F:84:ASN:OD1	2.22	0.40
8:H:19:VAL:CG2	8:H:21:LYS:HD3	2.52	0.40
10:J:71:LEU:O	10:J:72:VAL:HB	2.22	0.40
10:J:91:PRO:HB2	10:J:94:VAL:CG2	2.51	0.40
12:L:90:VAL:HG11	12:L:93:LEU:HD21	2.04	0.40
20:T:97:ALA:O	20:T:99:LEU:N	2.55	0.40
23:Z:38:A:C8	23:Z:38:A:OP2	2.75	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%)	150 (65%)	50 (22%)	32 (14%)	0 3
3	C	204/239 (85%)	123 (60%)	48 (24%)	33 (16%)	0 2
4	D	206/208 (99%)	140 (68%)	45 (22%)	21 (10%)	0 7
5	E	148/161 (92%)	115 (78%)	30 (20%)	3 (2%)	7 39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
6	F	99/101 (98%)	74 (75%)	21 (21%)	4 (4%)	3 24
7	G	153/155 (99%)	116 (76%)	28 (18%)	9 (6%)	1 15
8	H	136/138 (99%)	100 (74%)	27 (20%)	9 (7%)	1 13
9	I	125/128 (98%)	94 (75%)	18 (14%)	13 (10%)	0 7
10	J	96/104 (92%)	61 (64%)	19 (20%)	16 (17%)	0 2
11	K	117/129 (91%)	84 (72%)	25 (21%)	8 (7%)	1 13
12	L	123/135 (91%)	88 (72%)	23 (19%)	12 (10%)	0 7
13	M	123/126 (98%)	79 (64%)	26 (21%)	18 (15%)	0 3
14	N	58/60 (97%)	33 (57%)	14 (24%)	11 (19%)	0 2
15	O	86/88 (98%)	72 (84%)	11 (13%)	3 (4%)	3 27
16	P	81/88 (92%)	60 (74%)	18 (22%)	3 (4%)	3 26
17	Q	102/104 (98%)	82 (80%)	14 (14%)	6 (6%)	1 15
18	R	71/88 (81%)	56 (79%)	9 (13%)	6 (8%)	1 9
19	S	78/92 (85%)	47 (60%)	22 (28%)	9 (12%)	0 6
20	T	97/106 (92%)	71 (73%)	16 (16%)	10 (10%)	0 7
21	V	22/26 (85%)	17 (77%)	3 (14%)	2 (9%)	1 8
All	All	2357/2532 (93%)	1662 (70%)	467 (20%)	228 (10%)	0 7

All (228) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	17	PHE
2	B	24	TRP
2	B	38	GLY
2	B	225	ALA
2	B	232	PRO
3	C	15	THR
3	C	47	LEU
3	C	60	ALA
3	C	61	ALA
3	C	100	ALA
3	C	101	LEU
3	C	108	ASN
3	C	154	SER
3	C	157	ILE
3	C	179	ARG

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Mol	Chain	Res	Type
3	C	180	ALA
3	C	188	LEU
3	C	189	ALA
4	D	29	PRO
4	D	30	LYS
4	D	36	ARG
4	D	88	VAL
4	D	131	ARG
4	D	179	GLU
5	E	26	PHE
7	G	7	ALA
7	G	17	VAL
7	G	53	LYS
7	G	155	ARG
8	H	3	THR
8	H	24	THR
8	H	91	ARG
9	I	31	GLN
9	I	127	LYS
10	J	32	ALA
10	J	54	PHE
10	J	57	LYS
10	J	60	ARG
10	J	82	ILE
10	J	86	MET
11	K	35	PRO
11	K	127	LYS
12	L	28	LYS
12	L	51	ALA
12	L	91	LYS
12	L	92	ASP
12	L	127	GLU
13	M	11	ARG
13	M	67	GLU
13	M	106	ASN
14	N	4	LYS
14	N	33	VAL
14	N	35	ARG
15	O	73	GLU
16	P	64	ALA
17	Q	69	LYS
18	R	26	LEU

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Mol	Chain	Res	Type
19	S	6	LYS
19	S	9	VAL
19	S	30	LEU
20	T	11	SER
20	T	73	HIS
2	B	74	LYS
2	B	76	GLN
2	B	95	GLN
2	B	131	PRO
2	B	168	THR
2	B	204	ASN
2	B	207	ALA
2	B	208	ILE
2	B	238	LEU
3	C	4	LYS
3	C	29	TYR
3	C	54	ARG
3	C	55	VAL
3	C	66	VAL
3	C	84	ILE
3	C	156	ARG
3	C	158	GLY
3	C	159	GLY
3	C	181	ASN
4	D	5	ILE
4	D	96	LEU
4	D	138	TYR
4	D	166	LYS
4	D	177	ASP
8	H	111	ILE
8	H	134	ILE
9	I	94	ALA
9	I	101	PHE
9	I	118	LYS
10	J	34	VAL
10	J	35	SER
10	J	36	GLY
10	J	51	ARG
10	J	72	VAL
10	J	84	GLN
11	K	27	ASN
11	K	76	GLY

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Mol	Chain	Res	Type
12	L	27	LEU
12	L	79	GLU
12	L	87	GLY
12	L	106	ASP
13	M	4	ILE
13	M	7	VAL
13	M	23	TYR
13	M	63	THR
13	M	124	PRO
14	N	50	LYS
15	O	88	ARG
16	P	76	GLN
17	Q	49	GLU
17	Q	80	GLY
18	R	38	GLU
18	R	54	ARG
20	T	50	GLU
20	T	96	GLY
20	T	102	GLY
20	T	103	GLY
21	V	3	LYS
2	B	20	GLU
2	B	52	GLU
2	B	123	ALA
2	B	155	LEU
2	B	191	ASP
2	B	195	ASP
2	B	227	GLY
3	C	16	ARG
3	C	32	LEU
3	C	168	ALA
4	D	25	ARG
4	D	99	SER
4	D	151	LYS
6	F	39	LYS
6	F	44	GLY
7	G	31	MET
7	G	149	ARG
9	I	55	ALA
9	I	119	ALA
10	J	78	ASN
10	J	90	LEU

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Mol	Chain	Res	Type
11	K	13	GLN
11	K	78	GLN
12	L	115	LYS
13	M	24	GLY
13	M	68	GLY
13	M	97	PRO
13	M	116	THR
14	N	10	ALA
14	N	34	TYR
18	R	19	LYS
18	R	87	ARG
19	S	14	HIS
20	T	94	ALA
21	V	6	ARG
2	B	11	LEU
2	B	15	VAL
2	B	21	ARG
3	C	38	ARG
3	C	98	ASN
3	C	206	GLU
4	D	85	LYS
4	D	159	ARG
5	E	27	ARG
6	F	96	PRO
7	G	42	ILE
8	H	82	HIS
9	I	24	GLY
9	I	81	ILE
9	I	121	ARG
10	J	27	ALA
10	J	76	ASN
11	K	15	ALA
12	L	56	ALA
13	M	38	GLY
13	M	118	ALA
13	M	125	ARG
14	N	32	SER
14	N	36	PHE
14	N	38	GLY
16	P	57	ARG
17	Q	34	LYS
17	Q	98	LEU

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Mol	Chain	Res	Type
19	S	39	THR
19	S	69	HIS
20	T	98	PRO
2	B	75	LYS
2	B	113	HIS
2	B	116	GLU
2	B	151	GLY
2	B	181	PHE
2	B	183	PRO
3	C	116	VAL
3	C	146	ALA
4	D	3	ARG
4	D	171	GLY
5	E	107	ARG
9	I	34	ASN
9	I	78	LYS
12	L	116	SER
13	M	21	TYR
15	O	46	HIS
19	S	53	ASN
2	B	228	GLY
4	D	16	GLY
4	D	40	PRO
6	F	98	LEU
17	Q	97	SER
18	R	63	GLN
19	S	31	ILE
20	T	9	ASN
20	T	97	ALA
7	G	81	GLY
8	H	83	ILE
13	M	123	ALA
14	N	51	GLY
2	B	91	PRO
9	I	89	ASN
13	M	6	GLY
3	C	7	PRO
3	C	195	VAL
4	D	178	VAL
8	H	67	PRO
8	H	73	ASP
7	G	9	VAL

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Mol	Chain	Res	Type
11	K	90	GLY
14	N	56	VAL
19	S	59	PRO

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%)	177 (88%)	25 (12%)	4 23
3	C	160/188 (85%)	136 (85%)	24 (15%)	3 17
4	D	180/180 (100%)	157 (87%)	23 (13%)	4 22
5	E	115/122 (94%)	102 (89%)	13 (11%)	6 27
6	F	90/90 (100%)	84 (93%)	6 (7%)	16 48
7	G	126/126 (100%)	112 (89%)	14 (11%)	6 28
8	H	119/119 (100%)	105 (88%)	14 (12%)	5 25
9	I	98/99 (99%)	89 (91%)	9 (9%)	9 36
10	J	88/91 (97%)	77 (88%)	11 (12%)	4 23
11	K	90/99 (91%)	84 (93%)	6 (7%)	16 48
12	L	104/111 (94%)	94 (90%)	10 (10%)	8 34
13	M	100/101 (99%)	90 (90%)	10 (10%)	7 32
14	N	49/49 (100%)	44 (90%)	5 (10%)	7 32
15	O	79/79 (100%)	73 (92%)	6 (8%)	13 43
16	P	72/74 (97%)	62 (86%)	10 (14%)	3 20
17	Q	96/96 (100%)	84 (88%)	12 (12%)	4 23
18	R	64/77 (83%)	58 (91%)	6 (9%)	8 35
19	S	71/79 (90%)	64 (90%)	7 (10%)	8 33
20	T	76/82 (93%)	70 (92%)	6 (8%)	12 41
21	V	19/21 (90%)	19 (100%)	0	100 100
All	All	1998/2103 (95%)	1781 (89%)	217 (11%)	6 29

All (217) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	8	LYS
2	B	21	ARG
2	B	23	ARG
2	B	24	TRP
2	B	25	ASN
2	B	49	GLU
2	B	52	GLU
2	B	58	ILE
2	B	71	VAL
2	B	76	GLN
2	B	82	ARG
2	B	84	GLU
2	B	90	MET
2	B	92	TYR
2	B	98	LEU
2	B	117	GLU
2	B	118	LEU
2	B	144	ARG
2	B	154	LEU
2	B	156	LYS
2	B	176	GLU
2	B	178	ARG
2	B	187	LEU
2	B	215	LEU
2	B	231	GLU
3	C	3	ASN
3	C	5	ILE
3	C	17	ASP
3	C	26	LYS
3	C	29	TYR
3	C	39	ILE
3	C	40	ARG
3	C	52	LEU
3	C	59	ARG
3	C	79	ARG
3	C	93	LYS
3	C	95	THR
3	C	101	LEU
3	C	102	ASN
3	C	156	ARG
3	C	162	GLN
3	C	165	THR

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Mol	Chain	Res	Type
3	C	167	TRP
3	C	175	LEU
3	C	179	ARG
3	C	190	ARG
3	C	191	THR
3	C	195	VAL
3	C	204	LEU
4	D	9	CYS
4	D	10	ARG
4	D	11	LEU
4	D	12	CYS
4	D	15	GLU
4	D	26	CYS
4	D	27	TYR
4	D	29	PRO
4	D	50	ARG
4	D	62	GLN
4	D	74	GLN
4	D	80	GLU
4	D	106	TYR
4	D	110	PHE
4	D	112	VAL
4	D	122	ARG
4	D	127	THR
4	D	144	ASP
4	D	153	ARG
4	D	155	LEU
4	D	157	LEU
4	D	199	ASN
4	D	201	GLN
5	E	12	LEU
5	E	41	VAL
5	E	43	LEU
5	E	47	LYS
5	E	64	ARG
5	E	79	GLU
5	E	98	THR
5	E	100	VAL
5	E	101	ILE
5	E	116	THR
5	E	126	ARG
5	E	147	ASP

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Mol	Chain	Res	Type
5	E	150	ARG
6	F	1	MET
6	F	10	LEU
6	F	28	ARG
6	F	30	LEU
6	F	74	ASP
6	F	100	ASN
7	G	8	GLU
7	G	11	GLN
7	G	37	ASN
7	G	50	ILE
7	G	75	VAL
7	G	78	ARG
7	G	113	GLU
7	G	114	ARG
7	G	126	ASP
7	G	136	LYS
7	G	140	ASP
7	G	142	GLU
7	G	144	MET
7	G	149	ARG
8	H	19	VAL
8	H	26	VAL
8	H	67	PRO
8	H	80	ILE
8	H	81	HIS
8	H	84	ARG
8	H	85	ARG
8	H	88	LYS
8	H	91	ARG
8	H	92	ARG
8	H	105	ARG
8	H	107	LEU
8	H	119	LEU
8	H	127	LEU
9	I	3	GLN
9	I	23	ASN
9	I	38	GLN
9	I	65	VAL
9	I	79	LEU
9	I	102	LEU
9	I	104	ARG

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Mol	Chain	Res	Type
9	I	114	TYR
9	I	127	LYS
10	J	4	ILE
10	J	6	ILE
10	J	21	GLN
10	J	29	ARG
10	J	45	ARG
10	J	57	LYS
10	J	60	ARG
10	J	65	LEU
10	J	71	LEU
10	J	79	ARG
10	J	86	MET
11	K	29	ILE
11	K	35	PRO
11	K	54	ARG
11	K	84	VAL
11	K	93	GLN
11	K	109	VAL
12	L	15	ARG
12	L	23	LYS
12	L	41	ARG
12	L	53	ARG
12	L	81	SER
12	L	89	ARG
12	L	93	LEU
12	L	113	ARG
12	L	122	THR
12	L	126	LYS
13	M	3	ARG
13	M	12	ASN
13	M	80	ARG
13	M	98	VAL
13	M	102	ARG
13	M	108	ARG
13	M	110	ARG
13	M	121	LYS
13	M	124	PRO
13	M	125	ARG
14	N	3	ARG
14	N	12	ARG
14	N	16	PHE

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Mol	Chain	Res	Type
14	N	23	ARG
14	N	44	LEU
15	O	6	GLU
15	O	10	LYS
15	O	14	GLU
15	O	26	GLU
15	O	31	LEU
15	O	45	VAL
16	P	2	VAL
16	P	8	ARG
16	P	20	VAL
16	P	22	THR
16	P	45	THR
16	P	51	VAL
16	P	53	VAL
16	P	62	VAL
16	P	67	THR
16	P	81	ARG
17	Q	26	GLN
17	Q	34	LYS
17	Q	36	ILE
17	Q	38	ARG
17	Q	48	GLU
17	Q	68	ARG
17	Q	70	ARG
17	Q	78	GLU
17	Q	93	GLN
17	Q	96	GLN
17	Q	98	LEU
17	Q	101	ARG
18	R	26	LEU
18	R	28	GLU
18	R	54	ARG
18	R	55	ARG
18	R	69	THR
18	R	88	LYS
19	S	3	ARG
19	S	7	LYS
19	S	15	LEU
19	S	17	GLU
19	S	20	LEU
19	S	65	ASN

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Mol	Chain	Res	Type
19	S	78	ARG
20	T	10	LEU
20	T	25	ARG
20	T	62	LEU
20	T	64	ASP
20	T	68	LYS
20	T	73	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	25	ASN
2	B	37	ASN
2	B	78	GLN
2	B	95	GLN
2	B	113	HIS
2	B	135	GLN
2	B	224	GLN
2	B	240	GLN
3	C	69	HIS
3	C	102	ASN
3	C	107	GLN
3	C	110	ASN
3	C	123	GLN
3	C	139	GLN
3	C	162	GLN
3	C	170	GLN
4	D	62	GLN
4	D	74	GLN
4	D	77	ASN
4	D	123	HIS
4	D	199	ASN
5	E	20	GLN
5	E	65	ASN
5	E	130	ASN
6	F	13	ASN
6	F	16	GLN
6	F	18	GLN
6	F	27	GLN
6	F	32	ASN
6	F	57	GLN
6	F	94	GLN

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Mol	Chain	Res	Type
7	G	28	ASN
7	G	37	ASN
7	G	56	GLN
7	G	64	GLN
7	G	68	ASN
7	G	106	GLN
7	G	148	ASN
9	I	3	GLN
9	I	23	ASN
9	I	73	GLN
10	J	13	HIS
10	J	78	ASN
11	K	13	GLN
11	K	62	GLN
11	K	104	GLN
11	K	117	ASN
12	L	49	ASN
12	L	75	HIS
13	M	40	ASN
13	M	62	ASN
14	N	49	HIS
15	O	13	GLN
15	O	37	ASN
16	P	76	GLN
16	P	82	GLN
17	Q	16	GLN
17	Q	93	GLN
17	Q	94	ASN
19	S	14	HIS
19	S	23	ASN
19	S	65	ASN
20	T	75	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1508/1522 (99%)	250 (16%)	30 (1%)
22	W	5/6 (83%)	1 (20%)	0
23	Z	14/15 (93%)	10 (71%)	3 (21%)
All	All	1527/1543 (98%)	261 (17%)	33 (2%)

All (261) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	G
1	A	7	G
1	A	9	G
1	A	30	U
1	A	31	G
1	A	32	A
1	A	39	G
1	A	47	C
1	A	48	C
1	A	51	A
1	A	52	G
1	A	55	A
1	A	60	A
1	A	61	G
1	A	62	U
1	A	65	U
1	A	66	G
1	A	81	U
1	A	109	A
1	A	119	A
1	A	120	A
1	A	121	C
1	A	129(A)	G
1	A	130	A
1	A	131	C
1	A	156	G
1	A	164	U
1	A	189(F)	U
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	224	C
1	A	232	G
1	A	244	U
1	A	245	C
1	A	247	G
1	A	250	A
1	A	251	G
1	A	266	G

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Mol	Chain	Res	Type
1	A	267	C
1	A	274	A
1	A	275	G
1	A	280	C
1	A	289	G
1	A	306	G
1	A	321	A
1	A	328	C
1	A	329	A
1	A	343	U
1	A	345	C
1	A	346	G
1	A	347	G
1	A	351	G
1	A	352	C
1	A	354	G
1	A	367	U
1	A	369	C
1	A	372	C
1	A	373	A
1	A	390	C
1	A	397	A
1	A	406	G
1	A	410	G
1	A	411	A
1	A	412	A
1	A	414	A
1	A	418	C
1	A	419	C
1	A	421	U
1	A	422	C
1	A	428	G
1	A	429	U
1	A	430	A
1	A	448	A
1	A	452	A
1	A	470	C
1	A	479	C
1	A	485	G
1	A	486	U
1	A	498	U
1	A	500	G

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Mol	Chain	Res	Type
1	A	510	A
1	A	511	C
1	A	512	U
1	A	518	C
1	A	527	G
1	A	532	A
1	A	533	A
1	A	547	A
1	A	548	G
1	A	559	A
1	A	567	G
1	A	568	G
1	A	572	A
1	A	573	A
1	A	576	G
1	A	588	G
1	A	620	C
1	A	653	A
1	A	665	A
1	A	686	U
1	A	688	G
1	A	721	G
1	A	722	A
1	A	733	A
1	A	749	C
1	A	750	G
1	A	755	G
1	A	777	A
1	A	794	A
1	A	817	C
1	A	839	U
1	A	840	C
1	A	841	U
1	A	859	A
1	A	872	A
1	A	885	G
1	A	889	A
1	A	890	G
1	A	914	A
1	A	926	G
1	A	927	G
1	A	934	C

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Mol	Chain	Res	Type
1	A	935	A
1	A	960	U
1	A	966	G
1	A	969	A
1	A	971	G
1	A	974	A
1	A	975	A
1	A	976	G
1	A	977	A
1	A	982	U
1	A	992	U
1	A	993	G
1	A	994	A
1	A	997	U
1	A	998	G
1	A	999	C
1	A	1001	A
1	A	1001(A)	G
1	A	1003	G
1	A	1004	A
1	A	1027	C
1	A	1029	C
1	A	1030	C
1	A	1030(A)	G
1	A	1034	G
1	A	1048	G
1	A	1054	C
1	A	1068	G
1	A	1081	G
1	A	1094	G
1	A	1095	U
1	A	1101	A
1	A	1102	A
1	A	1104	G
1	A	1114	C
1	A	1118	C
1	A	1119	C
1	A	1122	U
1	A	1125	U
1	A	1126	U
1	A	1129	C
1	A	1130	A

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Mol	Chain	Res	Type
1	A	1131	G
1	A	1136	U
1	A	1137	C
1	A	1139	G
1	A	1146	A
1	A	1148	U
1	A	1156	G
1	A	1157	A
1	A	1158	C
1	A	1159	U
1	A	1181	G
1	A	1182	G
1	A	1183	A
1	A	1184	G
1	A	1196	U
1	A	1197	G
1	A	1198	G
1	A	1202	G
1	A	1209	C
1	A	1211	U
1	A	1212	U
1	A	1213	A
1	A	1214	C
1	A	1215	G
1	A	1225	A
1	A	1227	A
1	A	1238	A
1	A	1241	G
1	A	1245	A
1	A	1248	A
1	A	1250	A
1	A	1256	A
1	A	1257	U
1	A	1267	C
1	A	1272	G
1	A	1278	U
1	A	1279	A
1	A	1280	A
1	A	1281	U
1	A	1282	C
1	A	1287	A
1	A	1297	C

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Mol	Chain	Res	Type
1	A	1298	C
1	A	1300	G
1	A	1301	U
1	A	1302	U
1	A	1305	G
1	A	1306	A
1	A	1311	G
1	A	1320	C
1	A	1323	G
1	A	1336	C
1	A	1338	G
1	A	1346	A
1	A	1363	C
1	A	1363(A)	A
1	A	1364	U
1	A	1379	G
1	A	1381	U
1	A	1386	G
1	A	1401	G
1	A	1442	G
1	A	1442(A)	G
1	A	1442(B)	A
1	A	1452	C
1	A	1456	G
1	A	1474	G
1	A	1475	G
1	A	1485	U
1	A	1492	A
1	A	1494	G
1	A	1497	G
1	A	1499	A
1	A	1503	A
1	A	1506	U
1	A	1517	G
1	A	1520	G
1	A	1525	G
1	A	1529	G
1	A	1530	G
1	A	1542	U
22	W	5	A
23	Z	29	G
23	Z	30	G

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Mol	Chain	Res	Type
23	Z	31	A
23	Z	32	U
23	Z	34	G
23	Z	38	A
23	Z	39	U
23	Z	40	C
23	Z	41	C
23	Z	42	C

All (33) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	30	U
1	A	51	A
1	A	119	A
1	A	197	A
1	A	243	A
1	A	250	A
1	A	279	A
1	A	372	C
1	A	410	G
1	A	428	G
1	A	429	U
1	A	485	G
1	A	496	A
1	A	793	U
1	A	871	U
1	A	974	A
1	A	975	A
1	A	992	U
1	A	1001	A
1	A	1101	A
1	A	1145	C
1	A	1181	G
1	A	1182	G
1	A	1196	U
1	A	1201	A
1	A	1281	U
1	A	1305	G
1	A	1363(A)	A
1	A	1447	A
1	A	1452	C

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Mol	Chain	Res	Type
23	Z	30	G
23	Z	39	U
23	Z	40	C

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 225 ligands modelled in this entry, 220 are monoatomic - leaving 5 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	$\#\|Z\| > 2$
26	AM2	A	3003	-	40,40,40	0.92	2 (5%)	53,60,60	0.90	1 (1%)
26	AM2	A	3002	-	40,40,40	0.98	2 (5%)	53,60,60	0.87	1 (1%)
26	AM2	A	3005	-	40,40,40	0.92	1 (2%)	53,60,60	0.80	1 (1%)
26	AM2	A	3004	-	40,40,40	0.88	0	53,60,60	0.85	1 (1%)
26	AM2	A	3001	-	40,40,40	0.87	1 (2%)	53,60,60	1.16	2 (3%)

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
26	AM2	A	3003	-	-	1/12/84/84	0/4/4/4
26	AM2	A	3002	-	-	3/12/84/84	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	AM2	A	3005	-	-	4/12/84/84	0/4/4/4
26	AM2	A	3004	-	-	2/12/84/84	0/4/4/4
26	AM2	A	3001	-	-	2/12/84/84	0/4/4/4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	3002	AM2	OB1-CB1	2.47	1.48	1.41
26	A	3003	AM2	CB5-CB4	2.10	1.56	1.52
26	A	3001	AM2	OB1-CB1	2.06	1.47	1.41
26	A	3005	AM2	OB1-CB1	2.05	1.47	1.41
26	A	3002	AM2	OA4-CA1	2.03	1.47	1.41
26	A	3003	AM2	OB1-CB1	2.01	1.47	1.41

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	A	3001	AM2	CA9-NA7-CA7	6.70	124.14	114.38
26	A	3003	AM2	CA9-NA7-CA7	5.19	121.94	114.38
26	A	3004	AM2	CA9-NA7-CA7	4.75	121.30	114.38
26	A	3005	AM2	CA9-NA7-CA7	4.17	120.46	114.38
26	A	3002	AM2	CA9-NA7-CA7	4.04	120.26	114.38
26	A	3001	AM2	CA1-OA1-CC1	-2.43	111.96	117.96

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
26	A	3001	AM2	CA8-CA7-NA7-CA9
26	A	3002	AM2	CA8-CA7-NA7-CA9
26	A	3005	AM2	CC6-CC1-OA1-CA1
26	A	3002	AM2	OB1-CB5-CB6-OB6
26	A	3004	AM2	OB1-CB5-CB6-OB6
26	A	3003	AM2	OB1-CB5-CB6-OB6
26	A	3001	AM2	OB1-CB5-CB6-OB6
26	A	3005	AM2	OB1-CB5-CB6-OB6
26	A	3002	AM2	CA6-CA7-NA7-CA9
26	A	3004	AM2	CA8-CA7-NA7-CA9
26	A	3005	AM2	CA8-CA7-NA7-CA9
26	A	3005	AM2	CA2-CA1-OA1-CC1

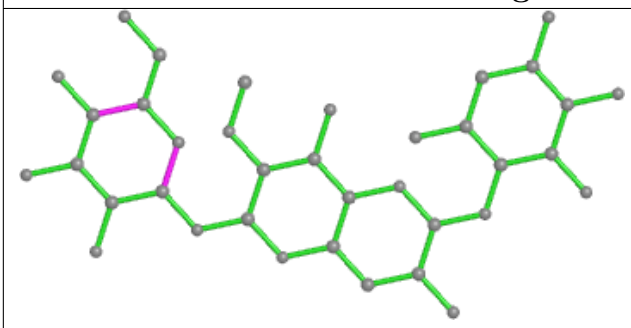
There are no ring outliers.

3 monomers are involved in 9 short contacts:

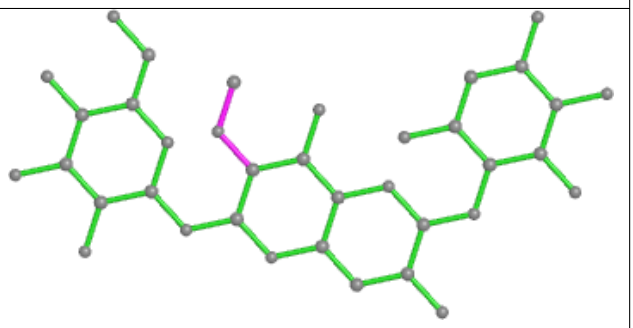
Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	A	3002	AM2	2	0
26	A	3005	AM2	5	0
26	A	3001	AM2	2	0

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.

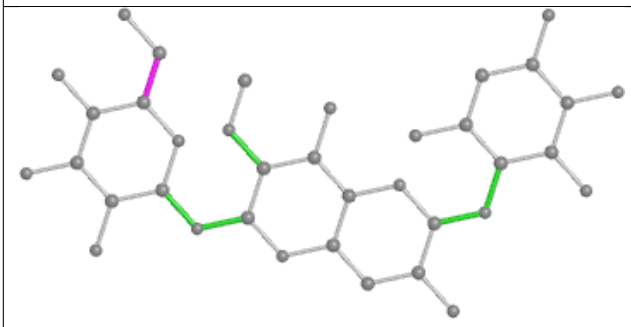
Ligand AM2 A 3003



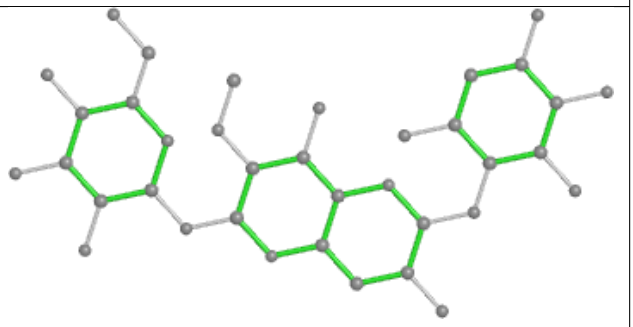
Bond lengths



Bond angles

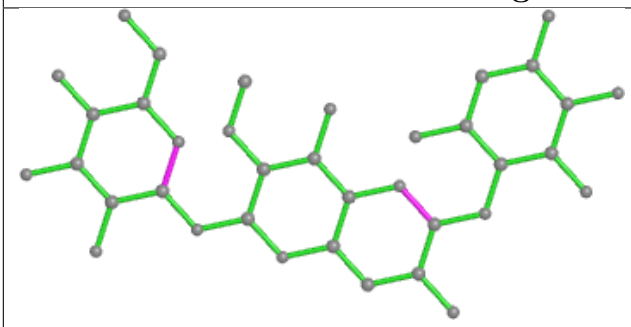


Torsions

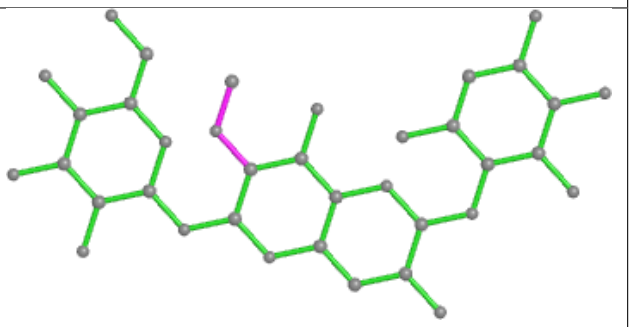


Rings

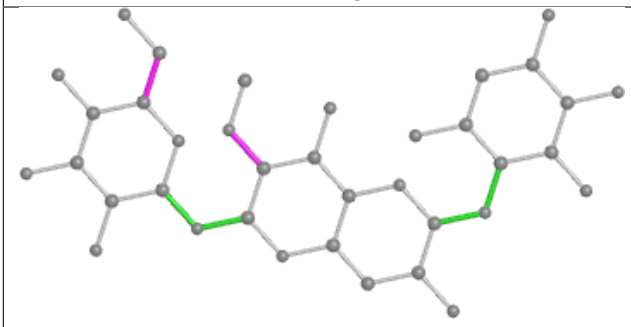
Ligand AM2 A 3002



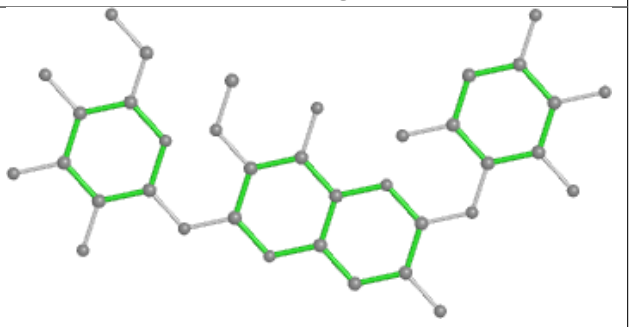
Bond lengths



Bond angles

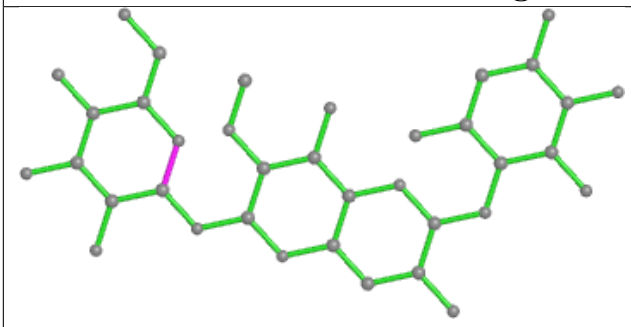


Torsions

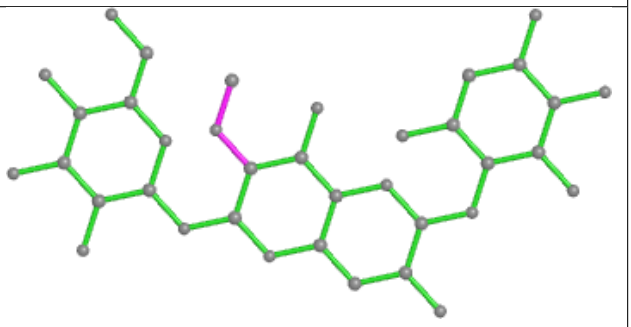


Rings

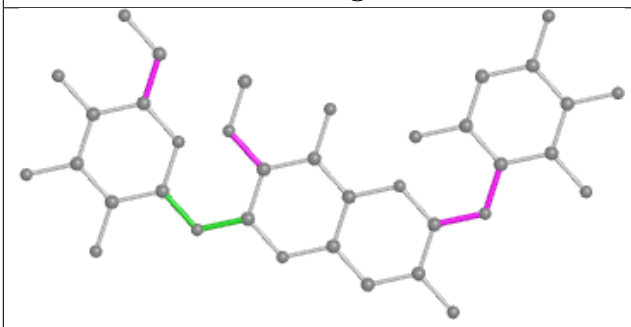
Ligand AM2 A 3005



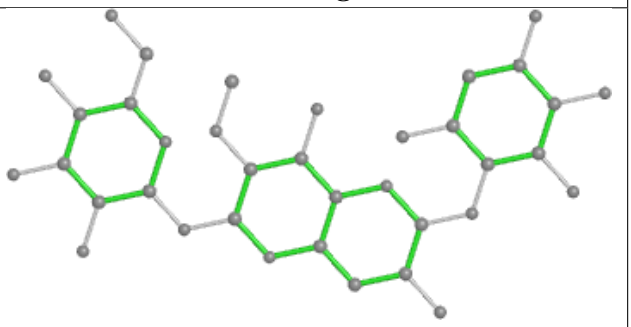
Bond lengths



Bond angles

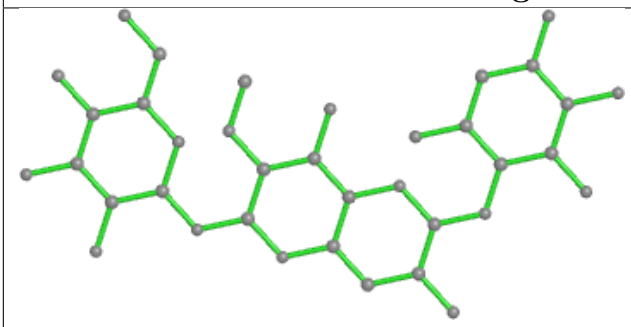


Torsions

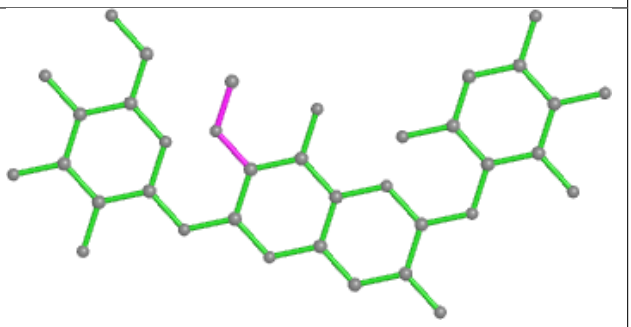


Rings

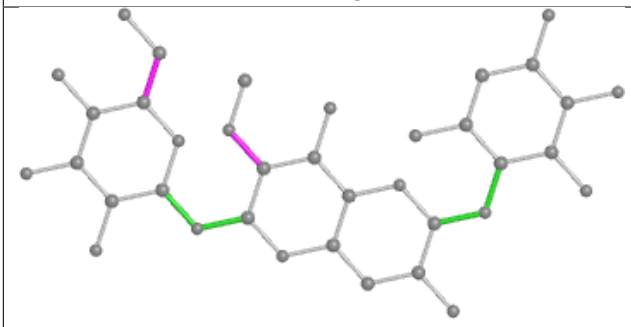
Ligand AM2 A 3004



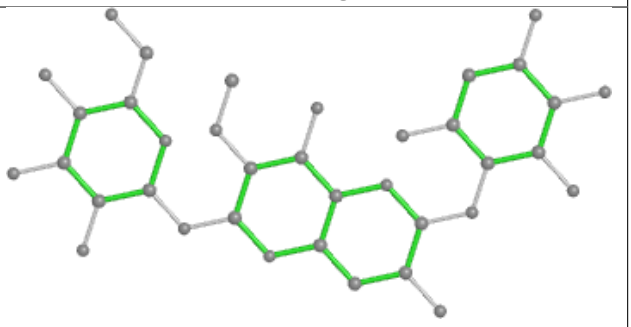
Bond lengths



Bond angles

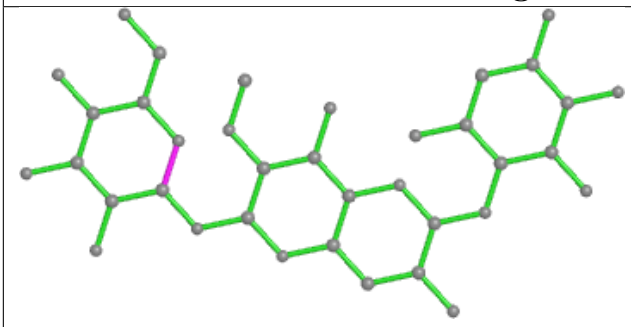


Torsions

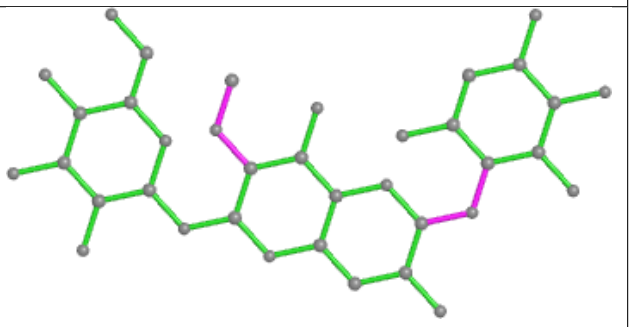


Rings

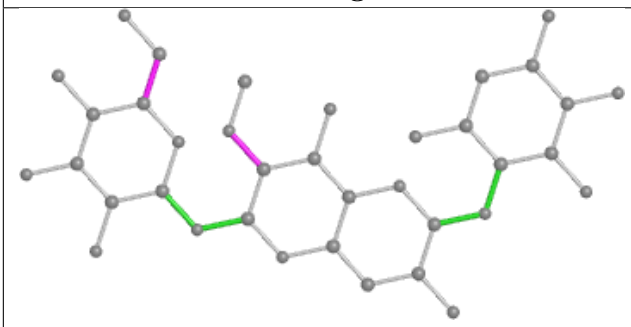
Ligand AM2 A 3001



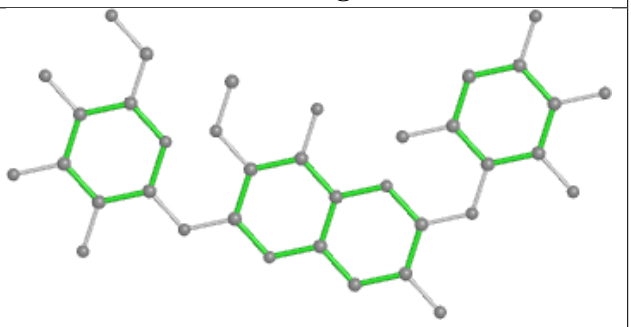
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	1510/1522 (99%)	-0.12	4 (0%) 94 91	82, 115, 181, 202	0
2	B	234/256 (91%)	-0.16	5 (2%) 63 58	84, 153, 190, 202	0
3	C	206/239 (86%)	-0.28	1 (0%) 91 88	86, 139, 185, 202	0
4	D	208/208 (100%)	-0.23	8 (3%) 40 36	90, 133, 184, 202	0
5	E	150/161 (93%)	-0.27	0 100 100	83, 108, 153, 196	0
6	F	101/101 (100%)	-0.35	0 100 100	104, 143, 177, 186	0
7	G	155/155 (100%)	-0.47	1 (0%) 89 86	89, 131, 186, 202	0
8	H	138/138 (100%)	-0.39	0 100 100	76, 105, 141, 163	0
9	I	127/128 (99%)	-0.17	1 (0%) 86 81	89, 144, 178, 202	0
10	J	98/104 (94%)	0.77	17 (17%) 1 1	97, 168, 202, 202	0
11	K	119/129 (92%)	-0.13	2 (1%) 70 64	79, 113, 161, 197	0
12	L	125/135 (92%)	-0.27	2 (1%) 72 66	74, 108, 155, 202	0
13	M	125/126 (99%)	0.23	9 (7%) 15 15	100, 133, 171, 200	0
14	N	60/60 (100%)	0.03	2 (3%) 46 41	93, 136, 178, 198	0
15	O	88/88 (100%)	-0.20	0 100 100	78, 123, 166, 192	0
16	P	83/88 (94%)	-0.38	0 100 100	79, 105, 138, 196	0
17	Q	104/104 (100%)	-0.15	4 (3%) 40 36	78, 106, 161, 202	0
18	R	73/88 (82%)	-0.16	5 (6%) 17 16	93, 130, 184, 196	0
19	S	80/92 (86%)	-0.13	0 100 100	103, 152, 188, 202	0
20	T	99/106 (93%)	-0.27	1 (1%) 82 77	80, 112, 164, 200	0
21	V	24/26 (92%)	0.76	2 (8%) 11 12	82, 126, 160, 173	0
22	W	6/6 (100%)	0.82	1 (16%) 1 2	112, 125, 180, 197	0
23	Z	15/15 (100%)	0.49	1 (6%) 17 16	97, 137, 200, 202	0
All	All	3928/4075 (96%)	-0.15	66 (1%) 70 64	74, 123, 184, 202	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	M	123	ALA	10.1
10	J	33	GLN	9.7
13	M	124	PRO	8.3
13	M	121	LYS	7.8
11	K	128	ALA	6.8
13	M	122	LYS	6.7
1	A	1001(A)	G	6.6
17	Q	105	ALA	6.4
13	M	125	ARG	6.3
10	J	34	VAL	6.3
13	M	126	LYS	6.0
2	B	130	ARG	5.9
17	Q	104	LYS	5.6
10	J	74	ILE	5.4
10	J	32	ALA	5.2
2	B	131	PRO	4.9
13	M	120	LYS	4.7
11	K	129	SER	4.0
12	L	19	ARG	3.9
2	B	134	GLU	3.8
10	J	72	VAL	3.8
10	J	20	ALA	3.7
4	D	37	PRO	3.6
7	G	81	GLY	3.6
17	Q	103	GLY	3.3
10	J	73	ASP	3.3
2	B	132	LYS	3.3
20	T	103	GLY	3.2
4	D	35	ARG	3.1
2	B	133	LYS	2.9
10	J	35	SER	2.8
18	R	17	SER	2.8
9	I	128	ARG	2.8
10	J	75	ILE	2.7
21	V	22	ARG	2.7
14	N	12	ARG	2.7
22	W	6	A	2.6
10	J	36	GLY	2.6
13	M	7	VAL	2.5
4	D	33	MET	2.5
10	J	28	ARG	2.4
3	C	161	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
4	D	38	TYR	2.4
23	Z	39	U	2.4
10	J	6	ILE	2.4
12	L	129	ALA	2.4
1	A	202	U	2.4
4	D	42	GLN	2.3
10	J	3	LYS	2.3
10	J	4	ILE	2.3
4	D	36	ARG	2.3
10	J	5	ARG	2.3
4	D	43	HIS	2.2
4	D	44	GLY	2.2
18	R	48	GLY	2.2
18	R	18	ARG	2.2
18	R	16	PRO	2.2
21	V	18	TYR	2.2
10	J	31	GLY	2.2
18	R	88	LYS	2.1
13	M	118	ALA	2.1
14	N	13	THR	2.1
1	A	1531	A	2.0
1	A	1006	C	2.0
17	Q	101	ARG	2.0
10	J	24	VAL	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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
24	MG	A	2550	1/1	0.03	0.85	105,105,105,105	0
24	MG	A	2596	1/1	0.20	0.37	105,105,105,105	0
24	MG	A	2618	1/1	0.21	0.48	97,97,97,97	0
24	MG	A	2721	1/1	0.23	0.15	174,174,174,174	1
25	K	A	2680	1/1	0.26	0.82	180,180,180,180	0
24	MG	A	2557	1/1	0.27	0.55	110,110,110,110	0
24	MG	A	2613	1/1	0.31	0.51	89,89,89,89	0
24	MG	A	2554	1/1	0.34	1.30	134,134,134,134	0
25	K	A	2672	1/1	0.36	0.57	159,159,159,159	0
24	MG	A	2684	1/1	0.37	0.71	88,88,88,88	0
24	MG	A	2548	1/1	0.40	1.58	114,114,114,114	0
24	MG	A	2549	1/1	0.40	0.51	103,103,103,103	0
24	MG	A	2600	1/1	0.42	0.70	93,93,93,93	0
24	MG	A	2601	1/1	0.43	0.39	105,105,105,105	0
24	MG	A	2555	1/1	0.44	0.59	129,129,129,129	0
24	MG	A	2631	1/1	0.47	0.62	96,96,96,96	0
24	MG	A	2701	1/1	0.47	0.82	85,85,85,85	0
25	K	A	2679	1/1	0.47	0.30	126,126,126,126	0
24	MG	A	2716	1/1	0.47	0.85	122,122,122,122	0
24	MG	A	2715	1/1	0.48	0.39	113,113,113,113	0
24	MG	A	2661	1/1	0.50	0.51	107,107,107,107	0
25	K	A	2675	1/1	0.50	1.02	143,143,143,143	0
24	MG	A	2552	1/1	0.56	0.27	84,84,84,84	0
24	MG	A	2687	1/1	0.57	0.72	114,114,114,114	0
24	MG	A	2626	1/1	0.57	1.64	102,102,102,102	0
24	MG	A	2634	1/1	0.57	0.42	86,86,86,86	0
25	K	A	2671	1/1	0.58	0.34	117,117,117,117	0
25	K	A	2681	1/1	0.58	0.18	140,140,140,140	0
24	MG	A	2708	1/1	0.60	0.59	105,105,105,105	0
25	K	A	2670	1/1	0.60	0.55	147,147,147,147	0
24	MG	A	2696	1/1	0.61	0.69	92,92,92,92	0
24	MG	A	2735	1/1	0.62	0.54	98,98,98,98	1
24	MG	A	2563	1/1	0.63	0.87	87,87,87,87	0
24	MG	A	2584	1/1	0.65	0.41	108,108,108,108	0
24	MG	A	2663	1/1	0.65	0.57	88,88,88,88	0
24	MG	A	2722	1/1	0.66	0.72	93,93,93,93	0
24	MG	A	2580	1/1	0.66	0.87	76,76,76,76	0
24	MG	A	2689	1/1	0.66	1.22	101,101,101,101	0
24	MG	S	1143	1/1	0.67	0.68	115,115,115,115	0
25	K	A	2676	1/1	0.67	0.29	142,142,142,142	0
24	MG	A	2667	1/1	0.67	0.69	92,92,92,92	0
24	MG	A	2725	1/1	0.67	0.59	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
24	MG	A	2611	1/1	0.67	0.27	98,98,98,98	0
24	MG	A	2615	1/1	0.68	0.64	91,91,91,91	0
24	MG	A	2740	1/1	0.68	1.05	92,92,92,92	0
25	K	A	2678	1/1	0.68	0.29	131,131,131,131	0
24	MG	A	2562	1/1	0.69	0.40	108,108,108,108	0
24	MG	A	2565	1/1	0.69	0.44	77,77,77,77	0
24	MG	A	2741	1/1	0.71	0.64	105,105,105,105	0
24	MG	A	2744	1/1	0.71	0.61	90,90,90,90	0
24	MG	A	2714	1/1	0.72	0.59	92,92,92,92	0
24	MG	A	2609	1/1	0.72	0.66	94,94,94,94	0
24	MG	A	2698	1/1	0.72	0.79	115,115,115,115	0
24	MG	A	2621	1/1	0.72	0.39	105,105,105,105	0
24	MG	A	2683	1/1	0.72	0.59	116,116,116,116	0
24	MG	A	2662	1/1	0.73	0.68	109,109,109,109	0
25	K	A	2682	1/1	0.73	0.42	147,147,147,147	0
24	MG	A	2747	1/1	0.74	1.23	104,104,104,104	0
24	MG	A	2639	1/1	0.74	0.37	129,129,129,129	0
24	MG	A	2728	1/1	0.74	0.58	108,108,108,108	0
24	MG	A	2624	1/1	0.75	0.45	89,89,89,89	0
24	MG	A	2731	1/1	0.75	1.29	88,88,88,88	0
24	MG	A	2644	1/1	0.77	0.58	121,121,121,121	0
24	MG	A	2695	1/1	0.77	0.38	98,98,98,98	0
24	MG	A	2653	1/1	0.77	0.42	98,98,98,98	0
24	MG	H	1139	1/1	0.77	0.33	100,100,100,100	0
24	MG	A	2582	1/1	0.77	0.56	85,85,85,85	0
24	MG	A	2742	1/1	0.78	2.29	106,106,106,106	0
24	MG	A	2739	1/1	0.79	0.48	101,101,101,101	0
24	MG	A	2726	1/1	0.79	1.68	106,106,106,106	0
25	K	A	2674	1/1	0.80	0.19	133,133,133,133	0
24	MG	A	2641	1/1	0.80	0.28	98,98,98,98	0
24	MG	A	2629	1/1	0.80	0.72	78,78,78,78	0
24	MG	A	2688	1/1	0.80	2.29	109,109,109,109	0
24	MG	A	2553	1/1	0.81	0.40	69,69,69,69	0
24	MG	A	2569	1/1	0.81	0.92	83,83,83,83	0
24	MG	A	2589	1/1	0.81	0.15	93,93,93,93	0
24	MG	A	2593	1/1	0.81	0.20	112,112,112,112	0
24	MG	A	2617	1/1	0.81	0.97	72,72,72,72	0
24	MG	A	2575	1/1	0.81	0.61	108,108,108,108	0
24	MG	A	2576	1/1	0.81	0.31	83,83,83,83	0
24	MG	A	2651	1/1	0.81	0.27	78,78,78,78	0
24	MG	A	2724	1/1	0.81	1.35	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
24	MG	A	2551	1/1	0.81	0.28	121,121,121,121	0
24	MG	A	2625	1/1	0.81	1.07	81,81,81,81	0
25	K	A	2800	1/1	0.81	0.19	153,153,153,153	1
24	MG	A	2711	1/1	0.82	1.08	103,103,103,103	0
24	MG	A	2633	1/1	0.82	0.22	87,87,87,87	0
24	MG	A	2666	1/1	0.82	0.35	87,87,87,87	0
24	MG	A	2697	1/1	0.82	0.26	92,92,92,92	0
24	MG	A	2648	1/1	0.83	0.30	89,89,89,89	0
25	K	A	2673	1/1	0.83	0.57	126,126,126,126	0
24	MG	A	2577	1/1	0.83	0.60	94,94,94,94	0
24	MG	A	2743	1/1	0.83	1.72	121,121,121,121	0
24	MG	A	2590	1/1	0.83	0.92	76,76,76,76	0
24	MG	A	2566	1/1	0.83	0.40	91,91,91,91	0
24	MG	F	1102	1/1	0.83	0.15	128,128,128,128	0
24	MG	A	2630	1/1	0.83	0.21	99,99,99,99	0
24	MG	A	2720	1/1	0.83	1.42	128,128,128,128	0
24	MG	A	2699	1/1	0.83	0.29	88,88,88,88	0
24	MG	A	2608	1/1	0.83	0.23	106,106,106,106	0
24	MG	A	2581	1/1	0.84	0.45	69,69,69,69	0
24	MG	A	2692	1/1	0.84	0.30	69,69,69,69	0
24	MG	A	2604	1/1	0.84	0.38	89,89,89,89	0
24	MG	A	2745	1/1	0.84	0.64	101,101,101,101	0
24	MG	A	2700	1/1	0.84	0.52	115,115,115,115	0
24	MG	A	2660	1/1	0.84	0.17	128,128,128,128	0
24	MG	A	2719	1/1	0.84	1.21	96,96,96,96	0
24	MG	A	2594	1/1	0.85	0.41	100,100,100,100	0
24	MG	A	2664	1/1	0.85	0.58	97,97,97,97	0
24	MG	A	2558	1/1	0.85	1.70	74,74,74,74	0
24	MG	A	2646	1/1	0.85	0.26	96,96,96,96	0
24	MG	A	2606	1/1	0.86	0.39	83,83,83,83	0
24	MG	A	2636	1/1	0.86	0.20	92,92,92,92	0
24	MG	A	2598	1/1	0.86	0.56	60,60,60,60	0
24	MG	A	2658	1/1	0.86	0.14	121,121,121,121	0
24	MG	G	1158	1/1	0.86	0.35	112,112,112,112	1
24	MG	A	2603	1/1	0.87	0.72	135,135,135,135	0
24	MG	A	2713	1/1	0.87	0.43	104,104,104,104	0
24	MG	A	2619	1/1	0.87	0.71	82,82,82,82	0
24	MG	A	2642	1/1	0.87	0.47	101,101,101,101	0
24	MG	W	1008	1/1	0.87	0.52	157,157,157,157	1
24	MG	A	2597	1/1	0.87	0.21	80,80,80,80	0
24	MG	A	2717	1/1	0.87	0.29	99,99,99,99	0
24	MG	A	2559	1/1	0.87	0.34	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
24	MG	A	2710	1/1	0.87	0.33	99,99,99,99	0
24	MG	A	2723	1/1	0.88	1.24	79,79,79,79	0
24	MG	A	2595	1/1	0.88	0.94	112,112,112,112	0
24	MG	A	2622	1/1	0.88	0.31	73,73,73,73	0
24	MG	A	2614	1/1	0.88	0.18	83,83,83,83	0
24	MG	A	2637	1/1	0.88	0.21	110,110,110,110	0
24	MG	A	2605	1/1	0.88	0.24	79,79,79,79	0
24	MG	A	2632	1/1	0.88	0.44	89,89,89,89	0
24	MG	A	2703	1/1	0.88	0.83	101,101,101,101	0
24	MG	A	2705	1/1	0.88	0.26	104,104,104,104	0
24	MG	A	2665	1/1	0.88	0.33	89,89,89,89	0
24	MG	A	2654	1/1	0.88	0.48	112,112,112,112	1
24	MG	A	2655	1/1	0.89	0.33	76,76,76,76	0
24	MG	A	2561	1/1	0.89	0.61	66,66,66,66	0
25	K	V	1026	1/1	0.89	0.36	132,132,132,132	0
24	MG	A	2702	1/1	0.90	0.55	94,94,94,94	0
24	MG	A	2712	1/1	0.90	0.26	99,99,99,99	0
24	MG	A	2571	1/1	0.90	0.33	49,49,49,49	0
24	MG	A	2732	1/1	0.90	0.22	88,88,88,88	1
24	MG	A	2612	1/1	0.90	0.64	92,92,92,92	0
24	MG	A	2706	1/1	0.90	0.37	87,87,87,87	0
24	MG	A	2568	1/1	0.90	0.27	91,91,91,91	0
24	MG	A	2638	1/1	0.90	0.16	79,79,79,79	0
24	MG	A	2647	1/1	0.91	0.17	60,60,60,60	0
24	MG	A	2691	1/1	0.91	0.61	94,94,94,94	0
24	MG	A	2729	1/1	0.91	0.22	96,96,96,96	1
24	MG	A	2628	1/1	0.91	0.27	95,95,95,95	0
24	MG	A	2650	1/1	0.91	0.24	72,72,72,72	0
24	MG	A	2734	1/1	0.91	1.82	113,113,113,113	0
24	MG	A	2746	1/1	0.91	0.58	85,85,85,85	0
24	MG	A	2545	1/1	0.91	0.28	122,122,122,122	0
24	MG	A	2583	1/1	0.91	0.72	83,83,83,83	0
24	MG	A	2694	1/1	0.92	0.31	88,88,88,88	0
24	MG	A	2709	1/1	0.92	0.36	79,79,79,79	0
24	MG	A	2560	1/1	0.92	0.37	46,46,46,46	0
24	MG	A	2546	1/1	0.92	0.20	100,100,100,100	0
24	MG	A	2656	1/1	0.93	0.31	90,90,90,90	0
24	MG	A	2564	1/1	0.93	0.37	57,57,57,57	0
24	MG	L	1129	1/1	0.93	0.24	59,59,59,59	0
24	MG	A	2635	1/1	0.93	0.19	95,95,95,95	0
24	MG	A	2727	1/1	0.93	0.98	107,107,107,107	0
24	MG	A	2652	1/1	0.93	0.20	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
25	K	A	2677	1/1	0.93	0.33	117,117,117,117	0
26	AM2	A	3001	37/37	0.93	0.20	103,105,119,121	0
26	AM2	A	3002	37/37	0.93	0.42	116,119,127,128	0
26	AM2	A	3003	37/37	0.93	0.22	110,114,122,124	0
24	MG	A	2730	1/1	0.94	1.11	70,70,70,70	0
24	MG	A	2623	1/1	0.94	0.57	56,56,56,56	0
24	MG	A	2693	1/1	0.94	0.35	89,89,89,89	0
24	MG	A	2733	1/1	0.94	0.84	93,93,93,93	0
24	MG	A	2587	1/1	0.94	1.02	129,129,129,129	0
24	MG	A	2579	1/1	0.94	0.48	94,94,94,94	0
24	MG	A	2736	1/1	0.94	0.74	103,103,103,103	0
24	MG	A	2573	1/1	0.94	0.11	72,72,72,72	0
26	AM2	A	3004	37/37	0.94	0.25	130,133,141,143	0
26	AM2	A	3005	37/37	0.94	0.23	126,131,135,136	0
24	MG	G	1157	1/1	0.95	0.13	134,134,134,134	1
24	MG	A	2659	1/1	0.95	0.28	80,80,80,80	0
24	MG	A	2685	1/1	0.95	0.36	23,23,23,23	0
24	MG	J	1101	1/1	0.95	0.21	68,68,68,68	0
24	MG	A	2627	1/1	0.95	0.32	75,75,75,75	0
24	MG	A	2570	1/1	0.95	0.55	97,97,97,97	0
24	MG	A	2602	1/1	0.95	0.39	81,81,81,81	0
24	MG	A	2643	1/1	0.95	0.36	92,92,92,92	0
24	MG	A	2718	1/1	0.95	0.58	60,60,60,60	0
24	MG	A	2572	1/1	0.96	0.36	89,89,89,89	0
24	MG	A	2585	1/1	0.96	0.97	78,78,78,78	0
24	MG	A	2738	1/1	0.96	1.17	94,94,94,94	0
24	MG	A	2599	1/1	0.96	0.18	58,58,58,58	0
24	MG	A	2645	1/1	0.96	0.46	78,78,78,78	0
24	MG	D	1211	1/1	0.96	0.20	82,82,82,82	0
24	MG	Z	1043	1/1	0.96	0.16	123,123,123,123	0
24	MG	A	2567	1/1	0.96	0.29	69,69,69,69	0
24	MG	A	2690	1/1	0.96	0.14	56,56,56,56	0
24	MG	A	2737	1/1	0.97	0.69	61,61,61,61	0
24	MG	W	1007	1/1	0.97	0.06	81,81,81,81	0
24	MG	A	2574	1/1	0.97	0.20	2,2,2,2	0
24	MG	A	2686	1/1	0.97	0.27	140,140,140,140	0
24	MG	A	2620	1/1	0.97	0.09	89,89,89,89	1
24	MG	A	2704	1/1	0.97	0.36	94,94,94,94	0
24	MG	K	1130	1/1	0.97	0.12	69,69,69,69	0
24	MG	A	2657	1/1	0.97	0.09	132,132,132,132	0
24	MG	A	2707	1/1	0.98	0.22	78,78,78,78	0
24	MG	A	2610	1/1	0.98	0.81	75,75,75,75	0

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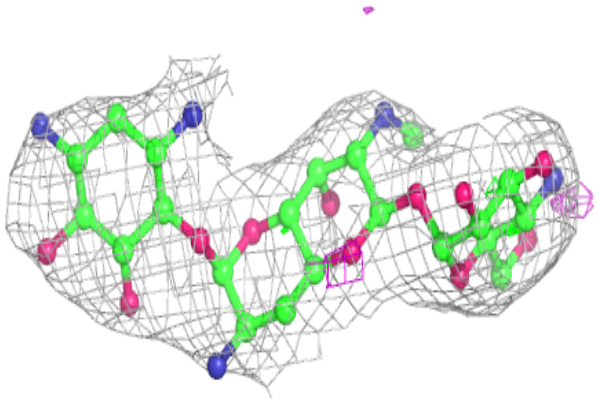
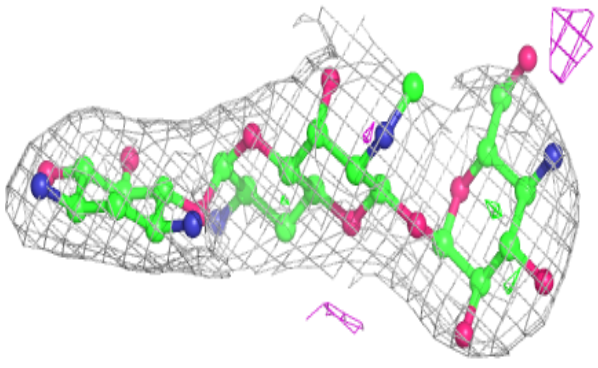
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
24	MG	A	2586	1/1	0.98	0.34	58,58,58,58	0
24	MG	A	2607	1/1	0.98	0.33	69,69,69,69	0
24	MG	A	2556	1/1	0.98	0.20	114,114,114,114	1
24	MG	A	2588	1/1	0.98	0.44	71,71,71,71	0
24	MG	A	2668	1/1	0.98	0.20	97,97,97,97	0
24	MG	M	1127	1/1	0.98	0.24	104,104,104,104	0
24	MG	A	2640	1/1	0.99	0.13	74,74,74,74	0
24	MG	A	2591	1/1	0.99	0.35	74,74,74,74	0
24	MG	A	2592	1/1	0.99	0.20	78,78,78,78	0
24	MG	A	2547	1/1	0.99	0.27	125,125,125,125	0
24	MG	A	2649	1/1	0.99	0.22	65,65,65,65	0
24	MG	A	2578	1/1	0.99	0.52	66,66,66,66	0
24	MG	A	2669	1/1	0.99	0.05	114,114,114,114	0
27	ZN	N	1062	1/1	0.99	0.22	172,172,172,172	0
27	ZN	D	1210	1/1	1.00	0.22	138,138,138,138	0
24	MG	A	2616	1/1	1.00	0.26	57,57,57,57	0

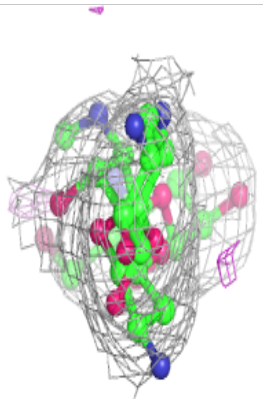
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around AM2 A 3001:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

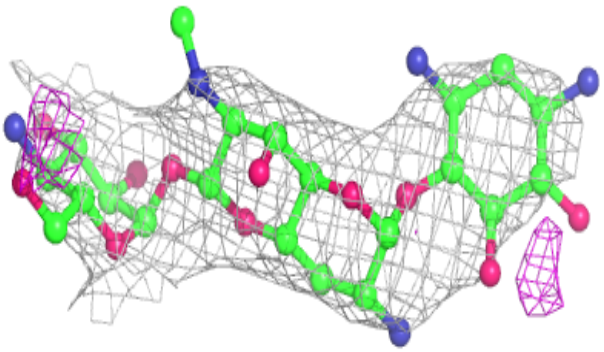


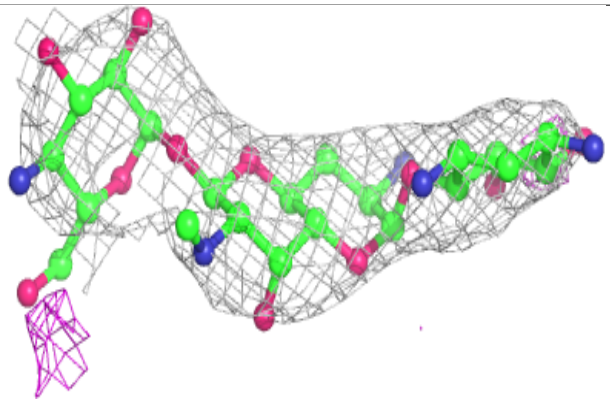


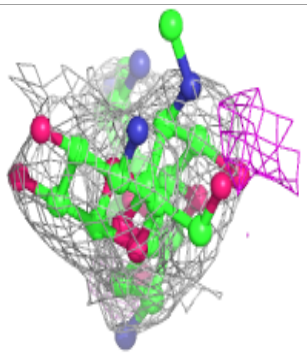


Electron density around AM2 A 3002:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

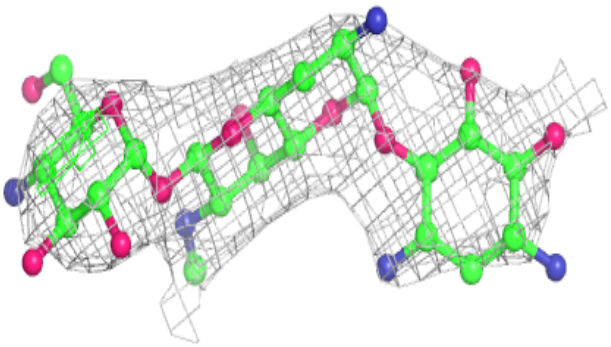


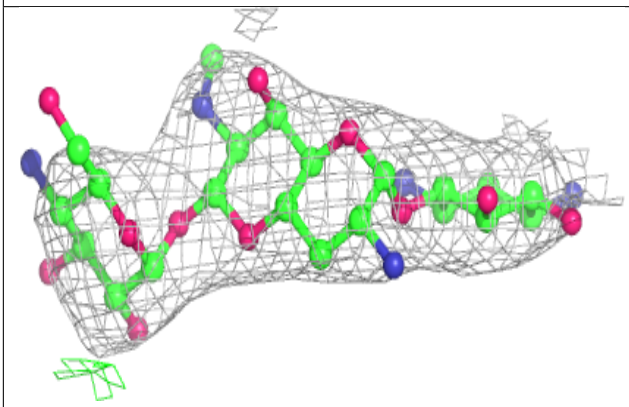


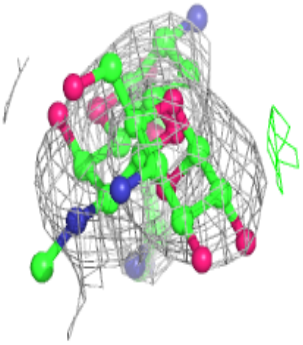


Electron density around AM2 A 3003:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

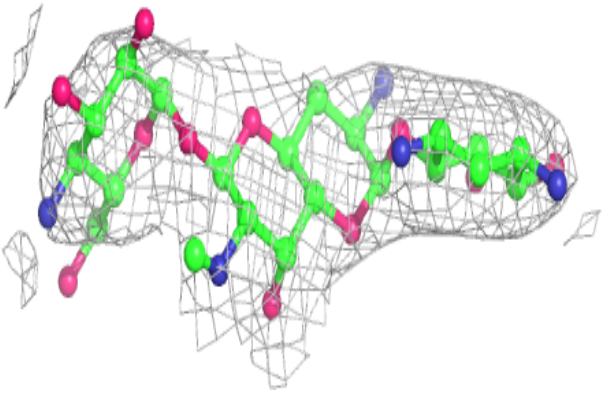


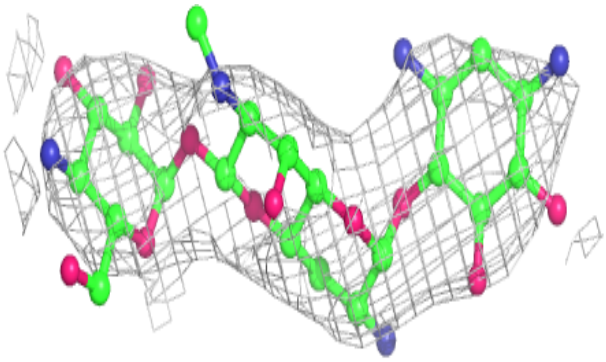


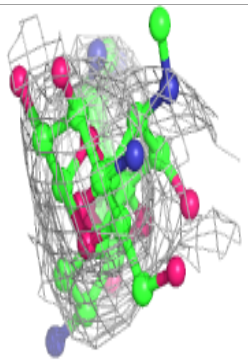


Electron density around AM2 A 3004:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

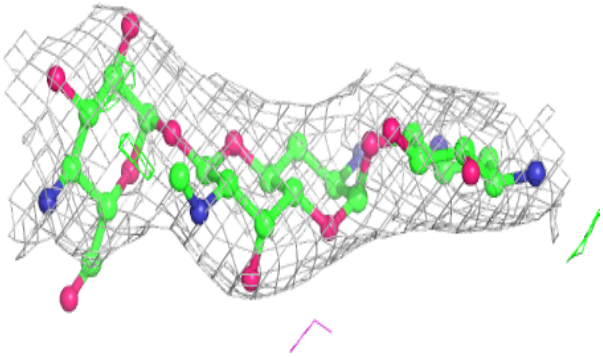


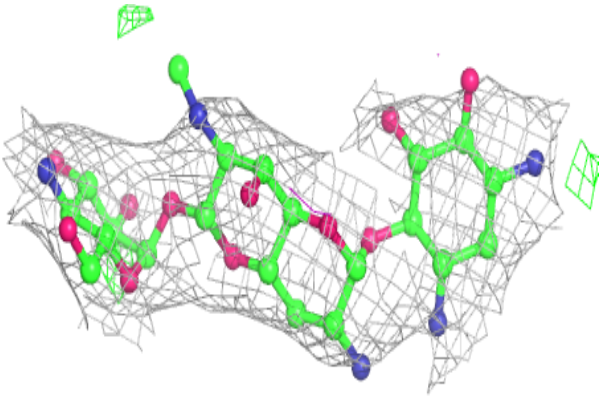


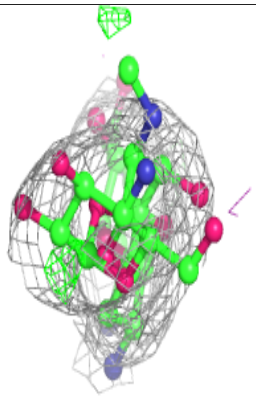


Electron density around AM2 A 3005:

$2mF_o$-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.