



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:59 PM GMT

PDB ID : 4JYA
Title : Crystal structures of pseudouridinylated stop codons with ASLs
Authors : Fernandez, I.S.; Ng, C.L.; Kelley, A.C.; Guowei, W.; Yu, Y.T.; Ramakrishnan, V.
Deposited on : 2013-03-29
Resolution : 3.10 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

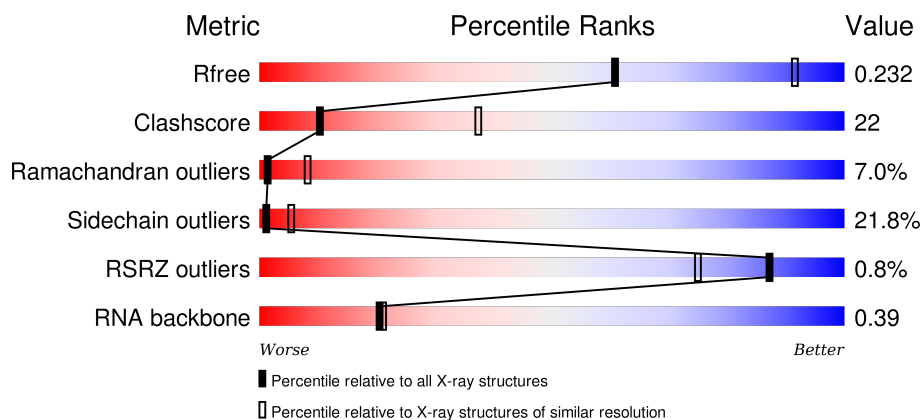
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

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








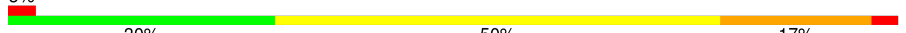







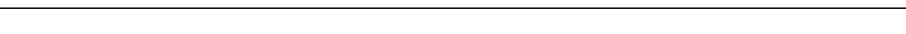




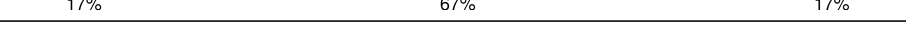
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)
RNA backbone	2183	1010 (3.52-2.68)

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

Mol	Chain	Length	Quality of chain
1	A	1516	<div> <div></div> <div>40%40%17%.</div> </div>
2	B	234	<div> <div>%</div> <div>38%43%18%.</div> </div>
3	C	206	<div> <div></div> <div>40%40%16%.</div> </div>
4	D	208	<div> <div></div> <div>50%35%13%.</div> </div>

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Mol	Chain	Length	Quality of chain
5	E	150	
6	F	101	
7	G	155	
8	H	138	
9	I	127	
10	J	98	
11	K	119	
12	L	125	
13	M	120	
14	N	60	
15	O	88	
16	P	83	
17	Q	99	
18	R	70	
19	S	78	
20	T	99	
21	U	24	
22	X	6	
23	Y	10	

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	1603	-	-	-	X
24	MG	A	1604	-	-	-	X
24	MG	A	1605	-	-	-	X
24	MG	A	1610	-	-	-	X

2 Entry composition

There are 25 unique types of molecules in this entry. The entry contains 52087 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
1	A	1516	Total	C	N	O	P	0	0	0
			32570	14499	6025	10531	1515			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	79	A	G	CONFLICT	GB 55771382

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

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

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

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

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

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

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

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

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

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

- 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
			1257	781	252	218	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
			1116	705	215	193	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
			1011	639	198	174			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	58	ARG	HIS	CONFLICT	UNP P80374

- 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
			885	549	168	165	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	0
			975	614	196	164	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	120	Total	C	N	O	S	0	0	0
			955	591	197	165	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
			492	312	104	72	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
			734	459	147	126	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	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	R	70	Total	C	N	O		0	0	0
			574	367	112	95				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	S	78	Total	C	N	O	S	0	0	0
			629	403	114	110	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
			763	470	162	129	2			

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

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

- Molecule 22 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	X	6	Total	C	N	O	P	0	0	0
			127	58	24	40	5			

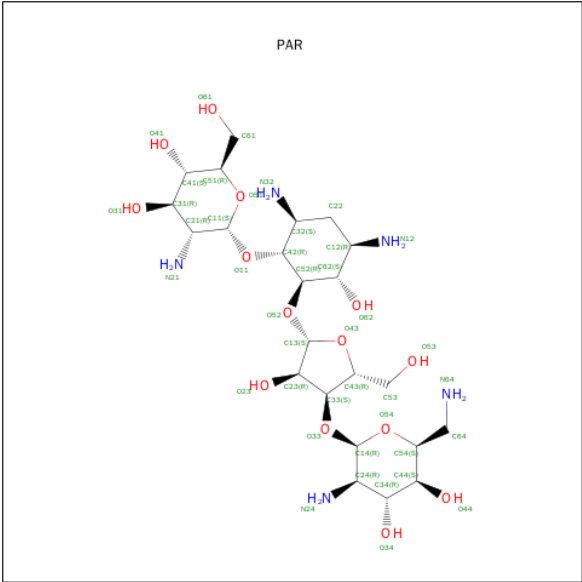
- Molecule 23 is a RNA chain called ASL-tRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	Y	10	Total	C	N	O	P	0	0	0
			214	96	38	70	10			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	X	1	Total	Mg	0	0
			1	1		
24	A	13	Total	Mg	0	0
			13	13		

- Molecule 25 is PAROMOMYCIN (three-letter code: PAR) (formula: C₂₃H₄₅N₅O₁₄).

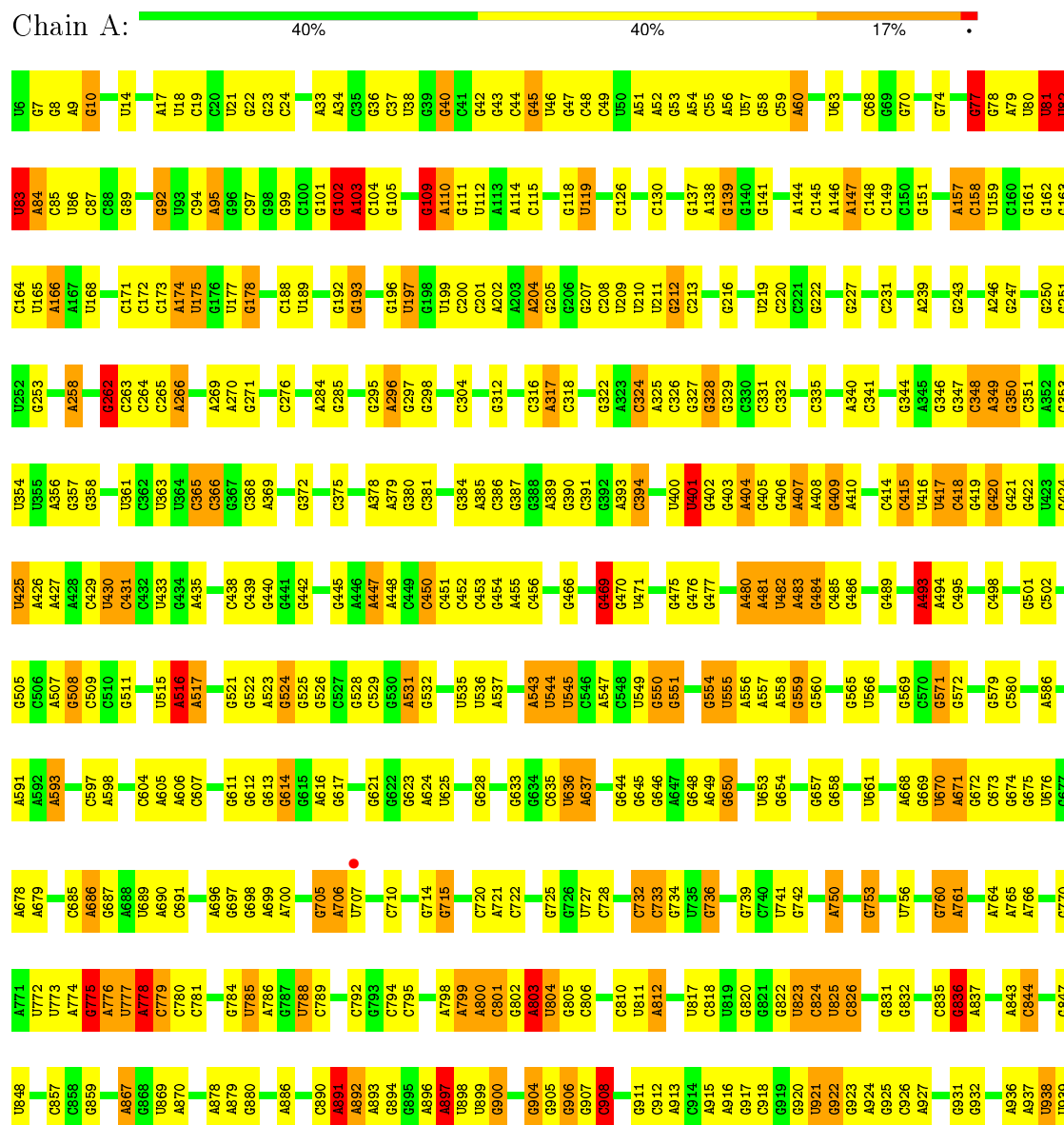


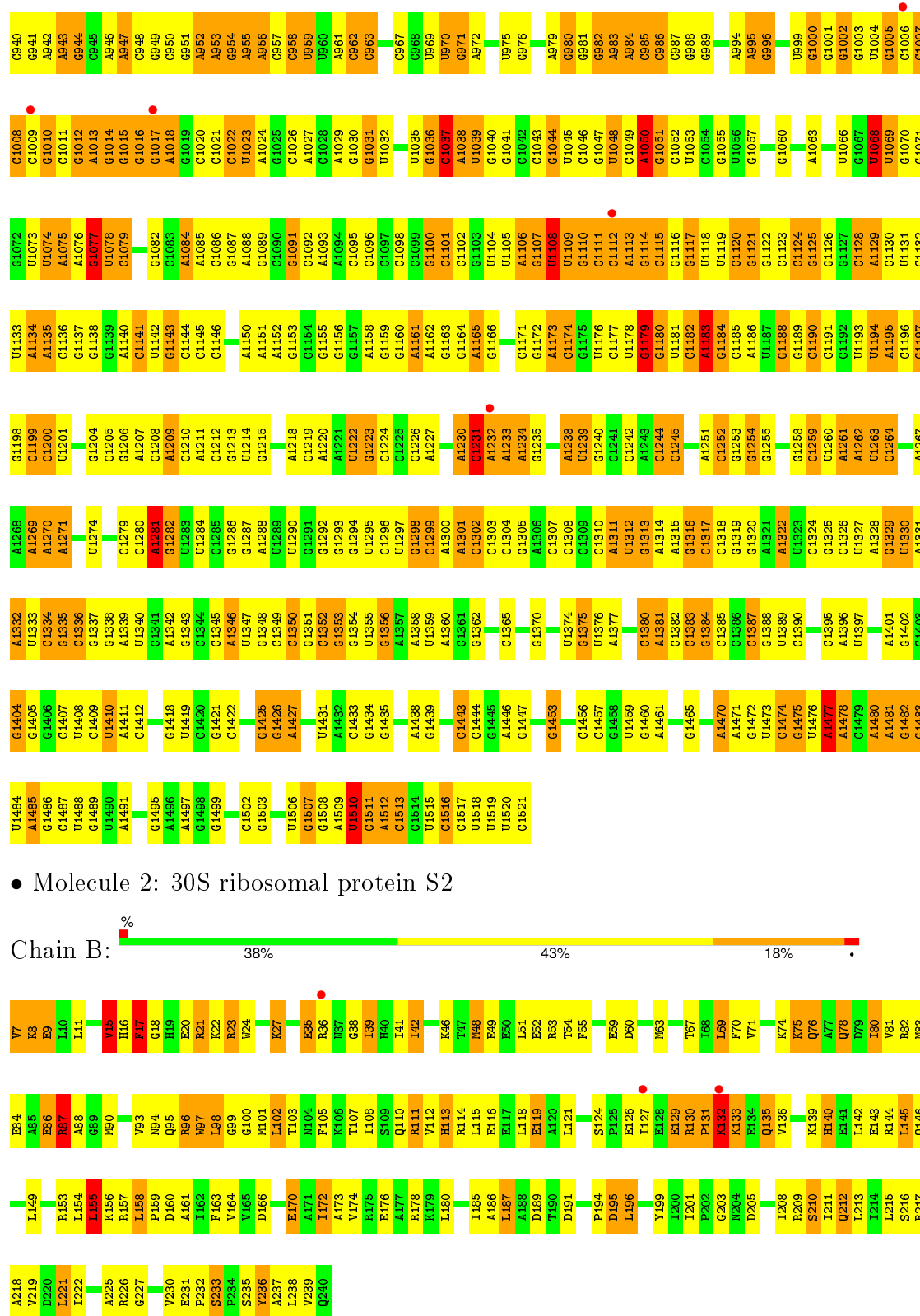
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	A	1	Total	C	N	O	0	0
			42	23	5	14		

3 Residue-property plots

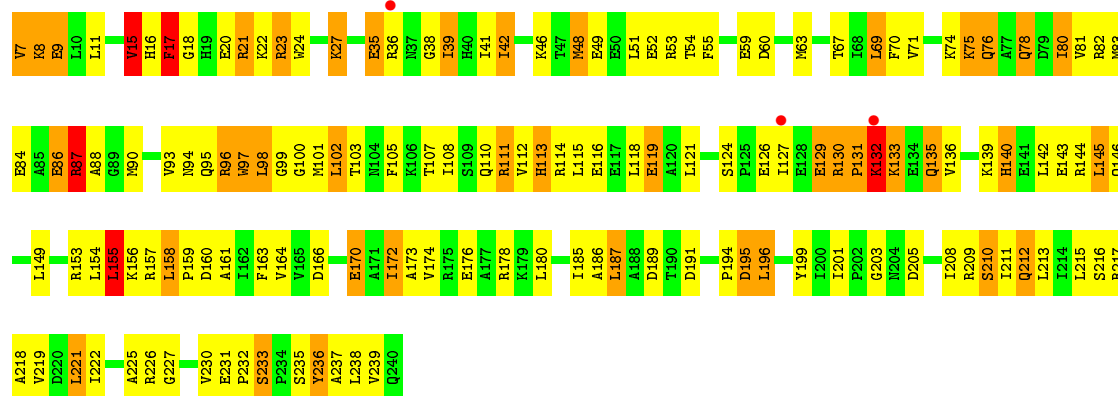
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($\text{RSRZ} > 2$). 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



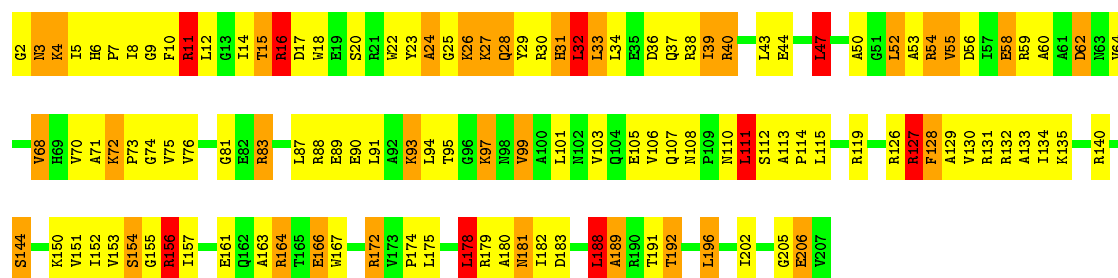


• Molecule 2: 30S ribosomal protein S2



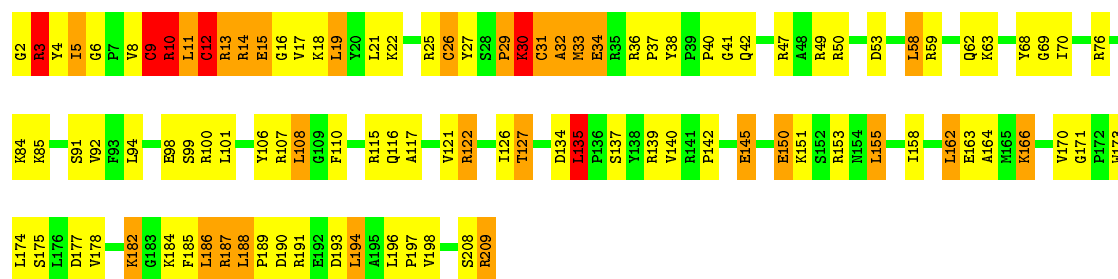
• Molecule 3: 30S ribosomal protein S3





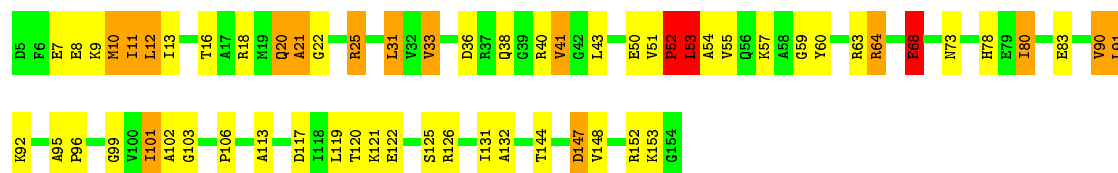
• Molecule 4: 30S ribosomal protein S4

Chain D: 50% 35% 13%



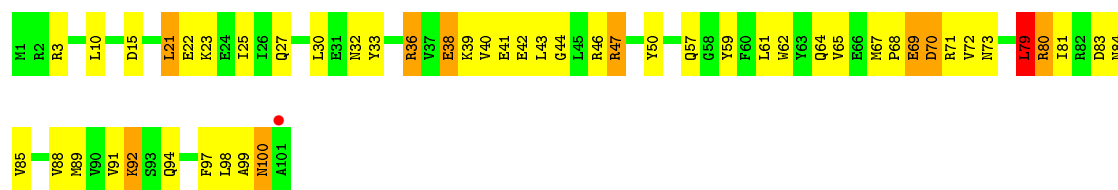
• Molecule 5: 30S ribosomal protein S5

Chain E: 59% 29% 10%



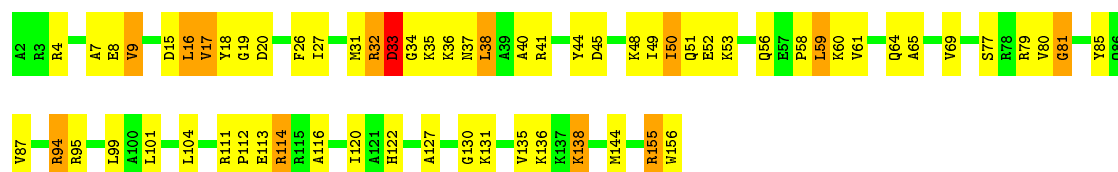
• Molecule 6: 30S ribosomal protein S6

Chain F: 50% 40% 9%

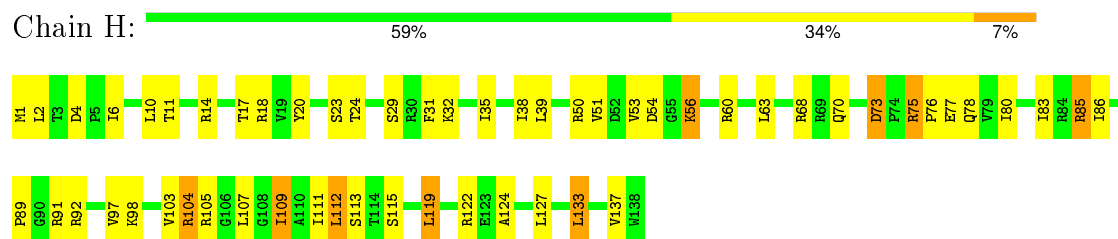


• Molecule 7: 30S ribosomal protein S7

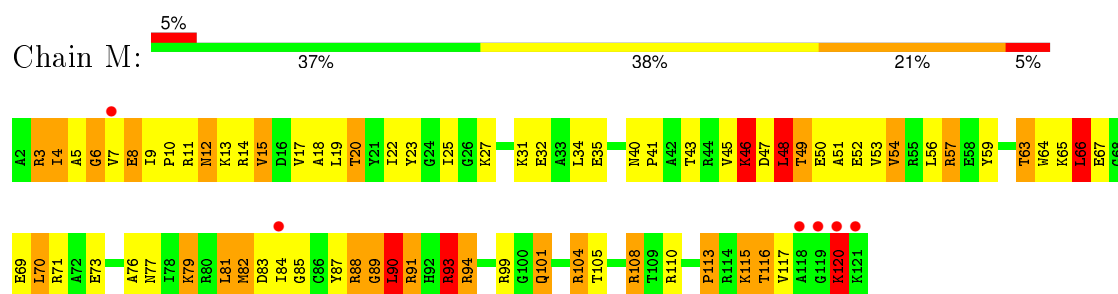
Chain G: 58% 34% 8%



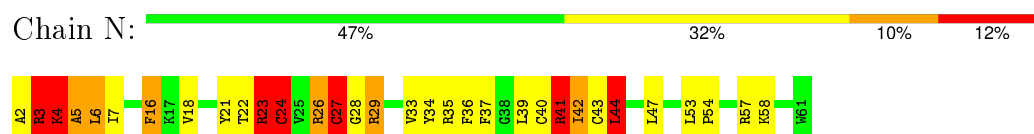
- Molecule 8: 30S ribosomal protein S8



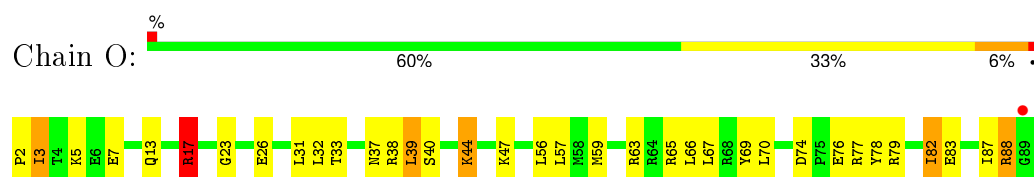
- Molecule 13: 30S ribosomal protein S13



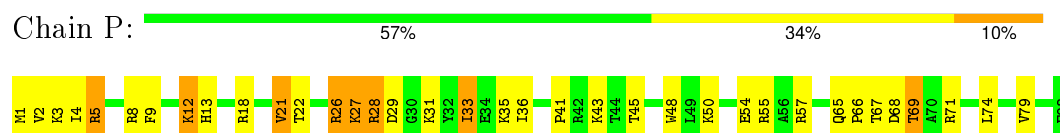
- Molecule 14: 30S ribosomal protein S14



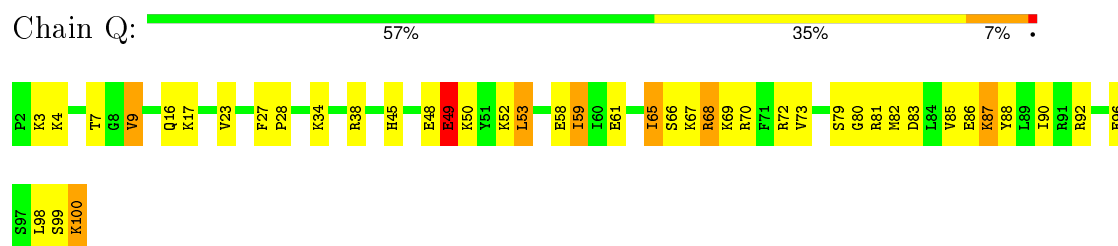
- Molecule 15: 30S ribosomal protein S15



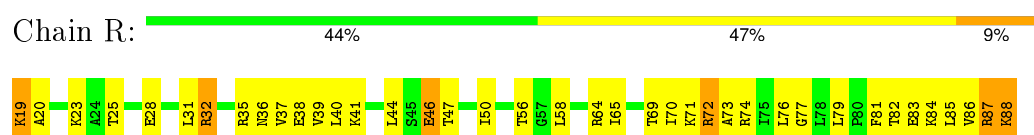
- Molecule 16: 30S ribosomal protein S16



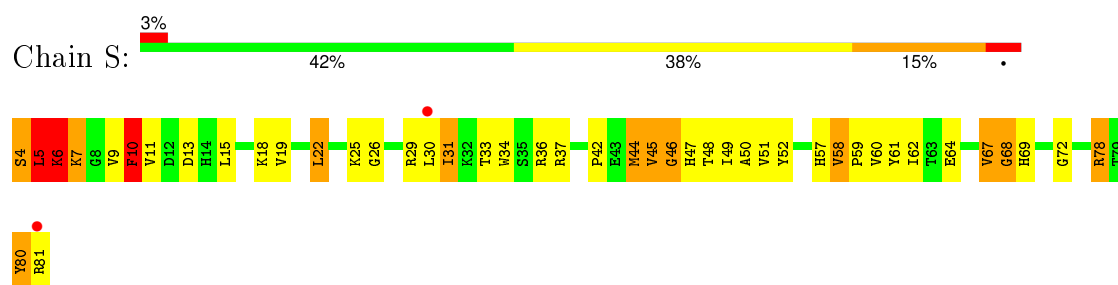
- Molecule 17: 30S ribosomal protein S17



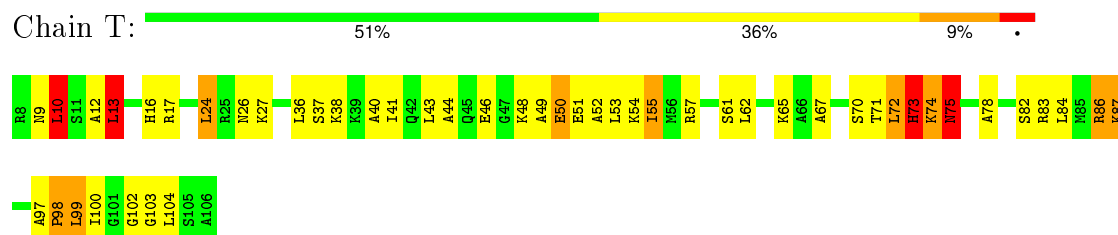
- Molecule 18: 30S ribosomal protein S18



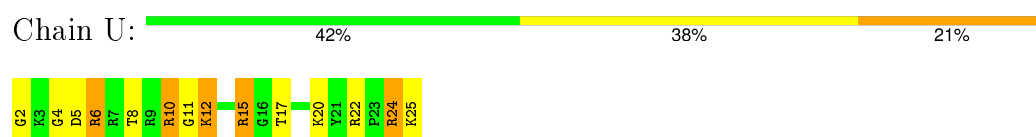
- Molecule 19: 30S ribosomal protein S19



- Molecule 20: 30S ribosomal protein S20



- Molecule 21: 30S ribosomal protein THX



- Molecule 22: mRNA



- Molecule 23: ASL-tRNA



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	402.32Å 402.32Å 174.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.93 – 3.10 48.93 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.0 (48.93-3.10) 99.0 (48.93-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.73 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.8.0021	Depositor
R, R_{free}	0.183 , 0.232 0.183 , 0.232	Depositor DCC
R_{free} test set	12741 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	78.5	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 58.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 254809 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	52087	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.40% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: PAR, MG, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.51	10/36456 (0.0%)	0.90	100/56897 (0.2%)
2	B	0.55	0/1935	0.86	1/2609 (0.0%)
3	C	0.63	0/1636	0.90	5/2205 (0.2%)
4	D	0.63	1/1733 (0.1%)	0.99	8/2318 (0.3%)
5	E	0.67	0/1162	0.95	2/1564 (0.1%)
6	F	0.49	0/856	0.82	1/1154 (0.1%)
7	G	0.51	0/1276	0.77	0/1709
8	H	0.63	0/1136	0.93	0/1527
9	I	0.55	0/1029	0.89	1/1378 (0.1%)
10	J	0.60	0/807	0.86	0/1085
11	K	0.53	0/900	0.84	1/1213 (0.1%)
12	L	0.67	0/991	1.02	2/1327 (0.2%)
13	M	0.57	0/965	0.93	3/1292 (0.2%)
14	N	0.73	0/501	1.11	3/664 (0.5%)
15	O	0.52	0/745	0.86	1/992 (0.1%)
16	P	0.60	0/716	0.91	1/963 (0.1%)
17	Q	0.63	0/836	0.98	2/1117 (0.2%)
18	R	0.52	0/579	0.86	1/768 (0.1%)
19	S	0.62	0/642	0.93	1/865 (0.1%)
20	T	0.58	0/765	1.00	1/1007 (0.1%)
21	U	0.69	0/212	0.96	0/277
22	X	0.83	0/102	1.65	2/160 (1.2%)
23	Y	0.42	0/239	0.84	1/370 (0.3%)
All	All	0.54	11/56219 (0.0%)	0.90	137/83461 (0.2%)

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
2	B	0	1
4	D	0	2
12	L	0	1
13	M	0	1
20	T	0	5
All	All	0	10

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	82	U	O3'-P	11.41	1.74	1.61
1	A	81	U	O3'-P	9.90	1.73	1.61
1	A	83	U	O3'-P	9.05	1.72	1.61
1	A	750	A	P-OP2	7.96	1.62	1.49
1	A	836	G	O3'-P	6.39	1.68	1.61
1	A	799	A	O3'-P	-6.38	1.53	1.61
1	A	77	G	O3'-P	-5.69	1.54	1.61
1	A	111	G	P-OP2	5.42	1.58	1.49
4	D	12	CYS	CA-CB	5.25	1.65	1.53
1	A	1108	U	O3'-P	5.20	1.67	1.61
1	A	82	U	C3'-O3'	5.07	1.49	1.42

All (137) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	X	3	A	O5'-P-OP1	-13.46	93.58	105.70
1	A	1477	A	O5'-P-OP1	-12.08	94.83	105.70
1	A	103	A	O5'-P-OP1	-9.71	96.96	105.70
1	A	891	A	C2'-C3'-O3'	9.37	130.10	109.50
1	A	1486	G	O5'-P-OP2	-9.13	97.48	105.70
1	A	778	A	O5'-P-OP2	-9.03	97.58	105.70
1	A	83	U	N1-C1'-C2'	9.01	125.71	114.00
1	A	1510	U	C2'-C3'-O3'	8.98	129.25	109.50
1	A	109	G	C2'-C3'-O3'	8.53	128.26	109.50
1	A	775	G	C2'-C3'-O3'	8.48	128.16	109.50
1	A	836	G	C4-N9-C1'	-8.47	115.48	126.50
1	A	558	A	O5'-P-OP1	-8.42	98.12	105.70
1	A	836	G	C8-N9-C1'	8.25	137.72	127.00
1	A	262	G	C2'-C3'-O3'	8.24	127.63	109.50
1	A	1050	A	C2'-C3'-O3'	8.12	127.36	109.50
1	A	775	G	O5'-P-OP1	-7.97	98.53	105.70
5	E	25	ARG	NE-CZ-NH2	-7.78	116.41	120.30
1	A	178	G	O5'-P-OP1	-7.76	98.72	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	671	A	C2'-C3'-O3'	7.66	126.35	109.50
1	A	836	G	O4'-C1'-N9	7.65	114.32	108.20
1	A	1179	G	O5'-P-OP2	-7.53	98.93	105.70
1	A	401	U	C2'-C3'-O3'	7.52	126.05	109.50
13	M	48	LEU	CA-CB-CG	7.42	132.37	115.30
1	A	469	G	C2'-C3'-O3'	7.37	125.72	109.50
1	A	82	U	P-O3'-C3'	7.37	128.55	119.70
4	D	188	LEU	CA-CB-CG	7.36	132.23	115.30
1	A	516	A	C2'-C3'-O3'	7.34	125.64	109.50
1	A	1288	A	O5'-P-OP2	-7.26	99.17	105.70
1	A	82	U	C2'-C3'-O3'	7.23	125.41	109.50
4	D	12	CYS	CA-CB-SG	7.05	126.69	114.00
1	A	1375	G	O5'-P-OP2	-7.00	99.40	105.70
1	A	1086	C	O5'-P-OP2	-6.96	99.43	105.70
1	A	736	G	O5'-P-OP2	-6.95	99.44	105.70
1	A	1486	G	O5'-P-OP1	6.91	118.99	110.70
12	L	92	ASP	CB-CG-OD2	-6.88	112.11	118.30
1	A	1066	U	O5'-P-OP1	-6.86	99.52	105.70
1	A	348	C	O5'-P-OP1	-6.86	99.53	105.70
1	A	1477	A	O5'-P-OP2	6.72	118.76	110.70
1	A	1037	C	C4'-C3'-O3'	-6.69	95.35	109.40
3	C	196	LEU	CA-CB-CG	6.67	130.64	115.30
14	N	27	CYS	CA-CB-SG	-6.67	102.00	114.00
1	A	493	A	C2'-C3'-O3'	6.66	124.36	113.70
4	D	12	CYS	N-CA-C	-6.63	93.10	111.00
1	A	906	G	O5'-P-OP1	-6.55	99.81	105.70
1	A	756	U	O5'-P-OP2	-6.51	99.84	105.70
1	A	1513	C	C4'-C3'-O3'	-6.50	95.75	109.40
19	S	5	LEU	CA-CB-CG	6.43	130.10	115.30
1	A	1134	A	C2'-C3'-O3'	6.35	123.86	113.70
1	A	297	G	O5'-P-OP2	-6.32	100.01	105.70
1	A	102	G	O4'-C4'-C3'	-6.31	97.69	104.00
1	A	785	U	O5'-P-OP1	-6.30	100.03	105.70
1	A	886	A	O5'-P-OP1	-6.28	100.05	105.70
3	C	11	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	A	1066	U	O5'-P-OP2	6.24	118.19	110.70
1	A	1089	G	O5'-P-OP2	6.21	118.16	110.70
1	A	356	A	O5'-P-OP1	-6.20	100.12	105.70
1	A	427	A	O5'-P-OP1	-6.17	100.14	105.70
1	A	103	A	O5'-P-OP2	6.17	118.10	110.70
1	A	593	A	O5'-P-OP1	-6.15	100.16	105.70
1	A	1231	C	C4'-C3'-O3'	6.02	125.05	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	558	A	O5'-P-OP2	6.01	117.92	110.70
1	A	427	A	O5'-P-OP2	6.00	117.90	110.70
1	A	551	G	O5'-P-OP1	-6.00	100.30	105.70
1	A	547	A	C4'-C3'-O3'	-5.94	96.92	109.40
17	Q	98	LEU	CA-CB-CG	5.94	128.97	115.30
1	A	262	G	P-O3'-C3'	5.94	126.83	119.70
1	A	63	U	O5'-P-OP2	-5.93	100.36	105.70
1	A	886	A	O5'-P-OP2	5.93	117.81	110.70
1	A	447	A	O5'-P-OP2	5.89	117.77	110.70
1	A	1281	A	N9-C1'-C2'	5.86	121.61	114.00
1	A	89	G	O5'-P-OP2	-5.85	100.44	105.70
1	A	803	A	C4'-C3'-O3'	-5.81	97.20	109.40
1	A	908	C	O4'-C4'-C3'	-5.78	98.22	104.00
1	A	493	A	O5'-P-OP1	-5.78	100.50	105.70
1	A	1480	A	N9-C1'-C2'	5.77	121.50	114.00
9	I	47	LEU	CA-CB-CG	5.77	128.57	115.30
1	A	1077	G	O5'-P-OP2	-5.77	100.51	105.70
14	N	24	CYS	CA-CB-SG	5.75	124.35	114.00
1	A	775	G	O5'-P-OP2	5.72	117.57	110.70
1	A	1183	A	C2'-C3'-O3'	5.70	122.81	113.70
2	B	155	LEU	CA-CB-CG	5.69	128.38	115.30
1	A	1206	G	O5'-P-OP1	5.68	117.52	110.70
1	A	686	A	N9-C1'-C2'	5.67	121.37	114.00
1	A	778	A	O5'-P-OP1	5.64	117.47	110.70
4	D	12	CYS	N-CA-CB	5.64	120.76	110.60
11	K	87	THR	N-CA-C	-5.64	95.77	111.00
1	A	628	G	O5'-P-OP2	-5.64	100.63	105.70
1	A	785	U	O5'-P-OP2	5.61	117.44	110.70
20	T	10	LEU	CA-CB-CG	5.58	128.15	115.30
6	F	79	LEU	CA-CB-CG	5.58	128.14	115.30
1	A	83	U	O4'-C1'-C2'	-5.58	100.22	105.80
1	A	82	U	O4'-C1'-N1	5.57	112.66	108.20
1	A	1031	G	C2'-C3'-O3'	5.57	122.61	113.70
1	A	803	A	C2'-C3'-O3'	5.56	122.60	113.70
1	A	836	G	O5'-P-OP1	-5.56	100.69	105.70
1	A	878	A	O5'-P-OP1	-5.56	100.69	105.70
1	A	670	U	C4'-C3'-O3'	-5.56	97.73	109.40
15	O	17	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	A	178	G	O5'-P-OP2	5.50	117.30	110.70
1	A	836	G	O5'-P-OP2	5.45	117.24	110.70
13	M	99	ARG	NE-CZ-NH2	-5.45	117.58	120.30
4	D	135	LEU	CA-CB-CG	5.44	127.81	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	R	31	LEU	CA-CB-CG	5.43	127.78	115.30
16	P	26	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	A	1380	C	C4'-C3'-O3'	-5.42	98.02	109.40
1	A	1060	G	O5'-P-OP2	-5.41	100.83	105.70
3	C	111	LEU	CA-CB-CG	5.38	127.66	115.30
1	A	897	A	O5'-P-OP1	-5.37	100.87	105.70
1	A	774	A	O5'-P-OP2	-5.35	100.88	105.70
1	A	119	U	O4'-C4'-C3'	-5.32	98.68	104.00
5	E	53	LEU	CA-CB-CG	5.31	127.50	115.30
1	A	867	A	C4'-C3'-O3'	-5.30	98.26	109.40
1	A	356	A	O5'-P-OP2	5.29	117.05	110.70
1	A	549	U	O5'-P-OP1	-5.29	100.94	105.70
4	D	186	LEU	CA-CB-CG	5.29	127.46	115.30
1	A	1377	A	O5'-P-OP1	-5.26	100.97	105.70
12	L	117	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	A	1179	G	O5'-P-OP1	5.25	117.00	110.70
1	A	792	C	O5'-P-OP2	5.23	116.98	110.70
4	D	9	CYS	C-N-CA	5.23	134.78	121.70
14	N	44	LEU	CB-CG-CD2	5.22	119.88	111.00
1	A	1305	G	O5'-P-OP1	-5.21	101.01	105.70
1	A	1305	G	O5'-P-OP2	5.21	116.95	110.70
1	A	836	G	C5'-C4'-O4'	-5.19	102.88	109.10
4	D	194	LEU	CA-CB-CG	5.18	127.22	115.30
1	A	848	U	O5'-P-OP1	-5.18	101.04	105.70
1	A	948	C	O5'-P-OP2	5.18	116.91	110.70
1	A	1068	U	O5'-P-OP1	-5.17	101.05	105.70
23	Y	35	A	O5'-P-OP2	5.12	116.85	110.70
1	A	422	G	O5'-P-OP2	-5.12	101.09	105.70
22	X	6	A	C2'-C3'-O3'	5.10	121.86	113.70
17	Q	9	VAL	CB-CA-C	-5.10	101.72	111.40
1	A	1510	U	O5'-P-OP2	-5.08	101.13	105.70
1	A	1380	C	O4'-C1'-N1	5.08	112.26	108.20
3	C	178	LEU	CA-CB-CG	5.05	126.91	115.30
3	C	11	ARG	NE-CZ-NH2	-5.03	117.78	120.30
13	M	93	ARG	NE-CZ-NH1	5.00	122.80	120.30

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	191	ASP	Peptide
4	D	30	LYS	Peptide

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Mol	Chain	Res	Type	Group
4	D	31	CYS	Peptide
12	L	87	GLY	Peptide
13	M	66	LEU	Peptide
20	T	13	LEU	Peptide
20	T	73	HIS	Peptide
20	T	75	ASN	Peptide
20	T	98	PRO	Peptide
20	T	99	LEU	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32570	0	16445	880	0
2	B	1900	0	1951	146	0
3	C	1612	0	1677	135	0
4	D	1703	0	1763	96	0
5	E	1146	0	1207	53	0
6	F	843	0	857	36	0
7	G	1257	0	1296	53	0
8	H	1116	0	1177	40	0
9	I	1011	0	1043	86	0
10	J	794	0	840	92	0
11	K	885	0	904	35	0
12	L	975	0	1062	68	0
13	M	955	0	1021	57	0
14	N	492	0	529	66	0
15	O	734	0	771	24	0
16	P	700	0	720	27	0
17	Q	823	0	891	32	0
18	R	574	0	644	39	0
19	S	629	0	652	56	0
20	T	763	0	861	38	0
21	U	208	0	221	15	0
22	X	127	0	65	20	0
23	Y	214	0	107	5	0
24	A	13	0	0	0	0
24	X	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	A	42	0	45	3	0
All	All	52087	0	36749	1905	0

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

All (1905) 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:1230:A:O2'	1:A:1231:C:H5''	1.32	1.29
1:A:1021:C:H2'	1:A:1022:C:O2	1.40	1.19
10:J:45:ARG:NH1	10:J:45:ARG:HB3	1.57	1.17
12:L:47:LYS:HB3	12:L:48:PRO:CD	1.76	1.16
10:J:8:LEU:HD13	10:J:20:ALA:CB	1.75	1.15
1:A:1338:G:H2'	1:A:1339:A:C8	1.82	1.14
4:D:150:GLU:HA	4:D:153:ARG:HD2	1.29	1.12
1:A:1108:U:C6	1:A:1108:U:H5''	1.84	1.11
2:B:111:ARG:HG2	2:B:111:ARG:HH11	1.15	1.11
19:S:6:LYS:CD	19:S:7:LYS:HE3	1.81	1.11
12:L:47:LYS:HB3	12:L:48:PRO:HD3	1.30	1.10
1:A:1043:C:C5	3:C:2:GLY:HA3	1.86	1.10
1:A:1013:A:H3'	1:A:1014:G:H5''	1.18	1.09
14:N:27:CYS:SG	14:N:27:CYS:O	2.10	1.09
1:A:197:U:H5''	1:A:197:U:H6	1.17	1.09
2:B:21:ARG:HD2	2:B:39:ILE:HG23	1.33	1.08
19:S:45:VAL:HG23	19:S:46:GLY:H	1.19	1.05
19:S:6:LYS:HD3	19:S:7:LYS:HE3	1.04	1.04
3:C:23:TYR:CD1	3:C:24:ALA:N	2.26	1.03
21:U:10:ARG:HH11	21:U:10:ARG:CG	1.71	1.03
1:A:957:C:H3'	1:A:958:C:H5''	1.39	1.01
2:B:84:GLU:HB3	2:B:219:VAL:HG21	1.40	1.01
10:J:90:LEU:H	10:J:91:PRO:HD3	1.23	1.01
1:A:1230:A:O2'	1:A:1231:C:C5'	2.09	1.01
1:A:1108:U:H6	1:A:1108:U:H5''	1.16	1.01
1:A:1233:A:H2'	1:A:1234:A:N7	1.74	1.00
1:A:1287:G:N2	1:A:1313:G:H2'	1.76	1.00
1:A:1043:C:H5	3:C:2:GLY:HA3	1.19	1.00
7:G:15:ASP:HB3	7:G:20:ASP:H	1.27	0.99
1:A:403:G:O2'	4:D:116:GLN:HG3	1.61	0.99
1:A:1108:U:O4	10:J:5:ARG:HD3	1.61	0.99
21:U:10:ARG:NH1	21:U:10:ARG:HG3	1.61	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:G:H5''	12:L:17:LYS:HE2	1.45	0.99
14:N:24:CYS:HB2	14:N:40:CYS:H	1.24	0.99
13:M:17:VAL:O	13:M:20:THR:HB	1.62	0.98
1:A:1233:A:O2'	1:A:1234:A:H8	1.44	0.98
10:J:7:LYS:HB2	10:J:97:GLU:HB2	1.44	0.98
10:J:45:ARG:HH11	10:J:45:ARG:HB3	0.81	0.98
1:A:1233:A:HO2'	1:A:1234:A:H8	1.12	0.98
21:U:10:ARG:HG3	21:U:10:ARG:HH11	0.81	0.98
1:A:1172:G:O2'	3:C:3:ASN:HB2	1.62	0.98
19:S:6:LYS:HD3	19:S:7:LYS:CE	1.93	0.97
2:B:18:GLY:HA2	2:B:42:ILE:HG23	1.47	0.96
3:C:110:ASN:ND2	3:C:140:ARG:HB3	1.79	0.96
12:L:27:LEU:O	12:L:29:GLY:N	1.99	0.96
20:T:50:GLU:HG2	20:T:100:ILE:HG21	1.46	0.96
16:P:28:ARG:HH11	16:P:28:ARG:HG2	1.28	0.95
10:J:45:ARG:HH11	10:J:45:ARG:CB	1.77	0.95
1:A:531:A:OP2	4:D:2:GLY:HA2	1.66	0.95
13:M:90:LEU:HA	13:M:93:ARG:HB2	1.48	0.95
1:A:1521:C:H41	2:B:23:ARG:HH22	1.09	0.95
1:A:77:G:H1	1:A:87:C:H5	0.95	0.94
1:A:1232:A:OP1	1:A:1232:A:O4'	1.86	0.93
12:L:47:LYS:CB	12:L:48:PRO:HD3	1.97	0.93
1:A:1013:A:H3'	1:A:1014:G:C5'	1.97	0.93
1:A:1521:C:H41	2:B:23:ARG:NH2	1.65	0.93
5:E:80:ILE:CD1	5:E:91:LEU:HB2	1.97	0.93
10:J:8:LEU:CD1	10:J:20:ALA:CB	2.45	0.93
10:J:8:LEU:CD1	10:J:20:ALA:HB1	1.98	0.93
14:N:27:CYS:HB3	14:N:43:CYS:HB3	1.47	0.93
3:C:70:VAL:HG12	3:C:72:LYS:H	1.32	0.93
3:C:154:SER:OG	3:C:155:GLY:N	1.97	0.93
12:L:90:VAL:O	12:L:91:LYS:HB3	1.68	0.92
1:A:197:U:H5''	1:A:197:U:C6	2.06	0.91
1:A:1239:U:H4'	1:A:1239:U:OP2	1.68	0.90
14:N:24:CYS:CB	14:N:40:CYS:HB3	2.02	0.90
1:A:1135:A:H5'	10:J:13:HIS:CD2	2.06	0.90
1:A:1108:U:H6	1:A:1108:U:C5'	1.82	0.90
10:J:49:VAL:O	10:J:60:ARG:HB3	1.72	0.90
1:A:1233:A:C2'	1:A:1234:A:C8	2.55	0.90
1:A:1039:U:H5'	3:C:163:ALA:HB2	1.54	0.90
1:A:1109:U:H2'	1:A:1109:U:O2	1.71	0.90
3:C:70:VAL:HG12	3:C:71:ALA:N	1.88	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1233:A:O2'	1:A:1234:A:C8	2.25	0.89
1:A:1013:A:C3'	1:A:1014:G:H5''	2.03	0.89
1:A:1069:U:H3	1:A:1082:G:H22	1.13	0.89
12:L:81:SER:O	12:L:106:ASP:HB2	1.73	0.89
1:A:1039:U:H5'	3:C:163:ALA:CB	2.04	0.88
23:Y:31:A:H2'	23:Y:31:A:N3	1.88	0.88
1:A:921:U:H2'	1:A:922:G:H5'	1.53	0.88
4:D:30:LYS:HB2	4:D:32:ALA:HA	1.54	0.88
10:J:5:ARG:HG3	10:J:73:ASP:OD1	1.73	0.88
1:A:648:G:H22	1:A:725:G:H1	1.18	0.88
1:A:1100:G:H4'	9:I:104:ARG:HH21	1.38	0.88
4:D:29:PRO:O	4:D:30:LYS:HD3	1.73	0.88
1:A:1230:A:HO2'	1:A:1231:C:H5''	1.34	0.87
5:E:91:LEU:HD12	5:E:120:THR:HG22	1.56	0.87
18:R:46:GLU:CD	18:R:46:GLU:H	1.77	0.87
1:A:1515:U:O2'	1:A:1516:C:OP2	1.93	0.87
15:O:17:ARG:HH11	15:O:17:ARG:HG3	1.39	0.86
4:D:33:MET:HE2	4:D:37:PRO:HA	1.57	0.86
3:C:108:ASN:HD21	3:C:144:SER:HB3	1.39	0.86
14:N:6:LEU:HD23	14:N:23:ARG:HH22	1.38	0.86
1:A:661:U:H3	1:A:697:G:H22	1.23	0.86
1:A:690:A:O2'	11:K:29:ILE:HD11	1.76	0.86
1:A:1349:C:H2'	1:A:1350:C:H6	1.39	0.86
1:A:77:G:N1	1:A:87:C:H5	1.72	0.86
1:A:690:A:N3	11:K:31:THR:HG21	1.91	0.86
20:T:50:GLU:HG2	20:T:100:ILE:CG2	2.06	0.85
1:A:433:U:H5''	4:D:155:LEU:HD22	1.56	0.85
20:T:73:HIS:O	20:T:74:LYS:HG3	1.75	0.85
3:C:205:GLY:O	3:C:206:GLU:HB2	1.77	0.84
10:J:79:ARG:HH11	10:J:82:ILE:HD12	1.38	0.84
10:J:50:ILE:H	10:J:50:ILE:HD12	1.39	0.84
3:C:110:ASN:O	3:C:111:LEU:HD23	1.75	0.84
1:A:1172:G:O2'	3:C:3:ASN:CB	2.25	0.84
2:B:140:HIS:HA	2:B:143:GLU:HG2	1.58	0.83
3:C:70:VAL:HG12	3:C:71:ALA:H	1.41	0.83
1:A:1233:A:C8	9:I:68:GLY:HA2	2.13	0.83
14:N:24:CYS:HB2	14:N:40:CYS:N	1.92	0.83
3:C:23:TYR:CE1	3:C:24:ALA:O	2.30	0.83
3:C:39:ILE:HG22	3:C:40:ARG:N	1.93	0.83
1:A:1521:C:N4	2:B:23:ARG:HH22	1.77	0.83
1:A:1334:C:H2'	1:A:1335:G:C8	2.14	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:430:U:H2'	1:A:431:C:C6	2.14	0.83
18:R:32:ARG:HA	18:R:69:THR:HG21	1.61	0.83
1:A:1307:C:O3'	21:U:17:THR:HG21	1.78	0.83
20:T:57:ARG:NH1	20:T:102:GLY:HA2	1.94	0.83
13:M:108:ARG:HH11	13:M:108:ARG:HG3	1.44	0.82
2:B:172:ILE:H	2:B:172:ILE:HD12	1.43	0.82
1:A:1233:A:H2'	1:A:1234:A:C8	2.14	0.82
2:B:158:LEU:H	2:B:158:LEU:HD12	1.44	0.82
18:R:85:LEU:HD23	18:R:88:LYS:HG3	1.62	0.82
12:L:24:VAL:HG12	12:L:24:VAL:O	1.77	0.82
16:P:74:LEU:O	16:P:79:VAL:HG23	1.80	0.82
1:A:1351:G:H2'	1:A:1352:C:H5'	1.61	0.82
4:D:11:LEU:C	4:D:13:ARG:N	2.30	0.82
1:A:1130:C:H4'	9:I:5:TYR:HE2	1.44	0.82
9:I:9:ARG:HG3	9:I:14:VAL:HG13	1.62	0.81
13:M:67:GLU:HG3	13:M:67:GLU:O	1.79	0.81
2:B:88:ALA:HB2	2:B:219:VAL:CG1	2.09	0.81
1:A:906:G:O2'	1:A:1511:C:OP1	1.97	0.81
17:Q:67:LYS:HA	17:Q:70:ARG:HH12	1.45	0.81
5:E:80:ILE:CD1	5:E:91:LEU:CB	2.59	0.81
1:A:614:G:H5''	1:A:614:G:H8	1.45	0.81
1:A:1322:A:H8	1:A:1322:A:H5''	1.45	0.80
1:A:921:U:C2'	1:A:922:G:H5'	2.11	0.80
1:A:931:G:H5'	1:A:943:A:H61	1.46	0.80
1:A:81:U:OP2	1:A:81:U:H6	1.64	0.80
4:D:190:ASP:HB3	4:D:193:ASP:OD1	1.81	0.80
5:E:101:ILE:HD11	5:E:119:LEU:HD23	1.61	0.80
2:B:23:ARG:HG2	2:B:23:ARG:O	1.80	0.80
5:E:101:ILE:HD11	5:E:119:LEU:CD2	2.12	0.80
1:A:1240:G:H1	1:A:1259:C:H42	1.30	0.79
11:K:48:ILE:HG22	11:K:49:GLY:H	1.46	0.79
14:N:27:CYS:HB3	14:N:43:CYS:CB	2.12	0.79
1:A:1349:C:H2'	1:A:1350:C:C6	2.17	0.79
1:A:1470:A:H1'	22:X:5:G:O2'	1.82	0.79
4:D:30:LYS:HB2	4:D:32:ALA:CA	2.11	0.79
3:C:95:THR:HG22	3:C:97:LYS:HB2	1.62	0.79
1:A:1014:G:N3	1:A:1015:G:O6	2.16	0.79
19:S:45:VAL:O	19:S:47:HIS:N	2.15	0.79
1:A:1287:G:H22	1:A:1313:G:H2'	1.45	0.79
18:R:56:THR:HB	18:R:58:LEU:HD13	1.65	0.78
1:A:953:A:H4'	1:A:954:G:H5''	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:45:VAL:HG23	19:S:46:GLY:N	1.97	0.78
1:A:1295:U:OP1	19:S:6:LYS:HG3	1.84	0.78
1:A:1374:U:H2'	1:A:1375:G:C8	2.19	0.78
21:U:6:ARG:HH21	21:U:15:ARG:HG2	1.48	0.78
1:A:1135:A:H5'	10:J:13:HIS:HD2	1.45	0.78
1:A:1418:G:H2'	1:A:1419:U:C6	2.19	0.78
1:A:788:U:H5''	1:A:789:C:OP2	1.82	0.78
22:X:4:PSU:H2'	22:X:5:G:H5''	1.64	0.77
1:A:779:C:H5''	1:A:780:C:OP2	1.84	0.77
1:A:972:A:N3	1:A:972:A:H2'	1.99	0.77
1:A:1296:C:OP2	19:S:6:LYS:HE2	1.84	0.77
1:A:1008:C:H3'	1:A:1008:C:H6	1.50	0.77
1:A:1313:G:H4'	1:A:1313:G:OP1	1.83	0.77
3:C:39:ILE:HG22	3:C:40:ARG:H	1.47	0.77
10:J:38:ILE:CD1	10:J:71:LEU:HD23	2.14	0.77
23:Y:34:G:H2'	23:Y:35:A:C8	2.20	0.76
1:A:1512:A:H2'	1:A:1513:C:H5'	1.65	0.76
1:A:961:A:H5'	1:A:962:C:OP2	1.85	0.76
1:A:953:A:C5'	1:A:953:A:H8	1.99	0.76
18:R:36:ASN:OD1	18:R:39:VAL:HB	1.86	0.76
9:I:88:TYR:O	9:I:89:ASN:HB2	1.86	0.76
1:A:1311:A:H2'	1:A:1312:U:H5'	1.65	0.76
1:A:1231:C:O2'	9:I:73:GLN:NE2	2.18	0.76
14:N:24:CYS:HB3	14:N:40:CYS:HB3	1.68	0.75
1:A:1104:U:H2'	1:A:1105:U:C6	2.20	0.75
15:O:33:THR:HG23	15:O:63:ARG:NH1	2.01	0.75
1:A:1349:C:O2'	1:A:1350:C:H5'	1.87	0.75
1:A:1230:A:H4'	1:A:1231:C:OP1	1.86	0.75
1:A:1104:U:H2'	1:A:1105:U:H6	1.51	0.75
15:O:33:THR:HG23	15:O:63:ARG:HH12	1.50	0.75
2:B:111:ARG:HG2	2:B:111:ARG:NH1	1.92	0.75
6:F:69:GLU:O	6:F:72:VAL:HG12	1.86	0.75
3:C:11:ARG:O	3:C:14:ILE:O	2.04	0.75
1:A:1351:G:C2'	1:A:1352:C:H5'	2.17	0.75
19:S:6:LYS:O	19:S:7:LYS:HD3	1.86	0.75
10:J:90:LEU:N	10:J:91:PRO:HD3	1.99	0.75
3:C:76:VAL:HG21	3:C:103:VAL:HG21	1.69	0.75
1:A:924:A:H2'	1:A:925:G:C8	2.22	0.75
1:A:417:U:O2	3:C:127:ARG:NH2	2.20	0.75
23:Y:34:G:H2'	23:Y:35:A:H8	1.52	0.74
5:E:68:GLU:HG3	5:E:68:GLU:O	1.84	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:28:ARG:HG2	16:P:28:ARG:NH1	2.03	0.74
3:C:15:THR:HG22	3:C:15:THR:O	1.85	0.74
1:A:1208:C:N4	13:M:104:ARG:HG2	2.03	0.74
1:A:1233:A:H8	9:I:68:GLY:HA2	1.52	0.74
4:D:6:GLY:O	4:D:8:VAL:HG23	1.87	0.74
3:C:110:ASN:HD21	3:C:140:ARG:HB3	1.48	0.74
8:H:109:ILE:CG2	8:H:137:VAL:HB	2.17	0.74
12:L:89:ARG:HA	12:L:97:ARG:HA	1.70	0.74
1:A:1151:A:H2'	1:A:1152:A:C8	2.22	0.74
10:J:8:LEU:HD11	10:J:20:ALA:HB1	1.70	0.74
1:A:1480:A:H2	1:A:1483:G:H1	1.34	0.73
1:A:1049:C:C2'	1:A:1050:A:H5'	2.17	0.73
10:J:4:ILE:HG22	10:J:74:ILE:HG13	1.68	0.73
14:N:24:CYS:HB2	14:N:40:CYS:HB3	1.69	0.73
1:A:957:C:C3'	1:A:958:C:H5''	2.17	0.73
13:M:10:PRO:HB2	13:M:18:ALA:HB1	1.71	0.73
7:G:50:ILE:HG21	7:G:61:VAL:HG21	1.70	0.73
1:A:1100:G:H4'	9:I:104:ARG:NH2	2.04	0.73
4:D:26:CYS:HA	4:D:31:CYS:HA	1.71	0.73
8:H:89:PRO:HA	8:H:92:ARG:NH1	2.04	0.73
1:A:1011:C:H2'	1:A:1012:G:H5'	1.71	0.73
1:A:79:A:H61	1:A:85:C:H42	1.36	0.73
1:A:1334:C:H2'	1:A:1335:G:H8	1.53	0.73
1:A:1049:C:H2'	1:A:1050:A:H5'	1.69	0.73
1:A:969:U:C5	1:A:1194:U:H1'	2.24	0.73
7:G:37:ASN:OD1	9:I:41:VAL:HG23	1.89	0.72
1:A:1308:C:OP1	21:U:12:LYS:NZ	2.21	0.72
1:A:961:A:N3	1:A:961:A:H3'	2.03	0.72
1:A:836:G:N7	1:A:847:G:N7	2.37	0.72
7:G:65:ALA:O	7:G:69:VAL:HG23	1.90	0.72
8:H:109:ILE:HG22	8:H:137:VAL:HB	1.71	0.72
2:B:97:TRP:HZ3	2:B:176:GLU:OE2	1.72	0.72
1:A:1244:C:H2'	1:A:1245:C:C6	2.24	0.72
13:M:3:ARG:HA	13:M:8:GLU:O	1.90	0.72
17:Q:65:ILE:N	17:Q:65:ILE:HD12	2.04	0.72
10:J:79:ARG:HH11	10:J:82:ILE:CD1	2.02	0.72
1:A:859:G:P	12:L:12:ARG:HH22	2.13	0.72
5:E:101:ILE:CD1	5:E:119:LEU:HD23	2.19	0.71
1:A:1184:G:C4	14:N:42:ILE:HD12	2.25	0.71
1:A:250:G:OP1	17:Q:67:LYS:O	2.09	0.71
1:A:1408:U:H3	1:A:1453:G:H1	1.34	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1338:G:H2'	1:A:1339:A:H8	1.53	0.71
3:C:73:PRO:O	3:C:76:VAL:HG22	1.91	0.71
1:A:982:G:N3	1:A:983:A:H1'	2.05	0.71
4:D:58:LEU:HD22	4:D:62:GLN:HG2	1.72	0.71
10:J:42:THR:HG23	10:J:67:THR:O	1.91	0.71
4:D:18:LYS:HD2	4:D:31:CYS:HB2	1.71	0.71
1:A:1233:A:H5'	9:I:12:GLU:OE1	1.91	0.71
10:J:49:VAL:HG22	14:N:41:ARG:HB2	1.72	0.71
12:L:25:PRO:C	12:L:27:LEU:H	1.94	0.71
2:B:80:ILE:CD1	2:B:212:GLN:HA	2.20	0.71
1:A:1231:C:H2'	1:A:1232:A:OP1	1.91	0.70
1:A:1183:A:H4'	1:A:1184:G:O5'	1.91	0.70
3:C:30:ARG:HH11	3:C:30:ARG:HB2	1.56	0.70
3:C:55:VAL:HG12	3:C:55:VAL:O	1.90	0.70
10:J:8:LEU:HD13	10:J:20:ALA:HB3	1.73	0.70
2:B:208:ILE:HD12	2:B:208:ILE:H	1.56	0.70
1:A:1135:A:C5'	10:J:13:HIS:CD2	2.74	0.70
1:A:1198:G:H5''	14:N:5:ALA:HB2	1.74	0.70
22:X:3:A:H8	22:X:3:A:H5''	1.56	0.70
2:B:97:TRP:CZ3	2:B:176:GLU:OE2	2.44	0.70
5:E:80:ILE:HD13	5:E:91:LEU:HB2	1.72	0.70
3:C:23:TYR:HD1	3:C:24:ALA:N	1.84	0.70
13:M:50:GLU:O	13:M:54:VAL:HG23	1.91	0.70
1:A:1108:U:C6	1:A:1108:U:C5'	2.65	0.70
1:A:1342:A:H2'	1:A:1343:G:C8	2.27	0.70
2:B:74:LYS:HG2	2:B:75:LYS:HE3	1.72	0.70
1:A:211:U:H4'	1:A:212:G:O5'	1.92	0.70
19:S:22:LEU:HD12	19:S:26:GLY:HA3	1.74	0.69
1:A:953:A:H5'	1:A:953:A:H8	1.58	0.69
1:A:1329:G:H22	1:A:1356:G:H2'	1.56	0.69
1:A:1120:C:O2'	1:A:1121:G:N2	2.24	0.69
1:A:1232:A:P	1:A:1232:A:O4'	2.50	0.69
1:A:957:C:H3'	1:A:958:C:C5'	2.18	0.69
1:A:779:C:C5'	1:A:780:C:OP2	2.39	0.69
13:M:53:VAL:HG12	13:M:57:ARG:HH21	1.56	0.69
1:A:981:G:H22	1:A:1022:C:H6	1.38	0.69
1:A:1231:C:H41	1:A:1270:A:H62	1.39	0.69
1:A:1322:A:C8	1:A:1322:A:H5''	2.27	0.69
1:A:9:A:N7	4:D:208:SER:HB3	2.08	0.69
10:J:55:LYS:HD2	10:J:55:LYS:O	1.92	0.69
1:A:482:U:O2'	1:A:483:A:OP2	2.10	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1108:U:O4	10:J:5:ARG:CD	2.40	0.69
4:D:30:LYS:HA	4:D:34:GLU:HB2	1.75	0.69
18:R:64:ARG:HG3	18:R:64:ARG:HH11	1.58	0.69
1:A:1208:C:C4	13:M:104:ARG:HG2	2.28	0.69
1:A:1329:G:N2	1:A:1356:G:H2'	2.06	0.69
2:B:114:ARG:HG3	2:B:114:ARG:HH11	1.57	0.69
1:A:1198:G:H5''	14:N:5:ALA:CB	2.23	0.69
7:G:138:LYS:C	7:G:138:LYS:HD3	2.13	0.69
5:E:10:MET:O	5:E:10:MET:HG3	1.90	0.69
4:D:173:TRP:O	4:D:186:LEU:HB2	1.92	0.69
1:A:1244:C:H2'	1:A:1245:C:H6	1.58	0.68
22:X:3:A:C8	22:X:3:A:H5''	2.28	0.68
1:A:9:A:N7	4:D:208:SER:CB	2.56	0.68
12:L:110:VAL:O	12:L:122:THR:HG21	1.93	0.68
1:A:523:A:H2'	1:A:524:G:C8	2.28	0.68
1:A:1210:C:OP1	13:M:115:LYS:HE3	1.92	0.68
10:J:33:GLN:HB2	10:J:75:ILE:HD11	1.75	0.68
19:S:64:GLU:O	19:S:67:VAL:HG23	1.93	0.68
1:A:1231:C:H4'	9:I:36:TYR:OH	1.93	0.68
2:B:51:LEU:HD22	2:B:55:PHE:HE2	1.57	0.68
2:B:118:LEU:HB2	2:B:142:LEU:HD12	1.74	0.68
8:H:112:LEU:HD12	8:H:113:SER:N	2.08	0.68
8:H:51:VAL:HG11	8:H:60:ARG:NH1	2.07	0.68
1:A:983:A:N7	1:A:1020:C:N3	2.42	0.68
4:D:98:GLU:HG2	4:D:189:PRO:HG3	1.76	0.68
2:B:215:LEU:O	2:B:219:VAL:HG23	1.93	0.68
5:E:80:ILE:HD12	5:E:91:LEU:HB2	1.75	0.68
1:A:1382:C:H4'	1:A:1383:C:H5''	1.75	0.68
1:A:1480:A:H2	1:A:1483:G:N1	1.91	0.68
1:A:614:G:C8	1:A:614:G:H5''	2.27	0.68
1:A:197:U:H6	1:A:197:U:C5'	2.00	0.68
1:A:1185:C:OP1	14:N:3:ARG:HD3	1.94	0.68
8:H:112:LEU:HD12	8:H:112:LEU:C	2.14	0.68
1:A:162:G:H2'	1:A:163:G:H8	1.57	0.68
1:A:372:G:H5''	16:P:5:ARG:HD3	1.76	0.68
12:L:60:LEU:HB2	12:L:64:TYR:O	1.94	0.68
3:C:91:LEU:HB3	3:C:99:VAL:HG11	1.75	0.67
13:M:81:LEU:HD21	13:M:88:ARG:NH1	2.10	0.67
9:I:118:LYS:O	9:I:119:ALA:HB3	1.94	0.67
16:P:57:ARG:NH1	16:P:79:VAL:O	2.26	0.67
9:I:104:ARG:O	9:I:105:ASP:HB3	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:971:G:H4'	1:A:972:A:OP2	1.94	0.67
13:M:11:ARG:O	13:M:13:LYS:N	2.22	0.67
3:C:150:LYS:HD3	3:C:152:ILE:HD11	1.75	0.67
6:F:97:PHE:HB2	18:R:32:ARG:NH2	2.10	0.67
1:A:954:G:N2	1:A:1345:C:OP2	2.27	0.67
1:A:1310:C:OP1	21:U:20:LYS:NZ	2.28	0.67
1:A:1171:C:P	10:J:51:ARG:HH22	2.17	0.67
14:N:4:LYS:C	14:N:6:LEU:H	1.95	0.67
1:A:1116:G:C2	1:A:1125:G:N1	2.63	0.67
1:A:1176:U:H2'	1:A:1177:C:H6	1.60	0.67
1:A:803:A:C8	1:A:803:A:H5''	2.30	0.67
10:J:8:LEU:HD13	10:J:20:ALA:HB2	1.75	0.67
14:N:27:CYS:CB	14:N:43:CYS:HB3	2.24	0.67
1:A:508:G:H2'	1:A:509:C:C6	2.30	0.67
1:A:1036:G:HO2'	1:A:1181:U:H5	1.43	0.67
3:C:114:PRO:HD3	3:C:183:ASP:OD2	1.95	0.67
1:A:953:A:C5'	1:A:953:A:C8	2.78	0.66
1:A:958:C:H5'	1:A:958:C:H6	1.60	0.66
2:B:96:ARG:HB2	2:B:96:ARG:CZ	2.25	0.66
4:D:25:ARG:O	4:D:27:TYR:N	2.28	0.66
1:A:1233:A:C2'	1:A:1234:A:N7	2.54	0.66
3:C:15:THR:HG23	3:C:181:ASN:HA	1.77	0.66
20:T:87:LYS:HE3	20:T:87:LYS:HA	1.78	0.66
17:Q:27:PHE:HB2	17:Q:28:PRO:HD2	1.76	0.66
1:A:1300:A:H5''	19:S:10:PHE:HD2	1.61	0.66
1:A:386:C:H2'	1:A:387:G:C8	2.30	0.66
1:A:836:G:C5	1:A:847:G:N7	2.63	0.66
4:D:163:GLU:HG3	4:D:166:LYS:HE2	1.77	0.66
1:A:349:A:C8	1:A:349:A:H5'	2.31	0.66
1:A:1111:C:H4'	9:I:16:ARG:HH12	1.59	0.66
14:N:24:CYS:HB2	14:N:40:CYS:CB	2.26	0.66
8:H:103:VAL:HG21	8:H:109:ILE:O	1.95	0.66
3:C:30:ARG:NH1	3:C:30:ARG:HB2	2.11	0.66
1:A:148:C:H42	1:A:163:G:H1	1.43	0.66
16:P:67:THR:HG22	16:P:69:THR:H	1.60	0.66
4:D:14:ARG:HB2	4:D:40:PRO:HD2	1.78	0.66
4:D:25:ARG:C	4:D:27:TYR:H	1.98	0.66
6:F:21:LEU:O	6:F:25:ILE:HG13	1.96	0.66
13:M:40:ASN:OD1	13:M:41:PRO:HD2	1.96	0.66
8:H:122:ARG:NH1	8:H:122:ARG:HB2	2.11	0.66
1:A:1068:U:H3'	1:A:1069:U:C5	2.30	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:430:U:H2'	1:A:431:C:H6	1.61	0.66
3:C:62:ASP:HA	3:C:97:LYS:HG2	1.78	0.66
1:A:722:C:OP2	6:F:92:LYS:NZ	2.25	0.66
1:A:1355:U:H2'	1:A:1356:G:O5'	1.95	0.66
1:A:1144:C:H2'	1:A:1145:C:C6	2.31	0.66
1:A:353:G:C2	1:A:354:U:C5	2.83	0.66
17:Q:66:SER:OG	17:Q:69:LYS:HB2	1.95	0.65
3:C:156:ARG:HH21	3:C:161:GLU:HA	1.59	0.65
22:X:2:G:H2'	22:X:3:A:C5'	2.25	0.65
1:A:365:C:C2'	1:A:366:C:O5'	2.45	0.65
1:A:653:U:H2'	1:A:654:G:C8	2.31	0.65
1:A:1130:C:H4'	9:I:5:TYR:CE2	2.29	0.65
1:A:523:A:OP1	12:L:114:LYS:HG2	1.97	0.65
1:A:1036:G:N7	1:A:1182:C:H5'	2.11	0.65
14:N:36:PHE:O	14:N:36:PHE:CD2	2.49	0.65
1:A:1473:U:H2'	1:A:1474:C:H6	1.61	0.65
1:A:1223:G:H2'	1:A:1224:C:H6	1.61	0.65
1:A:1008:C:H3'	1:A:1008:C:C6	2.31	0.65
3:C:39:ILE:CG2	3:C:40:ARG:N	2.60	0.65
9:I:53:VAL:HG23	9:I:55:ALA:H	1.61	0.65
1:A:1118:U:O2	1:A:1118:U:H2'	1.97	0.65
1:A:1078:U:P	1:A:1091:G:H1	2.19	0.65
1:A:1333:U:O4'	7:G:33:ASP:HB3	1.96	0.65
2:B:86:GLU:HA	2:B:86:GLU:OE2	1.95	0.65
2:B:21:ARG:HH21	2:B:38:GLY:HA3	1.61	0.65
1:A:1117:G:O5'	1:A:1117:G:H8	1.80	0.65
19:S:9:VAL:O	19:S:11:VAL:N	2.29	0.65
1:A:1311:A:C2'	1:A:1312:U:H5'	2.27	0.65
5:E:51:VAL:HB	5:E:52:PRO:CD	2.26	0.65
2:B:111:ARG:HD3	2:B:145:LEU:HD11	1.79	0.65
11:K:48:ILE:HD13	11:K:48:ILE:N	2.11	0.65
1:A:1325:G:H2'	1:A:1326:C:C6	2.32	0.65
10:J:23:ILE:O	10:J:23:ILE:HG22	1.97	0.65
9:I:114:TYR:HE2	10:J:60:ARG:H	1.46	0.64
14:N:27:CYS:O	14:N:29:ARG:HB3	1.96	0.64
1:A:954:G:C8	1:A:1340:U:O2	2.51	0.64
1:A:1109:U:O2	1:A:1109:U:C2'	2.45	0.64
14:N:24:CYS:CB	14:N:40:CYS:CB	2.75	0.64
1:A:1133:U:H4'	10:J:41:PRO:HG3	1.79	0.64
17:Q:86:GLU:O	17:Q:90:ILE:HG12	1.96	0.64
1:A:349:A:H8	1:A:349:A:H5'	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1233:A:H1'	1:A:1353:G:H4'	1.80	0.64
1:A:1259:C:H1'	1:A:1264:C:H1'	1.80	0.64
1:A:199:U:O4'	20:T:103:GLY:HA2	1.97	0.64
3:C:70:VAL:CG1	3:C:71:ALA:N	2.61	0.64
2:B:96:ARG:O	2:B:98:LEU:HD23	1.98	0.64
15:O:79:ARG:O	15:O:83:GLU:HG2	1.97	0.64
1:A:1252:C:OP2	21:U:24:ARG:NH2	2.31	0.64
17:Q:45:HIS:HB3	17:Q:72:ARG:HG2	1.79	0.64
8:H:35:ILE:HG23	8:H:111:ILE:HG21	1.80	0.64
10:J:90:LEU:H	10:J:91:PRO:CD	2.04	0.64
12:L:33:ARG:O	12:L:85:ILE:HG22	1.98	0.64
5:E:8:GLU:HA	5:E:33:VAL:O	1.97	0.64
1:A:836:G:C6	1:A:847:G:C8	2.86	0.64
1:A:400:U:O2'	1:A:401:U:H5'	1.97	0.64
1:A:1472:G:O2'	1:A:1473:U:H5'	1.98	0.64
15:O:70:LEU:HD23	15:O:78:TYR:HA	1.78	0.64
4:D:91:SER:OG	4:D:92:VAL:N	2.30	0.64
8:H:17:THR:HB	8:H:78:GLN:OE1	1.98	0.64
19:S:67:VAL:HG12	19:S:68:GLY:H	1.63	0.64
1:A:1316:G:H5''	1:A:1317:C:OP2	1.98	0.64
1:A:295:G:H2'	1:A:296:A:C8	2.33	0.64
2:B:21:ARG:HD2	2:B:39:ILE:CG2	2.20	0.63
3:C:43:LEU:O	3:C:47:LEU:HB2	1.98	0.63
15:O:39:LEU:CD1	15:O:56:LEU:HB2	2.28	0.63
5:E:91:LEU:CD1	5:E:120:THR:HG22	2.28	0.63
6:F:97:PHE:HB2	18:R:32:ARG:HH21	1.63	0.63
14:N:26:ARG:NH1	14:N:47:LEU:HD21	2.14	0.63
1:A:1477:A:H5'	1:A:1477:A:H8	1.64	0.63
2:B:107:THR:HA	2:B:110:GLN:NE2	2.13	0.63
1:A:1375:G:N2	1:A:1480:A:H8	1.96	0.63
1:A:68:C:O2'	1:A:166:A:H1'	1.99	0.63
12:L:41:ARG:HH22	12:L:57:LYS:HE2	1.62	0.63
8:H:73:ASP:OD1	8:H:75:ARG:HD3	1.99	0.63
12:L:46:LYS:NZ	12:L:47:LYS:HE3	2.13	0.63
1:A:1052:C:O2'	1:A:1174:C:H1'	1.98	0.63
9:I:88:TYR:CD1	9:I:88:TYR:O	2.52	0.63
1:A:1521:C:N4	2:B:23:ARG:NH2	2.42	0.63
9:I:89:ASN:OD1	9:I:91:ASP:HB2	1.98	0.63
15:O:39:LEU:HD12	15:O:56:LEU:HB2	1.81	0.63
2:B:69:LEU:HD12	2:B:70:PHE:N	2.13	0.63
21:U:10:ARG:NH1	21:U:10:ARG:CG	2.38	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:59:ARG:HG2	3:C:64:VAL:HG12	1.80	0.63
3:C:6:HIS:CE1	3:C:8:ILE:HB	2.34	0.63
17:Q:80:GLY:O	17:Q:82:MET:N	2.32	0.63
11:K:92:GLU:HA	11:K:95:ILE:HG13	1.80	0.63
20:T:73:HIS:O	20:T:74:LYS:CG	2.47	0.63
19:S:22:LEU:HD12	19:S:26:GLY:CA	2.29	0.63
2:B:158:LEU:H	2:B:158:LEU:CD1	2.11	0.62
1:A:1207:A:H2'	1:A:1208:C:C5	2.33	0.62
1:A:1329:G:C5	9:I:107:ARG:NH2	2.64	0.62
1:A:1481:A:H5'	1:A:1509:A:C1'	2.28	0.62
2:B:105:PHE:HE1	2:B:155:LEU:HD12	1.63	0.62
3:C:188:LEU:O	3:C:189:ALA:HB2	1.99	0.62
1:A:1261:A:H5''	1:A:1262:A:OP1	1.99	0.62
2:B:158:LEU:N	2:B:158:LEU:HD12	2.12	0.62
1:A:81:U:OP2	1:A:81:U:C6	2.50	0.62
1:A:1384:G:C2	1:A:1385:C:H1'	2.33	0.62
1:A:1515:U:O2'	1:A:1516:C:P	2.57	0.62
1:A:1232:A:H1'	1:A:1233:A:N7	2.14	0.62
19:S:5:LEU:HA	19:S:6:LYS:NZ	2.14	0.62
4:D:11:LEU:O	4:D:12:CYS:C	2.37	0.62
1:A:45:G:C2	1:A:46:U:H1'	2.35	0.62
4:D:5:ILE:HG22	4:D:5:ILE:O	2.00	0.62
1:A:429:C:H2'	1:A:430:U:H5'	1.80	0.62
1:A:231:C:H5'	17:Q:70:ARG:HG2	1.81	0.62
1:A:1198:G:O2'	1:A:1199:C:H5'	2.00	0.62
1:A:1128:C:H4'	1:A:1129:A:O5'	1.99	0.62
3:C:7:PRO:O	3:C:11:ARG:HG3	2.00	0.62
1:A:1300:A:H5''	19:S:10:PHE:CD2	2.35	0.62
10:J:50:ILE:CD1	10:J:50:ILE:H	2.08	0.62
1:A:1408:U:H2'	1:A:1409:C:C6	2.34	0.62
6:F:67:MET:HB2	6:F:68:PRO:HD2	1.81	0.62
1:A:668:A:O2'	11:K:38:ASN:HB3	1.99	0.62
9:I:53:VAL:HG11	9:I:85:LEU:HD11	1.82	0.62
7:G:51:GLN:O	7:G:53:LYS:N	2.33	0.62
18:R:85:LEU:HD23	18:R:88:LYS:CG	2.28	0.61
1:A:1176:U:H2'	1:A:1177:C:C6	2.34	0.61
7:G:51:GLN:OE1	7:G:51:GLN:HA	2.00	0.61
1:A:144:A:H2'	1:A:145:C:C6	2.34	0.61
1:A:1313:G:C4'	1:A:1313:G:OP1	2.47	0.61
22:X:2:G:H2'	22:X:3:A:O5'	2.00	0.61
1:A:207:G:H2'	1:A:208:C:O4'	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:51:VAL:HB	5:E:52:PRO:HD3	1.83	0.61
10:J:49:VAL:C	10:J:60:ARG:HB3	2.21	0.61
6:F:23:LYS:NZ	6:F:42:GLU:OE2	2.33	0.61
5:E:144:THR:O	5:E:148:VAL:HG23	2.00	0.61
8:H:6:ILE:O	8:H:10:LEU:HG	2.01	0.61
1:A:1014:G:C2	1:A:1015:G:O6	2.54	0.61
2:B:21:ARG:HB3	2:B:39:ILE:HA	1.81	0.61
16:P:22:THR:HA	16:P:33:ILE:HG13	1.80	0.61
1:A:644:G:OP1	15:O:5:LYS:HD2	2.01	0.61
10:J:94:VAL:HG12	10:J:95:GLU:N	2.15	0.61
2:B:96:ARG:HB2	2:B:96:ARG:NH1	2.16	0.61
1:A:1078:U:H2'	1:A:1079:C:C6	2.35	0.61
19:S:6:LYS:CG	19:S:7:LYS:HE3	2.30	0.61
9:I:104:ARG:O	9:I:104:ARG:HD2	2.00	0.61
17:Q:66:SER:O	17:Q:70:ARG:NH1	2.34	0.61
3:C:70:VAL:CG1	3:C:72:LYS:H	2.09	0.61
1:A:482:U:O2'	1:A:483:A:P	2.58	0.61
1:A:1108:U:H5'	1:A:1109:U:O4	1.99	0.61
9:I:4:TYR:CZ	9:I:88:TYR:HD2	2.19	0.61
4:D:8:VAL:O	4:D:10:ARG:N	2.33	0.61
4:D:196:LEU:HD22	4:D:197:PRO:HD2	1.83	0.61
6:F:43:LEU:HD23	6:F:46:ARG:NH1	2.15	0.61
7:G:35:LYS:HE3	7:G:38:LEU:HD23	1.83	0.61
13:M:94:ARG:HH11	13:M:94:ARG:HA	1.64	0.61
1:A:952:A:OP1	1:A:952:A:H8	1.83	0.61
1:A:765:A:H5'	1:A:766:A:OP2	2.01	0.61
10:J:45:ARG:NH1	10:J:45:ARG:CB	2.49	0.60
1:A:265:C:H2'	1:A:266:A:C8	2.35	0.60
1:A:193:G:H8	1:A:193:G:H5''	1.65	0.60
10:J:96:ILE:H	10:J:96:ILE:CD1	2.13	0.60
1:A:958:C:C5'	1:A:958:C:H6	2.13	0.60
1:A:1375:G:H21	1:A:1480:A:H8	1.48	0.60
7:G:38:LEU:C	7:G:38:LEU:HD12	2.22	0.60
1:A:1184:G:C2'	1:A:1185:C:H5'	2.31	0.60
14:N:4:LYS:C	14:N:6:LEU:N	2.55	0.60
20:T:67:ALA:O	20:T:73:HIS:CE1	2.54	0.60
3:C:34:LEU:O	3:C:38:ARG:HG2	2.01	0.60
1:A:344:G:H2'	1:A:344:G:N3	2.16	0.60
9:I:99:LEU:HB2	9:I:101:PHE:CE1	2.37	0.60
13:M:32:GLU:O	13:M:35:GLU:HG2	2.00	0.60
2:B:51:LEU:HD22	2:B:55:PHE:CE2	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:110:ASN:HD22	3:C:140:ARG:HB3	1.63	0.60
21:U:17:THR:O	21:U:22:ARG:NH1	2.35	0.60
2:B:22:LYS:HD2	2:B:22:LYS:N	2.16	0.60
1:A:1043:C:H5	3:C:2:GLY:CA	2.04	0.60
20:T:10:LEU:O	20:T:13:LEU:HG	2.02	0.60
1:A:1137:G:H2'	1:A:1138:G:C8	2.37	0.60
14:N:29:ARG:HD3	14:N:40:CYS:HB2	1.84	0.60
17:Q:58:GLU:O	17:Q:59:ILE:HD13	2.00	0.60
18:R:73:ALA:HB3	18:R:79:LEU:HD12	1.83	0.60
2:B:111:ARG:HB3	2:B:149:LEU:HD11	1.84	0.60
9:I:114:TYR:CE2	10:J:59:SER:HA	2.37	0.60
1:A:1137:G:H2'	1:A:1138:G:H8	1.67	0.60
1:A:1223:G:H2'	1:A:1224:C:C6	2.36	0.59
1:A:1477:A:H5'	1:A:1477:A:C8	2.36	0.59
18:R:44:LEU:CD1	18:R:79:LEU:HD22	2.32	0.59
1:A:1037:C:OP2	1:A:1179:G:OP2	2.20	0.59
3:C:155:GLY:O	3:C:156:ARG:HB2	2.01	0.59
18:R:46:GLU:CD	18:R:46:GLU:N	2.53	0.59
1:A:835:C:H2'	1:A:836:G:O4'	2.02	0.59
1:A:516:A:O2'	1:A:517:A:OP1	2.14	0.59
1:A:438:C:H2'	1:A:439:C:H6	1.67	0.59
3:C:15:THR:O	3:C:15:THR:CG2	2.49	0.59
1:A:544:U:H5'	1:A:550:G:N2	2.17	0.59
16:P:26:ARG:HD2	16:P:31:LYS:O	2.01	0.59
1:A:1333:U:C2'	1:A:1334:C:H5'	2.33	0.59
1:A:1043:C:O2	1:A:1180:G:C2	2.55	0.59
12:L:28:LYS:O	12:L:30:ALA:N	2.32	0.59
1:A:1039:U:O2'	1:A:1040:G:H5'	2.02	0.59
1:A:778:A:H2'	1:A:779:C:C6	2.38	0.59
2:B:80:ILE:HD13	2:B:212:GLN:HA	1.84	0.59
1:A:82:U:C6	1:A:83:U:O2	2.56	0.59
9:I:53:VAL:O	9:I:54:ASP:HB2	2.02	0.59
10:J:33:GLN:CB	10:J:75:ILE:HD11	2.33	0.59
1:A:414:C:H2'	1:A:415:C:C6	2.37	0.59
3:C:131:ARG:HE	3:C:166:GLU:HG2	1.68	0.59
16:P:3:LYS:O	16:P:21:VAL:HA	2.02	0.59
1:A:1470:A:C2	22:X:5:G:H8	2.20	0.59
4:D:18:LYS:CD	4:D:31:CYS:HB2	2.32	0.59
4:D:150:GLU:HA	4:D:153:ARG:CD	2.19	0.59
12:L:25:PRO:C	12:L:27:LEU:N	2.56	0.59
10:J:38:ILE:HD11	10:J:71:LEU:HD23	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1057:G:O3'	2:B:103:THR:HG22	2.02	0.59
10:J:90:LEU:N	10:J:91:PRO:CD	2.65	0.59
3:C:15:THR:CG2	3:C:181:ASN:HA	2.33	0.59
19:S:10:PHE:HD1	19:S:10:PHE:H	1.46	0.58
3:C:70:VAL:CG1	3:C:71:ALA:H	2.15	0.58
14:N:26:ARG:NH1	14:N:47:LEU:CD2	2.66	0.58
5:E:147:ASP:OD1	5:E:147:ASP:N	2.36	0.58
7:G:16:LEU:H	7:G:16:LEU:HD23	1.69	0.58
2:B:74:LYS:HE3	2:B:205:ASP:O	2.03	0.58
8:H:122:ARG:CZ	8:H:122:ARG:HB2	2.33	0.58
2:B:71:VAL:HG12	2:B:93:VAL:HB	1.85	0.58
1:A:1074:U:H5''	1:A:1075:A:OP2	2.03	0.58
4:D:15:GLU:OE2	4:D:59:ARG:NH1	2.37	0.58
1:A:798:A:H2'	1:A:800:A:H5''	1.84	0.58
3:C:52:LEU:H	3:C:52:LEU:HD23	1.68	0.58
1:A:691:C:H4'	11:K:20:TYR:CD2	2.38	0.58
8:H:119:LEU:HD12	8:H:124:ALA:HB2	1.84	0.58
1:A:1184:G:H21	14:N:43:CYS:HB3	1.69	0.58
10:J:96:ILE:N	10:J:96:ILE:CD1	2.66	0.58
1:A:637:A:P	8:H:56:LYS:HZ1	2.25	0.58
1:A:197:U:C6	1:A:197:U:C5'	2.80	0.58
13:M:90:LEU:O	13:M:91:ARG:HB2	2.02	0.58
1:A:483:A:H4'	1:A:484:G:OP1	2.03	0.58
1:A:324:C:O2	1:A:324:C:C2'	2.50	0.58
1:A:251:G:O6	1:A:262:G:O6	2.20	0.58
3:C:10:PHE:CE2	3:C:178:LEU:HD13	2.39	0.58
1:A:923:G:N3	1:A:923:G:H2'	2.17	0.58
1:A:469:G:H5'	1:A:471:U:O4'	2.03	0.58
1:A:1114:G:C6	1:A:1115:C:N4	2.72	0.58
2:B:136:VAL:O	2:B:140:HIS:HB2	2.03	0.58
9:I:44:VAL:O	9:I:51:ARG:NH2	2.35	0.58
1:A:1355:U:C2'	1:A:1356:G:O5'	2.51	0.58
19:S:5:LEU:HA	19:S:6:LYS:HZ1	1.67	0.58
1:A:1481:A:H5'	1:A:1509:A:H1'	1.84	0.58
4:D:100:ARG:NH1	4:D:137:SER:HA	2.18	0.58
1:A:1351:G:C2	1:A:1352:C:C5	2.92	0.58
1:A:1310:C:H2'	1:A:1311:A:O4'	2.04	0.58
1:A:1084:A:H4'	1:A:1085:A:O5'	2.04	0.58
2:B:80:ILE:HG13	2:B:80:ILE:O	2.01	0.58
1:A:165:U:O2'	1:A:166:A:H5'	2.04	0.58
15:O:74:ASP:O	15:O:76:GLU:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1158:A:H3'	1:A:1159:G:C8	2.39	0.58
20:T:73:HIS:C	20:T:74:LYS:CG	2.71	0.58
5:E:43:LEU:HD21	5:E:132:ALA:HB1	1.85	0.58
1:A:937:A:H5''	1:A:938:U:OP2	2.04	0.58
16:P:67:THR:HG22	16:P:68:ASP:N	2.19	0.57
1:A:898:U:H2'	1:A:899:U:C6	2.38	0.57
6:F:10:LEU:HB2	6:F:59:TYR:HB3	1.86	0.57
1:A:1014:G:H1'	1:A:1015:G:N1	2.19	0.57
9:I:114:TYR:HD1	9:I:114:TYR:H	1.52	0.57
1:A:1068:U:H3'	1:A:1069:U:H5	1.69	0.57
3:C:16:ARG:HB2	3:C:16:ARG:HH11	1.68	0.57
2:B:15:VAL:H	2:B:16:HIS:CE1	2.22	0.57
1:A:1043:C:C2'	1:A:1044:G:H5'	2.35	0.57
1:A:648:G:OP1	18:R:64:ARG:NE	2.32	0.57
1:A:1329:G:C6	9:I:107:ARG:NH2	2.73	0.57
1:A:1470:A:OP1	12:L:46:LYS:HB2	2.05	0.57
22:X:5:G:H5''	22:X:5:G:N3	2.19	0.57
14:N:43:CYS:SG	14:N:43:CYS:O	2.62	0.57
1:A:1145:C:H2'	1:A:1146:C:H6	1.68	0.57
3:C:188:LEU:O	3:C:189:ALA:CB	2.53	0.57
3:C:130:VAL:O	3:C:134:ILE:HG12	2.04	0.57
1:A:103:A:H2'	1:A:322:G:N2	2.19	0.57
1:A:1351:G:C2	1:A:1352:C:C6	2.92	0.57
1:A:1184:G:H2'	1:A:1185:C:H5'	1.87	0.57
1:A:417:U:H1'	1:A:418:C:OP1	2.03	0.57
1:A:932:G:H4'	13:M:120:LYS:HD2	1.86	0.57
17:Q:99:SER:OG	17:Q:100:LYS:N	2.38	0.57
1:A:1172:G:OP1	3:C:4:LYS:HA	2.04	0.57
4:D:175:SER:HB3	4:D:186:LEU:HD11	1.86	0.57
1:A:262:G:H5''	1:A:264:C:H41	1.69	0.57
1:A:1421:G:H2'	1:A:1422:C:C6	2.39	0.57
1:A:1190:C:H2'	1:A:1191:C:H6	1.69	0.57
1:A:171:C:H2'	1:A:172:C:H6	1.69	0.57
7:G:31:MET:SD	7:G:34:GLY:HA2	2.43	0.57
2:B:75:LYS:HB2	2:B:76:GLN:HE21	1.70	0.57
19:S:50:ALA:HB1	19:S:57:HIS:HB3	1.86	0.57
1:A:1022:C:C6	1:A:1023:U:C5	2.92	0.57
1:A:1297:U:H2'	1:A:1298:G:O4'	2.05	0.57
2:B:35:GLU:HG3	2:B:35:GLU:O	2.05	0.57
1:A:1135:A:O2'	1:A:1136:C:H5'	2.05	0.57
10:J:4:ILE:HA	10:J:100:THR:HG22	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1354:G:O2'	1:A:1355:U:H5'	2.05	0.57
9:I:79:LEU:HD23	9:I:101:PHE:O	2.05	0.57
4:D:63:LYS:HD2	4:D:198:VAL:CG2	2.35	0.57
18:R:86:VAL:O	18:R:87:ARG:HG2	2.04	0.57
20:T:36:LEU:HD12	20:T:62:LEU:HD12	1.87	0.57
1:A:1200:C:H2'	1:A:1201:U:C6	2.40	0.57
22:X:4:PSU:O5'	22:X:4:PSU:H6	1.87	0.57
5:E:102:ALA:HA	5:E:120:THR:OG1	2.04	0.57
1:A:528:G:OP1	4:D:59:ARG:NH2	2.38	0.57
10:J:96:ILE:H	10:J:96:ILE:HD12	1.70	0.57
1:A:1188:G:C6	1:A:1189:G:C5	2.93	0.57
1:A:1106:A:H4'	10:J:37:PRO:HD2	1.87	0.57
3:C:29:TYR:OH	14:N:54:PRO:HD2	2.04	0.56
4:D:13:ARG:HA	4:D:33:MET:HE3	1.87	0.56
1:A:1395:C:H2'	1:A:1396:A:C8	2.39	0.56
1:A:1261:A:O2'	1:A:1263:U:OP2	2.23	0.56
8:H:4:ASP:OD2	8:H:85:ARG:NH1	2.35	0.56
1:A:1295:U:O4	19:S:4:SER:N	2.39	0.56
12:L:82:VAL:HB	12:L:106:ASP:OD2	2.04	0.56
1:A:1116:G:H2'	1:A:1117:G:C8	2.40	0.56
13:M:34:LEU:CD1	13:M:41:PRO:HA	2.35	0.56
3:C:22:TRP:CZ2	3:C:32:LEU:O	2.58	0.56
2:B:71:VAL:CG2	2:B:164:VAL:HG22	2.36	0.56
1:A:604:C:C2	4:D:135:LEU:HG	2.41	0.56
11:K:126:ARG:O	11:K:128:ALA:N	2.38	0.56
4:D:11:LEU:C	4:D:13:ARG:H	2.08	0.56
1:A:943:A:H4'	1:A:944:G:O5'	2.04	0.56
11:K:46:GLY:O	11:K:48:ILE:O	2.23	0.56
22:X:2:G:H2'	22:X:3:A:H5''	1.87	0.56
2:B:78:GLN:O	2:B:94:ASN:OD1	2.23	0.56
1:A:1502:C:OP1	11:K:120:ARG:NH1	2.39	0.56
1:A:890:C:O2'	1:A:891:A:H5'	2.06	0.56
1:A:1482:G:OP1	1:A:1485:A:H4'	2.05	0.56
1:A:1330:U:O2'	1:A:1331:A:H5'	2.05	0.56
1:A:430:U:H5'	1:A:430:U:H6	1.70	0.56
1:A:1145:C:H2'	1:A:1146:C:C6	2.40	0.56
3:C:37:GLN:O	3:C:40:ARG:HG3	2.06	0.56
6:F:23:LYS:O	6:F:27:GLN:HG2	2.05	0.56
18:R:37:VAL:O	18:R:41:LYS:HB3	2.06	0.56
12:L:68:ALA:HB1	12:L:100:ILE:HD12	1.88	0.56
1:A:1231:C:O2	1:A:1231:C:H3'	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:36:PHE:HD2	14:N:37:PHE:CE2	2.23	0.56
13:M:108:ARG:NH1	13:M:108:ARG:HG3	2.13	0.56
3:C:15:THR:O	3:C:16:ARG:HB2	2.06	0.56
15:O:56:LEU:HA	15:O:59:MET:HE2	1.87	0.56
1:A:606:A:C8	1:A:607:C:C5	2.93	0.56
6:F:47:ARG:HA	6:F:57:GLN:HG2	1.86	0.56
3:C:8:ILE:HG23	3:C:16:ARG:HG2	1.88	0.56
1:A:1073:U:H2'	1:A:1074:U:H6	1.71	0.56
1:A:36:G:H2'	1:A:37:C:C6	2.41	0.56
10:J:94:VAL:CG1	10:J:95:GLU:N	2.69	0.56
2:B:18:GLY:CA	2:B:42:ILE:HG23	2.30	0.56
1:A:144:A:H2'	1:A:145:C:H6	1.69	0.56
10:J:38:ILE:HD12	10:J:71:LEU:HD23	1.87	0.55
2:B:105:PHE:HE1	2:B:155:LEU:CD1	2.18	0.55
1:A:801:C:N3	1:A:1507:G:O6	2.38	0.55
1:A:378:A:H2'	1:A:379:A:C8	2.41	0.55
1:A:953:A:H5''	1:A:953:A:C8	2.41	0.55
9:I:36:TYR:HD2	9:I:37:PHE:CE1	2.24	0.55
5:E:80:ILE:CD1	5:E:91:LEU:HB3	2.35	0.55
9:I:4:TYR:HB2	9:I:19:LEU:HB2	1.88	0.55
9:I:48:GLU:N	9:I:49:PRO:CD	2.69	0.55
1:A:1132:C:O5'	1:A:1132:C:H6	1.89	0.55
1:A:365:C:H2'	1:A:366:C:O5'	2.06	0.55
7:G:51:GLN:C	7:G:53:LYS:H	2.08	0.55
1:A:262:G:C8	1:A:262:G:H5'	2.41	0.55
12:L:126:LYS:HA	12:L:129:ALA:O	2.06	0.55
19:S:5:LEU:HG	19:S:10:PHE:CE1	2.41	0.55
4:D:2:GLY:O	4:D:3:ARG:O	2.24	0.55
2:B:139:LYS:O	2:B:143:GLU:HG2	2.06	0.55
6:F:97:PHE:CB	18:R:32:ARG:HH21	2.18	0.55
1:A:9:A:N7	4:D:208:SER:HB2	2.21	0.55
18:R:73:ALA:CB	18:R:79:LEU:HD12	2.37	0.55
5:E:36:ASP:OD1	5:E:38:GLN:N	2.28	0.55
11:K:56:GLY:O	11:K:57:THR:O	2.25	0.55
2:B:153:ARG:HG3	2:B:154:LEU:HD23	1.89	0.55
1:A:825:U:H3'	1:A:826:C:O4'	2.05	0.55
20:T:43:LEU:HB3	20:T:52:ALA:HB2	1.89	0.55
1:A:1135:A:OP1	10:J:68:HIS:CE1	2.59	0.55
9:I:89:ASN:HB3	9:I:92:TYR:CD2	2.42	0.55
2:B:164:VAL:HB	2:B:186:ALA:HB2	1.88	0.55
1:A:1014:G:N3	1:A:1015:G:C6	2.75	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:48:ILE:HG22	11:K:49:GLY:N	2.19	0.55
1:A:162:G:H2'	1:A:163:G:C8	2.41	0.55
1:A:1477:A:O2'	1:A:1478:A:H5'	2.06	0.55
1:A:734:G:N3	15:O:23:GLY:HA3	2.22	0.55
1:A:386:C:O3'	16:P:28:ARG:NH2	2.40	0.55
1:A:324:C:H2'	1:A:324:C:O2	2.05	0.55
1:A:1140:A:H4'	1:A:1141:C:O5'	2.06	0.55
7:G:45:ASP:O	7:G:49:ILE:HG12	2.06	0.55
1:A:831:G:C2'	1:A:832:G:H5'	2.36	0.55
11:K:31:THR:HG22	11:K:42:TRP:HB3	1.89	0.55
2:B:78:GLN:NE2	2:B:94:ASN:O	2.39	0.55
19:S:29:ARG:C	19:S:31:ILE:H	2.10	0.55
1:A:1108:U:O2'	1:A:1263:U:O2	2.17	0.55
20:T:57:ARG:HH11	20:T:102:GLY:HA2	1.70	0.55
1:A:859:G:OP2	12:L:12:ARG:NH2	2.40	0.55
1:A:650:G:H5'	1:A:710:C:H1'	1.89	0.55
12:L:50:SER:O	12:L:51:ALA:HB2	2.07	0.55
15:O:7:GLU:OE1	15:O:38:ARG:NH2	2.40	0.55
10:J:38:ILE:HG13	10:J:71:LEU:HB3	1.88	0.55
13:M:4:ILE:HG22	13:M:5:ALA:N	2.22	0.55
1:A:1473:U:H2'	1:A:1474:C:C6	2.41	0.55
1:A:485:C:H2'	1:A:486:G:H8	1.72	0.55
9:I:65:VAL:O	9:I:66:ARG:HG3	2.06	0.55
22:X:5:G:C5'	22:X:5:G:N3	2.70	0.54
4:D:33:MET:CE	4:D:37:PRO:HA	2.35	0.54
1:A:1210:C:H4'	13:M:116:THR:HA	1.88	0.54
12:L:68:ALA:HB3	12:L:100:ILE:CD1	2.38	0.54
1:A:331:C:H2'	1:A:332:C:C6	2.43	0.54
3:C:126:ARG:O	3:C:128:PHE:N	2.40	0.54
1:A:962:C:H2'	1:A:963:C:H6	1.72	0.54
1:A:1270:A:C2	1:A:1334:C:H1'	2.42	0.54
1:A:1109:U:C6	1:A:1262:A:N7	2.74	0.54
19:S:6:LYS:HD2	19:S:6:LYS:N	2.22	0.54
2:B:35:GLU:HA	2:B:39:ILE:O	2.06	0.54
5:E:80:ILE:HD12	5:E:91:LEU:CB	2.33	0.54
1:A:417:U:OP2	1:A:417:U:H3'	2.08	0.54
4:D:196:LEU:CD2	4:D:197:PRO:HD2	2.38	0.54
9:I:99:LEU:HB2	9:I:101:PHE:HE1	1.70	0.54
1:A:954:G:OP2	1:A:1340:U:O2'	2.25	0.54
9:I:54:ASP:C	9:I:56:LEU:H	2.11	0.54
10:J:96:ILE:N	10:J:96:ILE:HD12	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:25:ILE:HD11	13:M:66:LEU:HD21	1.90	0.54
12:L:73:GLU:OE2	12:L:73:GLU:HA	2.07	0.54
10:J:50:ILE:HD13	14:N:41:ARG:HD3	1.89	0.54
1:A:429:C:C2'	1:A:430:U:H5'	2.37	0.54
2:B:78:GLN:HE22	2:B:95:GLN:NE2	2.05	0.54
1:A:485:C:H2'	1:A:486:G:C8	2.42	0.54
1:A:1100:G:H5''	1:A:1100:G:H8	1.72	0.54
1:A:721:A:H1'	6:F:73:ASN:HD21	1.73	0.54
2:B:55:PHE:HE1	2:B:218:ALA:HA	1.73	0.54
1:A:438:C:H2'	1:A:439:C:C6	2.42	0.54
12:L:68:ALA:CB	12:L:100:ILE:HD12	2.37	0.54
8:H:119:LEU:CD1	8:H:124:ALA:HA	2.37	0.54
8:H:80:ILE:O	8:H:80:ILE:HG22	2.07	0.54
2:B:86:GLU:C	2:B:88:ALA:H	2.11	0.54
2:B:105:PHE:CE1	2:B:155:LEU:CD1	2.91	0.54
21:U:5:ASP:O	21:U:11:GLY:HA3	2.08	0.54
1:A:406:G:H5''	1:A:407:A:OP1	2.07	0.54
17:Q:67:LYS:HA	17:Q:70:ARG:NH1	2.20	0.54
1:A:1374:U:H2'	1:A:1375:G:H8	1.68	0.54
15:O:74:ASP:C	15:O:76:GLU:H	2.11	0.54
18:R:50:ILE:HG12	18:R:70:ILE:HD13	1.89	0.54
13:M:59:TYR:O	13:M:63:THR:OG1	2.20	0.54
1:A:53:G:O2'	1:A:54:A:H5'	2.08	0.54
3:C:28:GLN:HA	3:C:31:HIS:CE1	2.43	0.54
5:E:53:LEU:O	5:E:57:LYS:HB2	2.07	0.54
13:M:45:VAL:O	13:M:48:LEU:HD22	2.08	0.54
1:A:1404:G:N2	1:A:1457:C:N3	2.51	0.54
20:T:73:HIS:C	20:T:74:LYS:HG3	2.28	0.53
1:A:970:U:H4'	1:A:971:G:O5'	2.08	0.53
12:L:41:ARG:HH22	12:L:57:LYS:CE	2.21	0.53
1:A:955:A:C2'	1:A:956:A:H5'	2.37	0.53
2:B:159:PRO:HB2	2:B:161:ALA:O	2.07	0.53
2:B:187:LEU:HD21	2:B:203:GLY:HA3	1.89	0.53
12:L:47:LYS:CB	12:L:48:PRO:CD	2.58	0.53
2:B:88:ALA:HB2	2:B:219:VAL:HG12	1.89	0.53
7:G:16:LEU:CD1	9:I:42:ARG:HA	2.38	0.53
10:J:6:ILE:HG22	10:J:98:ILE:HA	1.90	0.53
1:A:946:A:H4'	1:A:947:A:OP2	2.08	0.53
19:S:4:SER:O	19:S:5:LEU:HD22	2.08	0.53
12:L:81:SER:O	12:L:106:ASP:CB	2.51	0.53
4:D:14:ARG:HG3	4:D:15:GLU:N	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:612:G:O2'	1:A:613:G:H5'	2.08	0.53
6:F:62:TRP:CG	18:R:35:ARG:NH1	2.76	0.53
1:A:657:G:H2'	1:A:658:G:C8	2.42	0.53
1:A:1008:C:C3'	1:A:1008:C:C6	2.91	0.53
2:B:21:ARG:NH2	2:B:38:GLY:HA3	2.24	0.53
17:Q:68:ARG:N	17:Q:70:ARG:HH11	2.06	0.53
1:A:1057:G:O3'	2:B:103:THR:CG2	2.56	0.53
1:A:994:A:H2'	1:A:995:A:C8	2.43	0.53
1:A:675:G:O6	11:K:52:GLY:HA2	2.09	0.53
1:A:1030:G:O5'	1:A:1030:G:H8	1.90	0.53
12:L:47:LYS:HB3	12:L:48:PRO:HD2	1.80	0.53
1:A:921:U:C3'	1:A:922:G:H5'	2.38	0.53
4:D:18:LYS:HG3	4:D:31:CYS:CB	2.38	0.53
3:C:90:GLU:O	3:C:93:LYS:HB3	2.08	0.53
9:I:54:ASP:HA	9:I:56:LEU:HD12	1.91	0.53
3:C:152:ILE:HG13	3:C:167:TRP:HB2	1.91	0.53
2:B:187:LEU:HD23	2:B:201:ILE:O	2.09	0.53
12:L:29:GLY:O	12:L:30:ALA:O	2.25	0.53
3:C:70:VAL:HG12	3:C:72:LYS:N	2.13	0.53
7:G:38:LEU:HD12	7:G:38:LEU:O	2.08	0.53
1:A:1231:C:N4	1:A:1270:A:H62	2.05	0.53
1:A:1335:G:C2'	1:A:1336:C:H5'	2.38	0.53
1:A:1346:A:H1'	1:A:1348:G:N7	2.24	0.53
14:N:37:PHE:O	14:N:39:LEU:HG	2.09	0.53
1:A:1044:G:O2'	1:A:1045:U:H5'	2.08	0.53
1:A:971:G:N3	1:A:971:G:H2'	2.23	0.53
1:A:1101:C:H1'	1:A:1161:A:C4	2.44	0.53
3:C:18:TRP:CD1	14:N:54:PRO:HA	2.44	0.53
1:A:921:U:H2'	1:A:921:U:O2	2.08	0.53
1:A:1143:G:H2'	1:A:1144:C:O5'	2.09	0.53
3:C:22:TRP:O	3:C:22:TRP:CE3	2.62	0.53
17:Q:87:LYS:HA	17:Q:87:LYS:HE3	1.91	0.53
1:A:938:U:H2'	1:A:938:U:O2	2.08	0.53
3:C:87:LEU:HD23	3:C:90:GLU:OE2	2.09	0.53
14:N:41:ARG:HA	14:N:44:LEU:HD13	1.90	0.52
1:A:429:C:O2'	1:A:430:U:H5''	2.09	0.52
18:R:56:THR:CB	18:R:58:LEU:HD13	2.37	0.52
1:A:38:U:O2'	1:A:484:G:H4'	2.09	0.52
2:B:101:MET:O	2:B:105:PHE:HA	2.09	0.52
1:A:1426:G:H4'	1:A:1427:A:O5'	2.10	0.52
10:J:27:ALA:HB2	10:J:85:LEU:HD11	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:87:GLY:HA2	12:L:98:TYR:HA	1.91	0.52
1:A:1253:G:H8	1:A:1253:G:O5'	1.92	0.52
4:D:13:ARG:HA	4:D:33:MET:CE	2.39	0.52
14:N:4:LYS:HA	14:N:7:ILE:HG12	1.90	0.52
1:A:429:C:O2'	1:A:430:U:C5'	2.56	0.52
1:A:896:A:H2'	1:A:897:A:C8	2.43	0.52
1:A:623:G:O2'	1:A:624:A:H5'	2.09	0.52
12:L:47:LYS:CG	12:L:48:PRO:HD3	2.40	0.52
14:N:4:LYS:O	14:N:6:LEU:N	2.42	0.52
1:A:82:U:C5	1:A:83:U:O2	2.61	0.52
1:A:732:C:H4'	1:A:733:C:O5'	2.07	0.52
9:I:26:VAL:HG13	9:I:61:ALA:HB3	1.90	0.52
20:T:48:LYS:HB3	20:T:51:GLU:CD	2.30	0.52
6:F:80:ARG:HB3	6:F:88:VAL:HG21	1.91	0.52
1:A:953:A:H4'	1:A:954:G:C5'	2.38	0.52
1:A:1470:A:H2	22:X:5:G:H8	1.57	0.52
17:Q:68:ARG:H	17:Q:70:ARG:NH1	2.07	0.52
2:B:7:VAL:O	2:B:217:ARG:NH1	2.38	0.52
3:C:52:LEU:H	3:C:52:LEU:CD2	2.22	0.52
11:K:16:SER:O	11:K:35:PRO:HD3	2.09	0.52
7:G:16:LEU:O	7:G:17:VAL:HG23	2.08	0.52
9:I:88:TYR:CG	9:I:88:TYR:O	2.63	0.52
18:R:19:LYS:HD3	18:R:20:ALA:H	1.75	0.52
7:G:26:PHE:HB2	7:G:101:LEU:HD22	1.92	0.52
1:A:1332:A:C6	1:A:1333:U:N3	2.78	0.52
9:I:36:TYR:CD2	9:I:37:PHE:CE1	2.98	0.52
9:I:9:ARG:HB3	9:I:104:ARG:NH1	2.25	0.52
2:B:140:HIS:HA	2:B:143:GLU:CG	2.35	0.52
4:D:8:VAL:HG21	4:D:115:ARG:NH1	2.24	0.52
4:D:8:VAL:CG1	4:D:21:LEU:HB3	2.40	0.52
1:A:1324:C:O2'	1:A:1325:G:H5'	2.09	0.52
1:A:1131:U:H2'	1:A:1132:C:O4'	2.09	0.52
13:M:49:THR:HG22	13:M:51:ALA:H	1.75	0.52
1:A:741:U:H2'	1:A:742:G:O4'	2.10	0.52
1:A:1352:C:H2'	1:A:1353:G:O4'	2.09	0.52
10:J:45:ARG:NH2	14:N:36:PHE:CD1	2.78	0.52
14:N:29:ARG:HD3	14:N:40:CYS:CB	2.40	0.52
1:A:196:G:H2'	1:A:197:U:C6	2.44	0.52
7:G:15:ASP:OD2	7:G:18:TYR:HB2	2.10	0.52
1:A:386:C:H2'	1:A:387:G:H8	1.74	0.52
4:D:8:VAL:HG11	4:D:21:LEU:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1116:G:N3	1:A:1125:G:N2	2.56	0.52
1:A:1143:G:O6	1:A:1163:G:C6	2.62	0.52
1:A:193:G:H8	1:A:193:G:C5'	2.22	0.52
1:A:938:U:H1'	1:A:1205:C:H5'	1.91	0.52
1:A:1190:C:H2'	1:A:1191:C:C6	2.43	0.52
1:A:56:A:O2'	1:A:57:U:H5'	2.09	0.52
9:I:118:LYS:O	9:I:119:ALA:CB	2.57	0.52
4:D:142:PRO:HA	4:D:185:PHE:HD2	1.73	0.52
1:A:954:G:C8	1:A:1340:U:C2	2.98	0.52
14:N:44:LEU:O	14:N:44:LEU:HD23	2.10	0.52
1:A:1287:G:H5''	21:U:4:GLY:HA3	1.93	0.52
1:A:1254:G:H5''	1:A:1254:G:H8	1.75	0.52
1:A:1117:G:N1	1:A:1124:C:C4	2.78	0.52
2:B:142:LEU:O	2:B:146:GLN:HB2	2.09	0.52
8:H:119:LEU:HD12	8:H:124:ALA:CB	2.40	0.52
3:C:172:ARG:HD2	3:C:174:PRO:HG3	1.92	0.52
1:A:1352:C:O2	1:A:1352:C:H2'	2.10	0.51
1:A:1040:G:C4	1:A:1186:A:C2	2.98	0.51
1:A:18:U:H2'	1:A:19:C:C6	2.45	0.51
4:D:108:LEU:HD13	4:D:174:LEU:HD13	1.91	0.51
1:A:1238:A:N6	1:A:1260:U:OP2	2.43	0.51
1:A:958:C:H5'	1:A:958:C:C6	2.44	0.51
1:A:1107:G:N2	1:A:1110:G:N2	2.57	0.51
1:A:1078:U:OP1	1:A:1091:G:N2	2.42	0.51
2:B:16:HIS:HB3	2:B:210:SER:OG	2.10	0.51
2:B:124:SER:O	2:B:127:ILE:HB	2.10	0.51
1:A:1446:A:H2'	1:A:1447:G:O4'	2.10	0.51
1:A:1087:G:OP1	2:B:144:ARG:NH1	2.43	0.51
8:H:1:MET:O	8:H:1:MET:HG2	2.09	0.51
14:N:40:CYS:O	14:N:42:ILE:N	2.44	0.51
1:A:1177:C:H2'	1:A:1177:C:O2	2.11	0.51
1:A:1472:G:N7	25:A:1614:PAR:N32	2.58	0.51
2:B:67:THR:HG22	2:B:90:MET:HE2	1.92	0.51
6:F:33:TYR:HA	6:F:71:ARG:HH21	1.75	0.51
10:J:29:ARG:HH12	10:J:84:GLN:HE21	1.57	0.51
4:D:8:VAL:HG13	4:D:21:LEU:HD13	1.92	0.51
2:B:105:PHE:CE1	2:B:155:LEU:HD12	2.42	0.51
1:A:824:C:H5'	1:A:826:C:O2	2.11	0.51
2:B:46:LYS:HA	2:B:49:GLU:HB2	1.93	0.51
12:L:54:LYS:N	12:L:54:LYS:HD3	2.26	0.51
13:M:15:VAL:HG22	13:M:43:THR:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:26:ARG:HH11	14:N:47:LEU:CG	2.23	0.51
1:A:1214:U:H5''	9:I:124:GLN:O	2.11	0.51
13:M:76:ALA:HA	13:M:79:LYS:HG2	1.91	0.51
4:D:31:CYS:N	4:D:33:MET:H	2.08	0.51
1:A:1209:A:H2'	1:A:1210:C:O5'	2.11	0.51
1:A:1222:U:H3'	1:A:1223:G:H5'	1.93	0.51
1:A:53:G:C2'	1:A:54:A:H5'	2.40	0.51
20:T:48:LYS:HB3	20:T:51:GLU:HG2	1.92	0.51
1:A:953:A:H5''	1:A:953:A:H8	1.74	0.51
16:P:9:PHE:CD1	16:P:18:ARG:HG3	2.46	0.51
1:A:22:G:H2'	1:A:23:G:C8	2.46	0.51
1:A:1292:G:H5'	13:M:77:ASN:ND2	2.25	0.51
2:B:194:PRO:O	2:B:196:LEU:N	2.44	0.51
2:B:52:GLU:HG2	2:B:53:ARG:N	2.26	0.51
1:A:1234:A:H2'	1:A:1234:A:N3	2.26	0.51
1:A:1205:C:P	19:S:78:ARG:HH21	2.33	0.51
1:A:598:A:C2	1:A:611:G:C2	2.99	0.51
1:A:1345:C:H5'	1:A:1346:A:O5'	2.11	0.51
1:A:1251:A:C2	1:A:1295:U:O4'	2.64	0.51
14:N:3:ARG:NE	14:N:3:ARG:O	2.44	0.51
10:J:82:ILE:O	10:J:82:ILE:HG22	2.11	0.51
15:O:70:LEU:CD2	15:O:78:TYR:HA	2.41	0.51
1:A:995:A:H2'	1:A:996:G:O4'	2.11	0.51
1:A:1010:G:N1	1:A:1015:G:N7	2.59	0.51
1:A:507:A:H61	12:L:92:ASP:HB2	1.76	0.51
2:B:102:LEU:O	2:B:105:PHE:HB2	2.11	0.51
19:S:51:VAL:O	19:S:57:HIS:HA	2.11	0.51
1:A:715:G:OP1	1:A:750:A:H1'	2.10	0.51
1:A:1358:A:C5	1:A:1359:U:C5	2.99	0.51
1:A:721:A:O2'	6:F:72:VAL:HG13	2.11	0.50
1:A:1036:G:O2'	1:A:1181:U:H5	1.94	0.50
1:A:1158:A:H3'	1:A:1159:G:H8	1.76	0.50
9:I:47:LEU:C	9:I:49:PRO:HD2	2.32	0.50
1:A:1007:C:O2'	1:A:1008:C:O4'	2.28	0.50
1:A:1510:U:H2'	1:A:1511:C:C6	2.47	0.50
1:A:1512:A:H2'	1:A:1513:C:C5'	2.38	0.50
2:B:98:LEU:O	2:B:100:GLY:N	2.44	0.50
22:X:1:PSU:H2'	22:X:2:G:H5'	1.93	0.50
3:C:31:HIS:C	3:C:33:LEU:H	2.13	0.50
1:A:316:C:H2'	1:A:317:A:C8	2.47	0.50
10:J:8:LEU:CD1	10:J:20:ALA:HB2	2.37	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1382:C:C2	1:A:1480:A:N6	2.80	0.50
2:B:96:ARG:O	2:B:98:LEU:CD2	2.59	0.50
1:A:1117:G:N2	1:A:1125:G:C4	2.79	0.50
1:A:172:C:OP1	20:T:65:LYS:NZ	2.43	0.50
19:S:51:VAL:O	19:S:58:VAL:HG22	2.11	0.50
5:E:60:TYR:CE1	5:E:64:ARG:NH2	2.79	0.50
1:A:1063:A:H5''	5:E:16:THR:HG21	1.93	0.50
3:C:72:LYS:HB3	3:C:75:VAL:HG23	1.93	0.50
3:C:11:ARG:HG3	3:C:11:ARG:HH11	1.76	0.50
10:J:23:ILE:O	10:J:23:ILE:CG2	2.59	0.50
8:H:20:TYR:CE2	8:H:75:ARG:HG2	2.46	0.50
2:B:15:VAL:C	2:B:16:HIS:CG	2.84	0.50
1:A:1443:C:H2'	1:A:1444:C:O4'	2.11	0.50
1:A:450:C:H2'	1:A:451:C:C6	2.47	0.50
6:F:3:ARG:HH11	6:F:64:GLN:HE21	1.60	0.50
2:B:116:GLU:HA	2:B:119:GLU:HB2	1.94	0.50
1:A:219:U:H2'	1:A:220:C:O4'	2.11	0.50
1:A:1335:G:O2'	1:A:1336:C:H5'	2.12	0.50
10:J:8:LEU:HD23	10:J:95:GLU:O	2.12	0.50
1:A:952:A:OP2	14:N:29:ARG:NH2	2.45	0.50
1:A:531:A:OP2	4:D:2:GLY:CA	2.50	0.50
2:B:218:ALA:O	2:B:222:ILE:HG13	2.12	0.50
1:A:36:G:O2'	12:L:118:SER:O	2.23	0.50
1:A:698:G:H2'	1:A:699:A:C8	2.47	0.50
9:I:93:ARG:O	9:I:95:LYS:N	2.45	0.50
1:A:1008:C:O2	1:A:1016:G:O6	2.30	0.50
3:C:70:VAL:O	3:C:106:VAL:HG23	2.11	0.50
12:L:69:TYR:CE2	12:L:71:PRO:HA	2.47	0.50
1:A:1118:U:O2	1:A:1120:C:H1'	2.12	0.50
1:A:1074:U:O2	1:A:1076:A:C8	2.65	0.50
4:D:49:ARG:HA	4:D:49:ARG:CZ	2.41	0.50
1:A:83:U:H1'	1:A:84:A:OP2	2.12	0.50
1:A:963:C:H2'	1:A:963:C:O2	2.12	0.50
9:I:51:ARG:HA	9:I:56:LEU:HG	1.93	0.50
1:A:1144:C:H2'	1:A:1145:C:H6	1.76	0.50
1:A:900:G:H8	1:A:900:G:H5''	1.76	0.50
1:A:822:G:H2'	1:A:823:U:H5''	1.93	0.50
9:I:43:ALA:HA	9:I:74:ILE:HD13	1.94	0.50
1:A:983:A:H2'	1:A:1021:C:O2	2.12	0.50
2:B:87:ARG:HH21	2:B:233:SER:HB2	1.77	0.50
1:A:349:A:C5'	1:A:349:A:H8	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:439:C:H2'	1:A:440:G:H8	1.77	0.50
9:I:33:PHE:CE2	9:I:47:LEU:HD21	2.47	0.50
6:F:80:ARG:NH1	6:F:88:VAL:HB	2.27	0.50
3:C:58:GLU:OE1	10:J:92:THR:HG21	2.10	0.50
1:A:953:A:C8	1:A:953:A:H5'	2.44	0.50
17:Q:67:LYS:O	17:Q:68:ARG:HG2	2.12	0.50
5:E:51:VAL:O	5:E:54:ALA:HB3	2.11	0.50
3:C:172:ARG:HB3	3:C:174:PRO:HD3	1.94	0.50
1:A:480:A:H4'	1:A:481:A:OP1	2.12	0.50
1:A:976:G:N2	1:A:1026:C:O2	2.40	0.50
14:N:37:PHE:CE1	14:N:53:LEU:HD13	2.46	0.49
1:A:1259:C:H2'	1:A:1261:A:H8	1.77	0.49
19:S:4:SER:C	19:S:5:LEU:HD13	2.32	0.49
1:A:1301:A:OP2	19:S:5:LEU:HD11	2.11	0.49
2:B:35:GLU:CG	2:B:35:GLU:O	2.60	0.49
1:A:1173:A:OP2	3:C:3:ASN:OD1	2.30	0.49
3:C:75:VAL:O	3:C:83:ARG:HD2	2.12	0.49
1:A:1516:C:H2'	1:A:1517:C:O4'	2.12	0.49
2:B:173:ALA:O	2:B:176:GLU:N	2.45	0.49
13:M:9:ILE:HG21	13:M:11:ARG:HH21	1.76	0.49
1:A:296:A:O5'	1:A:296:A:H8	1.95	0.49
18:R:44:LEU:HD11	18:R:79:LEU:HD22	1.92	0.49
1:A:612:G:H2'	1:A:613:G:C8	2.47	0.49
13:M:82:MET:O	13:M:85:GLY:HA2	2.12	0.49
15:O:26:GLU:OE2	15:O:77:ARG:NH1	2.45	0.49
14:N:57:ARG:HG2	14:N:58:LYS:H	1.77	0.49
1:A:130:C:O2	16:P:1:MET:HB2	2.12	0.49
1:A:83:U:H4'	1:A:84:A:C8	2.47	0.49
1:A:1143:G:C2'	1:A:1144:C:O5'	2.59	0.49
5:E:8:GLU:OE2	5:E:63:ARG:NH2	2.36	0.49
8:H:119:LEU:HD12	8:H:124:ALA:CA	2.42	0.49
1:A:1002:G:N3	1:A:1002:G:H2'	2.27	0.49
1:A:1231:C:H41	1:A:1270:A:N6	2.08	0.49
1:A:1109:U:H6	1:A:1262:A:N7	2.10	0.49
14:N:24:CYS:CB	14:N:40:CYS:H	2.11	0.49
1:A:952:A:P	14:N:41:ARG:HH12	2.35	0.49
13:M:108:ARG:NH1	13:M:113:PRO:O	2.45	0.49
9:I:5:TYR:CD1	9:I:6:GLY:N	2.80	0.49
1:A:1107:G:N2	1:A:1110:G:H21	2.09	0.49
3:C:15:THR:HG23	3:C:181:ASN:CA	2.43	0.49
1:A:923:G:C2	1:A:924:A:C8	2.99	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:30:ARG:CB	3:C:30:ARG:NH1	2.75	0.49
12:L:62:SER:HB2	12:L:64:TYR:HB2	1.95	0.49
13:M:81:LEU:HD21	13:M:88:ARG:HH11	1.77	0.49
1:A:1350:C:H4'	10:J:48:THR:HG21	1.93	0.49
19:S:67:VAL:O	19:S:69:HIS:N	2.41	0.49
14:N:26:ARG:HD3	14:N:47:LEU:HD11	1.94	0.49
9:I:100:GLY:C	9:I:102:LEU:H	2.14	0.49
1:A:87:C:O4'	1:A:87:C:O2	2.31	0.49
1:A:158:C:H2'	1:A:159:U:O4'	2.12	0.49
5:E:11:ILE:HG22	5:E:12:LEU:HB2	1.93	0.49
1:A:1233:A:N6	1:A:1269:A:C5	2.81	0.49
1:A:614:G:C8	1:A:614:G:C5'	2.95	0.49
3:C:47:LEU:HD21	3:C:68:VAL:HG11	1.94	0.49
14:N:26:ARG:HH11	14:N:47:LEU:HG	1.78	0.49
1:A:1350:C:C2	1:A:1351:G:C8	3.00	0.49
19:S:10:PHE:CD1	19:S:10:PHE:N	2.72	0.49
1:A:211:U:H6	1:A:211:U:H5'	1.78	0.49
1:A:1481:A:H5'	1:A:1509:A:O4'	2.12	0.49
15:O:74:ASP:C	15:O:76:GLU:N	2.66	0.49
5:E:12:LEU:HB3	5:E:31:LEU:HB2	1.95	0.49
19:S:15:LEU:O	19:S:19:VAL:HG23	2.12	0.49
1:A:1438:A:H2'	1:A:1439:G:O4'	2.12	0.49
1:A:1300:A:OP1	19:S:10:PHE:CE2	2.66	0.49
1:A:932:G:H4'	13:M:120:LYS:CD	2.42	0.49
6:F:80:ARG:HB3	6:F:88:VAL:CG2	2.41	0.49
16:P:18:ARG:HD3	16:P:35:LYS:HD2	1.94	0.49
20:T:37:SER:O	20:T:38:LYS:C	2.50	0.49
9:I:43:ALA:C	9:I:45:ALA:H	2.16	0.49
3:C:15:THR:HG21	3:C:181:ASN:H	1.77	0.49
1:A:803:A:H8	1:A:803:A:H5''	1.74	0.49
3:C:22:TRP:CB	3:C:59:ARG:HB2	2.43	0.49
17:Q:59:ILE:HD11	17:Q:73:VAL:HG22	1.94	0.49
1:A:1302:C:O2	19:S:72:GLY:HA3	2.13	0.49
1:A:1520:U:H2'	1:A:1521:C:O4'	2.13	0.49
11:K:47:VAL:HG12	11:K:48:ILE:HD13	1.95	0.49
18:R:36:ASN:OD1	18:R:39:VAL:CB	2.59	0.49
2:B:90:MET:CE	2:B:90:MET:HA	2.42	0.49
12:L:46:LYS:HE3	12:L:47:LYS:HG2	1.94	0.48
5:E:51:VAL:O	5:E:55:VAL:HG23	2.12	0.48
1:A:955:A:H2'	1:A:956:A:H5'	1.95	0.48
8:H:11:THR:HA	8:H:14:ARG:NH1	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:124:LYS:HD2	11:K:125:PHE:CZ	2.48	0.48
1:A:1425:G:C8	1:A:1425:G:H3'	2.48	0.48
1:A:1136:C:P	10:J:13:HIS:HE2	2.36	0.48
18:R:64:ARG:HG3	18:R:64:ARG:NH1	2.26	0.48
20:T:75:ASN:HA	20:T:78:ALA:H	1.77	0.48
1:A:1480:A:C2	1:A:1482:G:C2	3.01	0.48
3:C:14:ILE:O	3:C:16:ARG:N	2.46	0.48
4:D:63:LYS:HD2	4:D:198:VAL:HG23	1.94	0.48
4:D:117:ALA:O	4:D:121:VAL:HG23	2.14	0.48
5:E:13:ILE:HD12	5:E:13:ILE:O	2.13	0.48
1:A:81:U:O2	1:A:82:U:O2	2.31	0.48
4:D:25:ARG:C	4:D:27:TYR:N	2.61	0.48
16:P:67:THR:HG22	16:P:69:THR:N	2.26	0.48
1:A:1037:C:C6	1:A:1037:C:H5''	2.48	0.48
1:A:727:U:H2'	1:A:728:C:C6	2.48	0.48
1:A:1044:G:O4'	10:J:56:HIS:CD2	2.66	0.48
1:A:1184:G:H2'	1:A:1185:C:C5'	2.43	0.48
3:C:108:ASN:HD21	3:C:144:SER:CB	2.18	0.48
9:I:9:ARG:CG	9:I:14:VAL:HG13	2.40	0.48
9:I:5:TYR:HD1	9:I:6:GLY:N	2.10	0.48
1:A:836:G:OP2	1:A:836:G:H8	1.96	0.48
1:A:103:A:H4'	1:A:104:C:OP2	2.13	0.48
3:C:132:ARG:O	3:C:135:LYS:HB2	2.14	0.48
1:A:188:C:H2'	1:A:189:U:O4'	2.12	0.48
14:N:36:PHE:O	14:N:36:PHE:CG	2.66	0.48
19:S:6:LYS:HD2	19:S:6:LYS:C	2.32	0.48
7:G:16:LEU:H	7:G:16:LEU:CD2	2.26	0.48
1:A:1172:G:O2'	3:C:3:ASN:HB3	2.11	0.48
1:A:57:U:H2'	1:A:58:G:C8	2.49	0.48
1:A:23:G:C6	1:A:24:C:C4	3.02	0.48
3:C:129:ALA:HB3	3:C:132:ARG:HG2	1.95	0.48
2:B:178:ARG:HH12	8:H:68:ARG:HH22	1.61	0.48
1:A:1519:U:H2'	1:A:1520:U:C1'	2.43	0.48
14:N:2:ALA:O	14:N:4:LYS:N	2.46	0.48
1:A:778:A:C2'	1:A:779:C:O5'	2.61	0.48
2:B:110:GLN:HA	2:B:113:HIS:HB2	1.96	0.48
13:M:49:THR:HB	13:M:52:GLU:H	1.79	0.48
2:B:121:LEU:HA	2:B:124:SER:HB2	1.95	0.48
16:P:43:LYS:HG2	16:P:48:TRP:CE2	2.49	0.48
1:A:1212:C:H2'	1:A:1213:G:H8	1.78	0.48
1:A:1389:U:C2'	1:A:1390:C:H5'	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:17:VAL:O	7:G:17:VAL:CG1	2.61	0.48
13:M:34:LEU:HD13	13:M:41:PRO:HA	1.95	0.48
13:M:66:LEU:C	13:M:70:LEU:HB2	2.34	0.48
1:A:1070:G:H2'	1:A:1071:G:C8	2.49	0.48
1:A:959:U:H5'	14:N:21:TYR:CE1	2.48	0.48
10:J:94:VAL:CG1	10:J:95:GLU:H	2.26	0.48
1:A:9:A:C6	4:D:209:ARG:HB3	2.49	0.48
4:D:91:SER:O	4:D:94:LEU:N	2.47	0.48
1:A:516:A:H5'	1:A:516:A:N3	2.29	0.48
11:K:87:THR:HA	11:K:91:ARG:HH11	1.78	0.48
1:A:442:G:O5'	1:A:442:G:H8	1.96	0.48
1:A:1331:A:H2'	1:A:1332:A:C8	2.48	0.48
1:A:1300:A:OP1	19:S:10:PHE:HE2	1.97	0.48
19:S:22:LEU:O	19:S:26:GLY:HA3	2.13	0.48
1:A:265:C:H2'	1:A:266:A:H8	1.78	0.48
1:A:1503:G:P	11:K:120:ARG:HH22	2.37	0.48
3:C:25:GLY:O	3:C:27:LYS:N	2.46	0.48
1:A:201:C:OP1	20:T:61:SER:OG	2.31	0.48
1:A:1311:A:C3'	1:A:1312:U:H5'	2.44	0.48
3:C:180:ALA:O	3:C:181:ASN:HB3	2.13	0.48
5:E:51:VAL:CB	5:E:52:PRO:CD	2.91	0.48
3:C:43:LEU:HD23	3:C:47:LEU:HD13	1.95	0.48
1:A:741:U:H5''	1:A:806:C:O2	2.14	0.48
8:H:86:ILE:HG21	8:H:133:LEU:HD13	1.95	0.48
10:J:81:THR:C	10:J:83:GLU:H	2.16	0.48
1:A:8:G:H21	5:E:121:LYS:HG2	1.79	0.48
4:D:158:ILE:O	4:D:162:LEU:HB2	2.14	0.48
10:J:47:PHE:CZ	14:N:37:PHE:HE2	2.32	0.47
22:X:4:PSU:C2'	22:X:5:G:H5''	2.38	0.47
12:L:53:ARG:NH1	12:L:92:ASP:OD2	2.45	0.47
1:A:1135:A:H2'	1:A:1136:C:C6	2.49	0.47
20:T:72:LEU:O	20:T:73:HIS:C	2.52	0.47
1:A:961:A:C5'	1:A:962:C:OP2	2.60	0.47
1:A:653:U:H2'	1:A:654:G:H8	1.79	0.47
13:M:45:VAL:O	13:M:46:LYS:C	2.53	0.47
12:L:78:GLN:O	12:L:79:GLU:C	2.53	0.47
1:A:1333:U:H2'	1:A:1334:C:H5'	1.96	0.47
3:C:111:LEU:HD21	3:C:144:SER:O	2.14	0.47
5:E:80:ILE:HD11	5:E:91:LEU:HB3	1.95	0.47
1:A:365:C:O2'	1:A:366:C:O5'	2.32	0.47
12:L:74:GLY:O	12:L:111:LYS:NZ	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:954:G:N7	1:A:1340:U:C2	2.82	0.47
14:N:36:PHE:HD2	14:N:37:PHE:CD2	2.31	0.47
7:G:58:PRO:O	7:G:60:LYS:N	2.48	0.47
3:C:150:LYS:HG2	3:C:151:VAL:N	2.30	0.47
1:A:349:A:C8	1:A:349:A:C5'	2.98	0.47
1:A:1506:U:O3'	1:A:1507:G:H3'	2.15	0.47
9:I:65:VAL:C	9:I:66:ARG:HG3	2.34	0.47
1:A:526:G:H5'	4:D:41:GLY:HA3	1.95	0.47
1:A:174:A:H2'	1:A:175:U:C6	2.50	0.47
9:I:13:ALA:HA	9:I:67:GLY:HA3	1.96	0.47
6:F:91:VAL:HG13	18:R:72:ARG:NH2	2.30	0.47
1:A:1290:U:H5'	13:M:110:ARG:HH11	1.80	0.47
2:B:17:PHE:CD1	2:B:18:GLY:N	2.82	0.47
2:B:18:GLY:HA3	2:B:41:ILE:HA	1.96	0.47
10:J:24:VAL:HG13	10:J:34:VAL:HG11	1.95	0.47
22:X:3:A:H8	22:X:3:A:C5'	2.27	0.47
1:A:1118:U:C2'	1:A:1118:U:O2	2.63	0.47
13:M:56:LEU:O	13:M:57:ARG:C	2.52	0.47
7:G:51:GLN:C	7:G:53:LYS:N	2.68	0.47
3:C:31:HIS:C	3:C:33:LEU:N	2.66	0.47
9:I:111:ARG:O	9:I:113:LYS:HD2	2.15	0.47
1:A:269:A:N6	1:A:270:A:C6	2.83	0.47
1:A:635:C:O2'	1:A:636:U:H5'	2.14	0.47
22:X:5:G:O6	23:Y:35:A:N1	2.47	0.47
4:D:11:LEU:O	4:D:13:ARG:N	2.45	0.47
10:J:34:VAL:HG13	10:J:74:ILE:HG23	1.95	0.47
1:A:1407:C:H2'	1:A:1408:U:O4'	2.15	0.47
2:B:212:GLN:O	2:B:213:LEU:C	2.52	0.47
17:Q:3:LYS:HB3	17:Q:61:GLU:HB3	1.95	0.47
12:L:46:LYS:HZ1	12:L:47:LYS:HE3	1.77	0.47
2:B:21:ARG:NH1	2:B:39:ILE:HG12	2.29	0.47
17:Q:68:ARG:H	17:Q:70:ARG:HH11	1.62	0.47
3:C:22:TRP:HB3	3:C:59:ARG:HB2	1.96	0.47
1:A:1421:G:H2'	1:A:1422:C:H6	1.78	0.47
3:C:113:ALA:HB2	3:C:202:ILE:HG13	1.96	0.47
19:S:49:ILE:O	19:S:60:VAL:HG12	2.15	0.47
1:A:101:G:H2'	1:A:102:G:H5'	1.97	0.47
1:A:1476:U:H4'	1:A:1497:A:C2	2.50	0.47
18:R:38:GLU:CD	18:R:38:GLU:H	2.17	0.47
1:A:1401:A:N6	1:A:1460:G:HO2'	2.12	0.47
1:A:1347:U:O2'	1:A:1348:G:H5'	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:981:G:N2	1:A:1022:C:C6	2.81	0.47
1:A:982:G:O5'	1:A:982:G:H8	1.98	0.47
1:A:1300:A:H5''	19:S:10:PHE:HB3	1.97	0.47
7:G:18:TYR:CD2	7:G:59:LEU:HB2	2.48	0.47
4:D:29:PRO:O	4:D:30:LYS:CD	2.53	0.47
1:A:1245:C:N3	1:A:1254:G:O6	2.47	0.47
1:A:522:G:H5''	12:L:114:LYS:HB2	1.96	0.47
9:I:99:LEU:CB	9:I:101:PHE:CE1	2.98	0.47
16:P:26:ARG:HD3	16:P:31:LYS:H	1.79	0.47
1:A:1188:G:C4	1:A:1189:G:C8	3.03	0.47
1:A:486:G:OP1	12:L:118:SER:CB	2.63	0.47
1:A:571:G:H1'	8:H:1:MET:HE1	1.97	0.47
1:A:157:A:C5	1:A:158:C:H1'	2.50	0.47
8:H:29:SER:OG	8:H:32:LYS:HD2	2.14	0.47
19:S:33:THR:OG1	19:S:34:TRP:N	2.48	0.47
1:A:817:U:H2'	1:A:818:C:C6	2.49	0.47
1:A:1405:G:N2	1:A:1456:C:O2	2.48	0.47
1:A:916:A:C6	1:A:917:G:C5	3.03	0.47
14:N:27:CYS:CB	14:N:43:CYS:CB	2.89	0.47
7:G:60:LYS:HA	7:G:60:LYS:HE2	1.97	0.47
17:Q:65:ILE:N	17:Q:65:ILE:CD1	2.74	0.47
3:C:112:SER:HB3	3:C:115:LEU:HD12	1.95	0.47
10:J:46:ARG:HB3	10:J:46:ARG:HH11	1.79	0.47
1:A:1231:C:HO2'	9:I:73:GLN:NE2	2.12	0.47
21:U:2:GLY:O	21:U:4:GLY:N	2.48	0.47
1:A:1052:C:HO2'	1:A:1174:C:H1'	1.78	0.47
1:A:1135:A:OP1	10:J:68:HIS:ND1	2.47	0.47
1:A:1039:U:H5'	3:C:163:ALA:HB3	1.94	0.47
22:X:2:G:C2'	22:X:3:A:O5'	2.63	0.47
1:A:1329:G:N7	9:I:10:ARG:NH2	2.62	0.47
1:A:1188:G:H4'	3:C:192:THR:O	2.15	0.47
1:A:831:G:H2'	1:A:832:G:H5'	1.96	0.47
1:A:1290:U:H5'	13:M:110:ARG:NH1	2.30	0.47
1:A:705:G:H4'	1:A:706:A:H5''	1.97	0.47
1:A:168:U:H6	1:A:205:G:HO2'	1.60	0.47
1:A:676:U:H2'	1:A:678:A:OP2	2.15	0.47
1:A:981:G:H2'	1:A:982:G:C8	2.50	0.47
13:M:67:GLU:CG	13:M:67:GLU:O	2.51	0.47
1:A:1382:C:H4'	1:A:1383:C:C5'	2.44	0.47
3:C:54:ARG:HG3	3:C:55:VAL:H	1.80	0.47
3:C:55:VAL:O	3:C:55:VAL:CG1	2.59	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:77:GLU:HG2	8:H:78:GLN:O	2.14	0.47
1:A:606:A:C8	1:A:607:C:C6	3.03	0.47
5:E:11:ILE:HG22	5:E:12:LEU:N	2.30	0.47
1:A:753:G:H4'	1:A:1491:A:H4'	1.96	0.47
9:I:104:ARG:HD2	9:I:104:ARG:C	2.35	0.46
1:A:1515:U:O5'	1:A:1515:U:H2'	2.15	0.46
1:A:1128:C:O2'	1:A:1129:A:H5''	2.15	0.46
3:C:11:ARG:HH11	3:C:11:ARG:CG	2.28	0.46
6:F:44:GLY:O	6:F:59:TYR:HA	2.15	0.46
1:A:92:G:H5''	1:A:92:G:H8	1.79	0.46
1:A:1351:G:C5	1:A:1352:C:H5	2.32	0.46
3:C:54:ARG:O	3:C:55:VAL:HG23	2.16	0.46
7:G:41:ARG:HG2	7:G:41:ARG:HH11	1.80	0.46
1:A:1302:C:C2	19:S:72:GLY:HA3	2.50	0.46
4:D:101:LEU:HD23	4:D:121:VAL:CG1	2.45	0.46
17:Q:83:ASP:N	17:Q:83:ASP:OD1	2.49	0.46
12:L:69:TYR:HE2	12:L:71:PRO:HA	1.80	0.46
18:R:70:ILE:HG22	18:R:71:LYS:N	2.30	0.46
1:A:956:A:O2'	1:A:1304:C:N3	2.43	0.46
1:A:907:G:H2'	1:A:908:C:O4'	2.16	0.46
1:A:10:G:OP1	5:E:122:GLU:HG3	2.16	0.46
9:I:32:ASP:HB3	9:I:35:GLU:HB2	1.97	0.46
1:A:764:A:C2	1:A:785:U:C5	3.03	0.46
1:A:1015:G:H1'	1:A:1016:G:H5'	1.96	0.46
1:A:403:G:H2'	1:A:404:A:C8	2.51	0.46
3:C:119:ARG:HG2	3:C:140:ARG:HH21	1.81	0.46
10:J:3:LYS:HA	10:J:75:ILE:HA	1.96	0.46
4:D:62:GLN:HA	4:D:62:GLN:OE1	2.14	0.46
1:A:483:A:H4'	1:A:484:G:H5'	1.98	0.46
1:A:959:U:O5'	1:A:959:U:H6	1.98	0.46
1:A:536:U:C2'	1:A:537:A:H5'	2.46	0.46
21:U:12:LYS:HB3	21:U:22:ARG:HD2	1.97	0.46
1:A:1111:C:H42	1:A:1126:G:H1	1.64	0.46
1:A:1117:G:C2	1:A:1125:G:C2	3.03	0.46
1:A:414:C:H2'	1:A:415:C:H6	1.80	0.46
1:A:1477:A:C2'	1:A:1478:A:H5'	2.46	0.46
8:H:119:LEU:HD12	8:H:124:ALA:HA	1.97	0.46
16:P:4:ILE:O	16:P:66:PRO:HA	2.15	0.46
1:A:843:A:C2'	1:A:844:C:H5'	2.46	0.46
1:A:253:G:O5'	1:A:253:G:H8	1.99	0.46
1:A:1007:C:C2'	1:A:1008:C:O4'	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:23:TYR:C	3:C:23:TYR:CD1	2.89	0.46
1:A:1173:A:H2'	1:A:1174:C:C6	2.51	0.46
12:L:24:VAL:CG1	12:L:24:VAL:O	2.46	0.46
3:C:180:ALA:O	3:C:181:ASN:CB	2.63	0.46
1:A:523:A:H2'	1:A:524:G:H8	1.76	0.46
16:P:67:THR:CG2	16:P:68:ASP:N	2.78	0.46
1:A:1411:A:H2'	1:A:1412:C:C6	2.50	0.46
2:B:129:GLU:O	2:B:130:ARG:HB2	2.15	0.46
1:A:1434:G:H2'	1:A:1435:G:O4'	2.15	0.46
1:A:770:G:C2	1:A:781:C:C2	3.04	0.46
1:A:312:G:OP2	1:A:347:G:O2'	2.33	0.46
14:N:36:PHE:CD2	14:N:37:PHE:CE2	3.03	0.46
2:B:36:ARG:HB2	2:B:41:ILE:HD13	1.96	0.46
3:C:50:ALA:HB1	3:C:70:VAL:HG11	1.97	0.46
1:A:1040:G:H2'	1:A:1041:G:O4'	2.16	0.46
1:A:775:G:C6	1:A:776:A:N7	2.83	0.46
1:A:476:G:H2'	1:A:477:G:H8	1.80	0.46
1:A:1051:G:H8	1:A:1051:G:OP2	1.99	0.46
19:S:6:LYS:HG2	19:S:7:LYS:HE3	1.97	0.46
7:G:16:LEU:HD11	9:I:42:ARG:HA	1.97	0.46
6:F:94:GLN:HB3	18:R:32:ARG:HD2	1.97	0.46
17:Q:59:ILE:HA	17:Q:59:ILE:HD12	1.62	0.46
1:A:892:A:C2'	1:A:893:A:H5'	2.45	0.46
11:K:102:GLY:O	11:K:103:LEU:C	2.54	0.46
16:P:12:LYS:O	16:P:13:HIS:HB2	2.16	0.46
1:A:1488:U:H2'	1:A:1489:G:C8	2.50	0.46
1:A:983:A:C8	1:A:1020:C:N3	2.84	0.46
2:B:140:HIS:CD2	2:B:143:GLU:HG3	2.50	0.46
1:A:1355:U:O2'	1:A:1356:G:H5'	2.15	0.46
4:D:121:VAL:O	4:D:134:ASP:HA	2.16	0.46
1:A:982:G:H2'	1:A:983:A:H1'	1.98	0.46
1:A:1238:A:H5''	1:A:1240:G:N3	2.31	0.46
2:B:97:TRP:CZ3	2:B:98:LEU:O	2.69	0.46
1:A:148:C:N4	1:A:163:G:H1	2.12	0.46
4:D:14:ARG:C	4:D:16:GLY:H	2.19	0.46
19:S:29:ARG:O	19:S:31:ILE:N	2.49	0.46
18:R:19:LYS:HE2	18:R:19:LYS:HA	1.97	0.46
11:K:87:THR:HG22	11:K:91:ARG:NH1	2.31	0.46
7:G:80:VAL:HG12	7:G:81:GLY:N	2.31	0.46
6:F:36:ARG:CZ	6:F:36:ARG:HB2	2.46	0.46
7:G:15:ASP:O	7:G:19:GLY:HA2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:108:ARG:CG	13:M:108:ARG:HH11	2.21	0.45
9:I:57:GLY:O	9:I:59:PHE:N	2.41	0.45
1:A:1208:C:H4'	1:A:1209:A:OP1	2.16	0.45
10:J:3:LYS:HA	10:J:74:ILE:O	2.16	0.45
1:A:85:C:H6	1:A:85:C:O5'	1.99	0.45
1:A:1387:C:H2'	1:A:1388:G:C8	2.51	0.45
1:A:86:U:O5'	1:A:86:U:H6	1.99	0.45
4:D:68:TYR:N	4:D:68:TYR:CD1	2.84	0.45
22:X:4:PSU:C5'	22:X:4:PSU:H6	2.28	0.45
25:A:1614:PAR:H21	25:A:1614:PAR:O53	2.16	0.45
3:C:131:ARG:HH11	5:E:50:GLU:HG2	1.81	0.45
1:A:1073:U:H2'	1:A:1074:U:C6	2.49	0.45
7:G:80:VAL:CG1	7:G:81:GLY:N	2.79	0.45
1:A:416:U:O2	1:A:420:G:C2	2.69	0.45
1:A:1349:C:C2'	1:A:1350:C:H5'	2.46	0.45
2:B:187:LEU:HA	2:B:201:ILE:HB	1.98	0.45
1:A:1327:U:C4	1:A:1360:A:C2	3.05	0.45
2:B:8:LYS:HB2	2:B:9:GLU:H	1.64	0.45
2:B:166:ASP:O	2:B:170:GLU:HB2	2.16	0.45
1:A:1258:G:N3	1:A:1264:C:O2'	2.48	0.45
1:A:531:A:H4'	1:A:532:G:O5'	2.17	0.45
1:A:81:U:H4'	1:A:82:U:OP1	2.15	0.45
21:U:6:ARG:HH21	21:U:15:ARG:CG	2.24	0.45
1:A:46:U:H2'	1:A:47:G:C8	2.51	0.45
1:A:34:A:N3	12:L:32:PHE:HE2	2.14	0.45
1:A:1333:U:O2'	1:A:1334:C:H5'	2.16	0.45
1:A:1519:U:H2'	1:A:1520:U:H1'	1.97	0.45
1:A:937:A:C2	1:A:1204:G:O4'	2.69	0.45
11:K:87:THR:HG22	11:K:91:ARG:HH12	1.81	0.45
1:A:1280:C:H4'	1:A:1281:A:O4'	2.17	0.45
1:A:42:G:H2'	1:A:43:G:C8	2.51	0.45
13:M:20:THR:C	13:M:22:ILE:H	2.19	0.45
1:A:778:A:H2'	1:A:779:C:O5'	2.15	0.45
1:A:1356:G:O5'	1:A:1356:G:H8	1.98	0.45
13:M:5:ALA:O	13:M:6:GLY:C	2.54	0.45
1:A:1472:G:C2'	1:A:1473:U:H5'	2.47	0.45
6:F:80:ARG:HA	6:F:85:VAL:HG11	1.99	0.45
7:G:40:ALA:O	7:G:41:ARG:C	2.53	0.45
3:C:132:ARG:HG3	3:C:133:ALA:N	2.32	0.45
1:A:97:C:P	20:T:17:ARG:HH21	2.39	0.45
4:D:107:ARG:HH21	4:D:194:LEU:HD12	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1013:A:N3	1:A:1013:A:OP2	2.50	0.45
18:R:32:ARG:HE	18:R:32:ARG:HB2	1.45	0.45
1:A:961:A:N3	1:A:961:A:C3'	2.76	0.45
2:B:100:GLY:HA2	2:B:176:GLU:OE2	2.17	0.45
2:B:101:MET:HA	2:B:108:ILE:HD12	1.98	0.45
11:K:51:LYS:H	11:K:54:ARG:HH21	1.65	0.45
10:J:32:ALA:HB3	10:J:76:ASN:HD21	1.82	0.45
1:A:1331:A:OP2	9:I:118:LYS:NZ	2.50	0.45
1:A:1354:G:C2'	1:A:1355:U:H5'	2.47	0.45
1:A:1176:U:C2	1:A:1177:C:C5	3.04	0.45
14:N:26:ARG:HH11	14:N:47:LEU:CD2	2.30	0.45
1:A:604:C:H2'	1:A:605:A:O4'	2.17	0.45
2:B:187:LEU:CD2	2:B:203:GLY:HA3	2.47	0.45
1:A:1280:C:OP2	7:G:114:ARG:NH2	2.46	0.45
5:E:103:GLY:O	5:E:106:PRO:HD2	2.16	0.45
11:K:40:ILE:HA	11:K:40:ILE:HD13	1.78	0.45
1:A:409:G:N2	1:A:424:G:H1'	2.32	0.45
1:A:1046:C:H3'	1:A:1047:G:H2'	1.97	0.45
1:A:1351:G:OP2	9:I:112:LYS:HG3	2.17	0.45
19:S:45:VAL:CG2	19:S:46:GLY:N	2.68	0.45
2:B:97:TRP:CH2	2:B:176:GLU:CD	2.90	0.45
1:A:559:G:C5	1:A:859:G:C2	3.05	0.45
1:A:400:U:H5'	4:D:122:ARG:HD2	1.98	0.45
1:A:414:C:H1'	1:A:524:G:O2'	2.17	0.45
6:F:10:LEU:HA	6:F:84:ASN:O	2.17	0.45
1:A:942:A:N3	1:A:947:A:O2'	2.50	0.45
1:A:896:A:H2'	1:A:897:A:O4'	2.16	0.45
1:A:1401:A:H61	1:A:1460:G:HO2'	1.63	0.45
1:A:1327:U:C2	1:A:1360:A:N1	2.85	0.45
5:E:20:GLN:O	5:E:21:ALA:C	2.55	0.45
20:T:40:ALA:HB2	20:T:55:ILE:HG22	1.99	0.45
10:J:47:PHE:HD1	14:N:34:TYR:CE2	2.35	0.45
15:O:33:THR:HG22	15:O:37:ASN:ND2	2.31	0.45
1:A:722:C:H5''	6:F:69:GLU:HB2	1.98	0.45
12:L:110:VAL:CG2	12:L:120:TYR:HB3	2.47	0.45
1:A:565:G:O6	1:A:742:G:H3'	2.16	0.45
2:B:67:THR:HG22	2:B:90:MET:CE	2.46	0.45
1:A:1047:G:H4'	1:A:1048:U:OP1	2.17	0.45
1:A:1270:A:H2	1:A:1334:C:H1'	1.82	0.44
3:C:119:ARG:HG2	3:C:140:ARG:NH2	2.32	0.44
9:I:19:LEU:HB3	9:I:59:PHE:CD2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:C:O2'	1:A:149:C:H5'	2.16	0.44
1:A:439:C:O2'	1:A:440:G:H5'	2.17	0.44
13:M:49:THR:CG2	13:M:51:ALA:HB3	2.47	0.44
17:Q:48:GLU:O	17:Q:49:GLU:C	2.55	0.44
1:A:14:U:C5	1:A:894:G:O6	2.70	0.44
4:D:126:ILE:HG22	4:D:127:THR:N	2.32	0.44
1:A:999:U:H2'	1:A:1000:G:C8	2.53	0.44
4:D:18:LYS:CG	4:D:31:CYS:HB2	2.47	0.44
20:T:73:HIS:O	20:T:74:LYS:CB	2.64	0.44
1:A:1480:A:C2	1:A:1483:G:N1	2.70	0.44
10:J:4:ILE:HD13	10:J:99:LYS:O	2.18	0.44
4:D:58:LEU:CD2	4:D:62:GLN:HG2	2.42	0.44
1:A:668:A:N6	1:A:669:G:C6	2.86	0.44
1:A:378:A:C2	1:A:379:A:C4	3.05	0.44
9:I:65:VAL:HG21	9:I:77:ILE:HD11	1.99	0.44
6:F:99:ALA:O	18:R:28:GLU:HA	2.17	0.44
2:B:132:LYS:HA	2:B:135:GLN:NE2	2.32	0.44
6:F:50:TYR:CE1	18:R:77:GLY:HA2	2.53	0.44
1:A:380:G:H2'	1:A:381:C:C6	2.52	0.44
7:G:32:ARG:O	7:G:34:GLY:N	2.50	0.44
1:A:1184:G:O2'	1:A:1185:C:H5'	2.17	0.44
1:A:1520:U:H3'	1:A:1521:C:C6	2.53	0.44
1:A:1375:G:O2'	1:A:1376:U:H5'	2.17	0.44
1:A:776:A:C4	1:A:778:A:C6	3.05	0.44
1:A:777:U:H5'	1:A:778:A:H5''	1.99	0.44
1:A:45:G:N2	1:A:46:U:H1'	2.32	0.44
1:A:700:A:N3	11:K:117:ASN:O	2.50	0.44
1:A:543:A:P	5:E:126:ARG:HH22	2.39	0.44
1:A:521:G:OP1	12:L:113:ARG:NH2	2.50	0.44
1:A:954:G:H5'	1:A:1340:U:O2'	2.17	0.44
2:B:213:LEU:O	2:B:217:ARG:HG2	2.17	0.44
19:S:78:ARG:HD2	19:S:81:ARG:NH1	2.32	0.44
4:D:49:ARG:NH1	4:D:49:ARG:HA	2.32	0.44
1:A:409:G:H21	1:A:424:G:H1'	1.82	0.44
1:A:385:A:H2'	1:A:385:A:N3	2.32	0.44
7:G:17:VAL:HG12	7:G:18:TYR:CD1	2.52	0.44
4:D:36:ARG:HD2	4:D:38:TYR:OH	2.17	0.44
1:A:161:G:H2'	1:A:162:G:H8	1.82	0.44
15:O:79:ARG:O	15:O:82:ILE:HD13	2.18	0.44
2:B:15:VAL:N	2:B:16:HIS:CE1	2.85	0.44
5:E:99:GLY:O	5:E:117:ASP:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:14:VAL:O	11:K:77:MET:HA	2.17	0.44
1:A:1331:A:C2'	1:A:1332:A:O5'	2.65	0.44
9:I:43:ALA:C	9:I:45:ALA:N	2.71	0.44
1:A:836:G:C5	1:A:847:G:C8	3.06	0.44
22:X:3:A:C8	22:X:3:A:C5'	2.99	0.44
13:M:34:LEU:HD12	13:M:41:PRO:HB3	2.00	0.44
1:A:1037:C:H6	1:A:1037:C:H5''	1.82	0.44
1:A:109:G:H1'	1:A:110:A:N7	2.32	0.44
1:A:917:G:H2'	1:A:918:C:C6	2.53	0.44
1:A:1410:U:H2'	1:A:1411:A:C8	2.53	0.44
1:A:43:G:H2'	1:A:44:C:O4'	2.17	0.44
1:A:927:A:C2	1:A:1215:G:N3	2.86	0.44
1:A:453:C:H2'	1:A:454:G:O4'	2.18	0.44
19:S:44:MET:SD	19:S:44:MET:N	2.90	0.44
1:A:1350:C:C2'	1:A:1351:G:O5'	2.66	0.44
15:O:17:ARG:HH11	15:O:17:ARG:CG	2.22	0.44
10:J:79:ARG:HD3	10:J:82:ILE:HD12	2.00	0.44
1:A:803:A:H8	1:A:803:A:C5'	2.30	0.44
2:B:102:LEU:CD1	2:B:102:LEU:N	2.80	0.44
1:A:104:C:H2'	1:A:105:G:O4'	2.18	0.44
1:A:60:A:H1'	1:A:350:G:N2	2.33	0.44
9:I:50:LEU:O	9:I:53:VAL:HG22	2.18	0.44
2:B:114:ARG:HG3	2:B:114:ARG:NH1	2.27	0.44
12:L:41:ARG:NH2	12:L:57:LYS:HE2	2.32	0.44
20:T:48:LYS:HB3	20:T:51:GLU:CG	2.48	0.44
1:A:380:G:H2'	1:A:381:C:H6	1.83	0.44
6:F:40:VAL:HG22	6:F:41:GLU:N	2.32	0.44
1:A:1238:A:N6	1:A:1259:C:H3'	2.33	0.44
7:G:15:ASP:CB	7:G:20:ASP:H	2.15	0.44
2:B:189:ASP:OD2	2:B:205:ASP:OD1	2.36	0.44
1:A:1188:G:C5	1:A:1189:G:N7	2.85	0.44
8:H:4:ASP:CG	8:H:85:ARG:HH11	2.20	0.44
1:A:956:A:H1'	1:A:1304:C:O2	2.17	0.44
9:I:97:LYS:O	9:I:100:GLY:N	2.46	0.44
1:A:1425:G:C8	1:A:1425:G:C3'	3.00	0.44
2:B:131:PRO:O	2:B:133:LYS:N	2.50	0.44
2:B:225:ALA:O	2:B:226:ARG:HG3	2.18	0.44
4:D:145:GLU:OE1	4:D:182:LYS:HD3	2.18	0.44
1:A:1231:C:C5	1:A:1271:A:N6	2.86	0.43
12:L:27:LEU:C	12:L:29:GLY:N	2.70	0.43
20:T:67:ALA:O	20:T:73:HIS:ND1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1162:A:H2'	1:A:1163:G:H5'	1.99	0.43
4:D:196:LEU:HA	4:D:196:LEU:HD23	1.55	0.43
1:A:715:G:H5'	1:A:750:A:H4'	2.00	0.43
14:N:57:ARG:HG2	14:N:58:LYS:N	2.32	0.43
11:K:54:ARG:HE	11:K:54:ARG:HB2	1.49	0.43
1:A:146:A:H2'	1:A:147:A:O4'	2.18	0.43
1:A:810:C:H2'	1:A:811:U:C6	2.53	0.43
20:T:44:ALA:C	20:T:46:GLU:H	2.22	0.43
1:A:812:A:OP1	1:A:812:A:H4'	2.18	0.43
5:E:80:ILE:H	5:E:80:ILE:HD12	1.84	0.43
1:A:720:C:H2'	1:A:721:A:C8	2.53	0.43
4:D:8:VAL:C	4:D:10:ARG:N	2.71	0.43
2:B:74:LYS:O	2:B:78:GLN:HG2	2.18	0.43
1:A:1117:G:N7	1:A:1118:U:H5	2.16	0.43
6:F:22:GLU:HA	6:F:25:ILE:HD12	2.00	0.43
25:A:1614:PAR:O43	25:A:1614:PAR:H11	2.19	0.43
4:D:99:SER:O	4:D:140:VAL:HG23	2.19	0.43
1:A:795:C:O2'	1:A:879:A:N1	2.44	0.43
1:A:1020:C:H6	1:A:1020:C:O5'	2.01	0.43
1:A:979:A:H2'	1:A:980:G:C8	2.53	0.43
3:C:50:ALA:O	3:C:72:LYS:HB2	2.18	0.43
4:D:13:ARG:HD2	4:D:38:TYR:O	2.18	0.43
10:J:38:ILE:HA	10:J:39:PRO:HD3	1.89	0.43
1:A:416:U:H1'	1:A:420:G:N2	2.33	0.43
6:F:100:ASN:ND2	18:R:23:LYS:O	2.48	0.43
1:A:1195:A:O2'	1:A:1197:G:N7	2.40	0.43
5:E:95:ALA:HA	5:E:96:PRO:HD2	1.75	0.43
7:G:111:ARG:HB3	7:G:112:PRO:HD2	1.99	0.43
5:E:152:ARG:NH2	8:H:107:LEU:O	2.49	0.43
7:G:32:ARG:O	7:G:33:ASP:C	2.56	0.43
1:A:1043:C:O2'	1:A:1044:G:H5'	2.18	0.43
2:B:84:GLU:O	2:B:219:VAL:HG11	2.19	0.43
3:C:110:ASN:HD21	3:C:140:ARG:HD2	1.82	0.43
4:D:19:LEU:O	4:D:31:CYS:SG	2.76	0.43
1:A:696:A:H2'	1:A:697:G:O4'	2.19	0.43
1:A:1150:A:H2'	1:A:1151:A:C8	2.54	0.43
1:A:836:G:O6	1:A:847:G:C8	2.71	0.43
1:A:524:G:H2'	1:A:525:G:O4'	2.19	0.43
6:F:67:MET:HB2	6:F:68:PRO:CD	2.48	0.43
12:L:68:ALA:CB	12:L:100:ILE:CD1	2.97	0.43
19:S:49:ILE:HD12	19:S:49:ILE:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:82:SER:O	20:T:83:ARG:C	2.56	0.43
1:A:924:A:H2'	1:A:925:G:H8	1.75	0.43
3:C:59:ARG:CG	3:C:64:VAL:HG12	2.45	0.43
1:A:331:C:H2'	1:A:332:C:H6	1.83	0.43
12:L:78:GLN:O	12:L:80:HIS:N	2.52	0.43
20:T:26:ASN:OD1	20:T:71:THR:HG23	2.19	0.43
1:A:979:A:C8	1:A:1024:A:C2	3.06	0.43
1:A:1039:U:O2	1:A:1039:U:H2'	2.18	0.43
19:S:22:LEU:HD12	19:S:26:GLY:C	2.39	0.43
3:C:91:LEU:CB	3:C:99:VAL:HG11	2.45	0.43
13:M:11:ARG:HG2	13:M:12:ASN:HB2	2.01	0.43
9:I:13:ALA:HB2	9:I:67:GLY:O	2.18	0.43
1:A:736:G:H4'	15:O:69:TYR:OH	2.18	0.43
12:L:43:VAL:HG12	12:L:44:THR:O	2.19	0.43
1:A:357:G:C2'	1:A:358:G:H5'	2.48	0.43
11:K:41:THR:HG21	11:K:71:LYS:HB3	2.01	0.43
1:A:760:G:HO2'	1:A:761:A:H8	1.65	0.43
1:A:493:A:C8	1:A:493:A:H3'	2.53	0.43
4:D:18:LYS:HG3	4:D:31:CYS:HB2	1.99	0.43
17:Q:68:ARG:N	17:Q:70:ARG:NH1	2.65	0.43
1:A:904:G:H2'	1:A:1483:G:N3	2.33	0.43
1:A:972:A:N7	1:A:1198:G:H4'	2.33	0.43
1:A:1117:G:C6	1:A:1124:C:N4	2.87	0.43
1:A:1222:U:C3'	1:A:1223:G:H5'	2.48	0.43
1:A:1503:G:OP1	11:K:120:ARG:NH2	2.52	0.43
15:O:57:LEU:HA	15:O:57:LEU:HD23	1.70	0.43
6:F:70:ASP:N	6:F:70:ASP:OD1	2.47	0.43
1:A:1270:A:H1'	1:A:1334:C:O2'	2.18	0.43
1:A:1335:G:N2	1:A:1336:C:C2	2.87	0.43
14:N:37:PHE:HB3	14:N:39:LEU:HB2	2.00	0.43
1:A:1299:C:H5''	1:A:1300:A:OP2	2.19	0.43
2:B:88:ALA:CB	2:B:219:VAL:CG1	2.91	0.43
1:A:1173:A:P	3:C:3:ASN:OD1	2.77	0.43
12:L:69:TYR:HB2	12:L:90:VAL:HG21	2.01	0.43
4:D:190:ASP:O	4:D:191:ARG:C	2.56	0.43
3:C:32:LEU:HD22	3:C:59:ARG:NH1	2.33	0.43
9:I:97:LYS:HA	9:I:102:LEU:HD12	2.01	0.43
7:G:9:VAL:HG13	7:G:94:ARG:HE	1.82	0.43
1:A:1218:A:O2'	1:A:1286:G:H4'	2.18	0.43
1:A:804:U:H4'	1:A:805:G:OP2	2.18	0.43
16:P:55:ARG:HD2	16:P:55:ARG:HA	1.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1017:G:N3	1:A:1017:G:H3'	2.34	0.43
1:A:1232:A:H5''	1:A:1232:A:N3	2.33	0.43
2:B:98:LEU:N	2:B:98:LEU:HD23	2.34	0.43
6:F:43:LEU:HD23	6:F:46:ARG:HH11	1.83	0.43
2:B:112:VAL:HG11	2:B:153:ARG:HA	2.01	0.43
2:B:52:GLU:HG2	2:B:53:ARG:H	1.82	0.43
5:E:31:LEU:HD23	5:E:31:LEU:HA	1.81	0.43
15:O:44:LYS:HE3	15:O:47:LYS:NZ	2.33	0.43
3:C:76:VAL:O	3:C:83:ARG:HB3	2.18	0.43
20:T:74:LYS:HB3	20:T:74:LYS:HE3	1.62	0.43
1:A:706:A:N3	1:A:706:A:H3'	2.34	0.43
1:A:60:A:H3'	1:A:327:G:H22	1.84	0.43
7:G:95:ARG:HG2	7:G:99:LEU:CD1	2.49	0.43
12:L:45:PRO:HG2	12:L:49:ASN:O	2.19	0.43
19:S:36:ARG:NH1	19:S:52:TYR:O	2.52	0.43
7:G:85:TYR:O	7:G:87:VAL:HG23	2.19	0.43
3:C:73:PRO:HG3	3:C:105:GLU:HG3	2.00	0.42
1:A:1049:C:O2'	1:A:1050:A:C5'	2.67	0.42
2:B:75:LYS:HE3	2:B:75:LYS:H	1.84	0.42
1:A:40:G:C4	1:A:482:U:O4	2.72	0.42
12:L:41:ARG:HH22	12:L:57:LYS:NZ	2.16	0.42
9:I:79:LEU:HD22	9:I:83:ARG:HG3	2.01	0.42
16:P:26:ARG:CG	16:P:27:LYS:N	2.82	0.42
1:A:1401:A:N6	1:A:1460:G:O2'	2.49	0.42
1:A:817:U:H2'	1:A:818:C:H6	1.84	0.42
13:M:101:GLN:HE21	13:M:101:GLN:HB3	1.64	0.42
1:A:953:A:N6	1:A:1349:C:O2'	2.50	0.42
14:N:44:LEU:C	14:N:44:LEU:HD23	2.39	0.42
12:L:53:ARG:HG2	12:L:69:TYR:HE1	1.83	0.42
1:A:83:U:H1'	1:A:84:A:P	2.59	0.42
1:A:1012:G:C8	1:A:1012:G:H5''	2.54	0.42
1:A:1356:G:H5''	7:G:36:LYS:HB2	2.01	0.42
5:E:7:GLU:O	5:E:8:GLU:HB3	2.19	0.42
1:A:1404:G:H1	1:A:1457:C:H42	1.67	0.42
17:Q:17:LYS:H	17:Q:49:GLU:HG2	1.84	0.42
2:B:63:MET:HB3	2:B:225:ALA:HB1	1.99	0.42
1:A:985:C:H2'	1:A:986:C:C6	2.54	0.42
5:E:41:VAL:HG22	5:E:113:ALA:HB2	2.01	0.42
1:A:625:U:O4'	8:H:115:SER:HB2	2.19	0.42
3:C:20:SER:O	14:N:54:PRO:HB3	2.19	0.42
8:H:112:LEU:CD1	8:H:112:LEU:C	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:188:LEU:HD13	3:C:189:ALA:H	1.83	0.42
1:A:1292:G:H5'	13:M:77:ASN:HD21	1.83	0.42
17:Q:88:TYR:OH	17:Q:92:ARG:NH1	2.53	0.42
19:S:48:THR:HG22	19:S:61:TYR:HA	2.00	0.42
10:J:15:THR:HA	10:J:18:ALA:HB3	2.01	0.42
1:A:1298:G:O2'	1:A:1300:A:N7	2.47	0.42
2:B:88:ALA:HB2	2:B:219:VAL:HG13	1.93	0.42
1:A:1521:C:O5'	1:A:1521:C:H6	2.02	0.42
12:L:93:LEU:HB2	12:L:96:VAL:CG2	2.50	0.42
15:O:17:ARG:HG3	15:O:17:ARG:NH1	2.18	0.42
1:A:82:U:O2'	1:A:82:U:H6	2.02	0.42
1:A:775:G:H3'	1:A:775:G:C8	2.54	0.42
1:A:1095:C:N3	3:C:178:LEU:HB2	2.35	0.42
7:G:65:ALA:HB1	7:G:127:ALA:HB3	2.00	0.42
9:I:10:ARG:HD3	9:I:75:ASP:HB2	2.02	0.42
4:D:209:ARG:HG3	4:D:209:ARG:HH11	1.83	0.42
7:G:138:LYS:O	7:G:138:LYS:HD3	2.18	0.42
8:H:75:ARG:HA	8:H:76:PRO:HD3	1.93	0.42
1:A:1075:A:H5''	7:G:4:ARG:CZ	2.49	0.42
19:S:50:ALA:HA	19:S:58:VAL:O	2.19	0.42
16:P:9:PHE:CD1	16:P:9:PHE:N	2.88	0.42
2:B:126:GLU:HA	2:B:129:GLU:HG3	2.01	0.42
2:B:235:SER:O	2:B:236:TYR:HD1	2.03	0.42
1:A:112:U:H3'	1:A:284:A:H61	1.84	0.42
1:A:1295:U:P	19:S:6:LYS:HG3	2.59	0.42
1:A:318:C:OP2	1:A:324:C:N4	2.52	0.42
12:L:68:ALA:HB3	12:L:100:ILE:HD11	2.02	0.42
1:A:569:G:N3	1:A:857:C:H4'	2.33	0.42
9:I:43:ALA:O	9:I:45:ALA:N	2.51	0.42
1:A:925:G:H2'	1:A:926:C:O4'	2.19	0.42
1:A:211:U:C6	1:A:211:U:C5'	3.02	0.42
2:B:118:LEU:HB2	2:B:142:LEU:CD1	2.48	0.42
1:A:1481:A:C8	1:A:1509:A:H1'	2.55	0.42
3:C:44:GLU:HA	3:C:52:LEU:HD11	2.01	0.42
16:P:18:ARG:HD3	16:P:35:LYS:CD	2.50	0.42
1:A:1460:G:HO2'	1:A:1461:A:H8	1.59	0.42
9:I:80:GLY:O	9:I:81:ILE:C	2.58	0.42
1:A:982:G:H2'	1:A:983:A:C1'	2.49	0.42
10:J:47:PHE:HD1	14:N:34:TYR:CD2	2.38	0.42
9:I:114:TYR:N	9:I:114:TYR:CD1	2.87	0.42
23:Y:31:A:C2'	23:Y:31:A:N3	2.70	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:9:ARG:HB3	9:I:104:ARG:HH11	1.83	0.42
2:B:211:ILE:H	2:B:211:ILE:HG13	1.70	0.42
1:A:1035:U:O4	1:A:1182:C:C2	2.73	0.42
1:A:192:G:H2'	1:A:193:G:H5''	2.02	0.42
1:A:439:C:H2'	1:A:440:G:C8	2.53	0.42
4:D:70:ILE:HD12	4:D:100:ARG:HD2	2.00	0.42
18:R:71:LYS:O	18:R:74:ARG:HB2	2.20	0.42
1:A:17:A:C2'	1:A:18:U:H5'	2.50	0.42
10:J:30:SER:HB3	10:J:84:GLN:HE22	1.85	0.42
2:B:81:VAL:HG12	2:B:82:ARG:N	2.34	0.42
17:Q:53:LEU:HD11	17:Q:85:VAL:HG11	2.01	0.42
1:A:784:G:O5'	1:A:784:G:H8	2.03	0.42
1:A:445:G:H4'	16:P:41:PRO:HB2	2.00	0.42
1:A:1335:G:H2'	1:A:1336:C:H5'	2.02	0.42
1:A:1346:A:C4	1:A:1348:G:C6	3.07	0.42
10:J:5:ARG:CG	10:J:73:ASP:OD1	2.58	0.42
4:D:30:LYS:HB2	4:D:32:ALA:C	2.40	0.42
1:A:1095:C:C2	3:C:178:LEU:HB2	2.55	0.42
1:A:1209:A:C2'	1:A:1210:C:O5'	2.68	0.42
1:A:1049:C:O2'	1:A:1050:A:H5'	2.19	0.42
11:K:92:GLU:HB3	11:K:96:ARG:NH1	2.35	0.42
10:J:40:LEU:N	10:J:69:ASN:O	2.51	0.42
1:A:139:G:H1	1:A:173:C:H42	1.67	0.42
1:A:177:U:C4	1:A:178:G:H1'	2.55	0.42
11:K:11:LYS:HA	11:K:11:LYS:HD2	1.92	0.42
3:C:101:LEU:CD2	3:C:101:LEU:O	2.67	0.42
5:E:78:HIS:CD2	5:E:78:HIS:C	2.93	0.42
5:E:131:ILE:HD13	5:E:131:ILE:HA	1.88	0.42
1:A:1382:C:C2	1:A:1384:G:C5	3.07	0.42
8:H:109:ILE:HG22	8:H:137:VAL:O	2.20	0.42
1:A:1049:C:C2'	1:A:1050:A:C5'	2.92	0.42
1:A:1146:C:C2	1:A:1156:G:N2	2.88	0.42
4:D:94:LEU:HD23	4:D:94:LEU:HA	1.68	0.42
7:G:116:ALA:O	7:G:120:ILE:HG12	2.20	0.42
2:B:27:LYS:HG2	2:B:195:ASP:OD2	2.20	0.42
1:A:1112:C:O5'	1:A:1113:A:O5'	2.37	0.42
3:C:12:LEU:HD23	3:C:12:LEU:HA	1.73	0.42
1:A:1471:A:C8	22:X:5:G:H1'	2.55	0.42
10:J:8:LEU:HD11	10:J:20:ALA:CB	2.37	0.42
14:N:24:CYS:HB2	14:N:40:CYS:CA	2.50	0.42
2:B:42:ILE:O	2:B:42:ILE:HG13	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:36:ASN:C	18:R:40:LEU:HD12	2.40	0.42
9:I:85:LEU:HD12	9:I:92:TYR:CD2	2.55	0.42
13:M:115:LYS:H	13:M:115:LYS:HD3	1.85	0.42
20:T:10:LEU:HD12	20:T:12:ALA:H	1.83	0.42
11:K:20:TYR:CE1	11:K:83:ILE:HD13	2.55	0.42
1:A:405:G:H3'	1:A:406:G:H8	1.85	0.42
1:A:1389:U:O2'	1:A:1390:C:H5'	2.20	0.42
1:A:475:G:H2'	1:A:476:G:H8	1.85	0.42
1:A:94:C:H2'	1:A:95:A:O4'	2.19	0.42
1:A:673:C:H2'	1:A:674:G:O4'	2.20	0.42
1:A:1269:A:H2'	1:A:1270:A:C8	2.55	0.41
1:A:1043:C:C4	3:C:2:GLY:HA3	2.48	0.41
1:A:1040:G:C5	1:A:1186:A:C2	3.08	0.41
2:B:216:SER:OG	2:B:217:ARG:N	2.53	0.41
14:N:26:ARG:HH11	14:N:47:LEU:HD21	1.84	0.41
1:A:544:U:H4'	1:A:545:U:H5''	2.02	0.41
18:R:37:VAL:HG12	18:R:41:LYS:HE3	2.02	0.41
12:L:126:LYS:CA	12:L:129:ALA:O	2.68	0.41
1:A:331:C:O2'	1:A:332:C:H5'	2.20	0.41
5:E:20:GLN:OE1	5:E:21:ALA:O	2.38	0.41
10:J:9:ARG:HG2	10:J:69:ASN:OD1	2.20	0.41
1:A:425:U:O2'	4:D:22:LYS:HE2	2.20	0.41
1:A:586:A:C2	1:A:621:G:C2	3.08	0.41
1:A:597:C:C6	1:A:597:C:H3'	2.55	0.41
19:S:18:LYS:HE2	19:S:18:LYS:HB2	1.68	0.41
10:J:57:LYS:HE2	10:J:60:ARG:HH22	1.86	0.41
2:B:84:GLU:HA	2:B:87:ARG:HB3	2.01	0.41
1:A:1107:G:H21	1:A:1110:G:N2	2.18	0.41
1:A:1208:C:N4	13:M:104:ARG:CG	2.79	0.41
4:D:8:VAL:CG1	4:D:21:LEU:CB	2.98	0.41
8:H:31:PHE:O	8:H:35:ILE:HG13	2.20	0.41
17:Q:80:GLY:O	17:Q:82:MET:HG2	2.20	0.41
3:C:87:LEU:C	3:C:89:GLU:H	2.24	0.41
13:M:49:THR:HG21	13:M:51:ALA:HB3	2.01	0.41
1:A:1281:A:C5'	1:A:1282:G:OP2	2.68	0.41
9:I:11:LYS:HG2	9:I:11:LYS:O	2.20	0.41
1:A:1023:U:O2	1:A:1023:U:H2'	2.20	0.41
2:B:21:ARG:CB	2:B:39:ILE:HA	2.47	0.41
12:L:92:ASP:C	12:L:93:LEU:HD23	2.41	0.41
17:Q:69:LYS:O	17:Q:70:ARG:HD2	2.21	0.41
1:A:1198:G:C2'	1:A:1199:C:H5'	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:109:ILE:HD12	8:H:109:ILE:HG21	1.90	0.41
2:B:208:ILE:HA	2:B:211:ILE:HD12	2.01	0.41
1:A:1117:G:C2	1:A:1124:C:C4	3.08	0.41
1:A:1219:C:H4'	1:A:1316:G:N2	2.35	0.41
1:A:47:G:O2'	1:A:361:U:H1'	2.19	0.41
12:L:50:SER:O	12:L:51:ALA:CB	2.68	0.41
1:A:1211:A:C2	1:A:1212:C:C4	3.08	0.41
10:J:81:THR:O	10:J:83:GLU:N	2.53	0.41
9:I:58:ARG:CZ	9:I:58:ARG:HB2	2.49	0.41
2:B:180:LEU:HD23	2:B:180:LEU:HA	1.87	0.41
1:A:982:G:C2'	1:A:983:A:H4'	2.50	0.41
12:L:47:LYS:HG3	12:L:48:PRO:HD3	2.02	0.41
2:B:88:ALA:CB	2:B:219:VAL:HG13	2.50	0.41
3:C:14:ILE:HG22	3:C:15:THR:H	1.84	0.41
1:A:1035:U:O2'	1:A:1038:A:OP2	2.32	0.41
1:A:344:G:C2'	1:A:344:G:N3	2.83	0.41
1:A:171:C:H2'	1:A:172:C:C6	2.54	0.41
18:R:74:ARG:HD3	18:R:81:PHE:CD2	2.55	0.41
2:B:163:PHE:HA	2:B:185:ILE:O	2.20	0.41
1:A:714:G:C5	1:A:715:G:H1'	2.55	0.41
17:Q:48:GLU:O	17:Q:50:LYS:N	2.53	0.41
1:A:59:C:O2'	1:A:384:G:N7	2.45	0.41
1:A:1351:G:N1	1:A:1352:C:C5	2.88	0.41
1:A:1108:U:H5'	1:A:1109:U:C4	2.55	0.41
9:I:114:TYR:HD2	10:J:60:ARG:HD2	1.86	0.41
14:N:24:CYS:SG	14:N:27:CYS:O	2.78	0.41
7:G:15:ASP:OD1	7:G:44:TYR:OH	2.35	0.41
16:P:28:ARG:HG2	16:P:29:ASP:OD1	2.20	0.41
12:L:90:VAL:O	12:L:91:LYS:CB	2.45	0.41
13:M:23:TYR:HB3	13:M:67:GLU:HA	2.02	0.41
1:A:83:U:O4'	1:A:83:U:OP1	2.38	0.41
18:R:58:LEU:N	18:R:58:LEU:HD12	2.36	0.41
1:A:1107:G:H4'	10:J:38:ILE:HD13	2.02	0.41
3:C:180:ALA:HB1	3:C:182:ILE:HG13	2.03	0.41
1:A:1084:A:OP2	2:B:96:ARG:NH2	2.53	0.41
1:A:1315:A:H2'	1:A:1316:G:O4'	2.20	0.41
1:A:765:A:C5	1:A:786:A:C2	3.09	0.41
1:A:193:G:C8	1:A:193:G:C5'	3.02	0.41
17:Q:99:SER:O	17:Q:100:LYS:HG3	2.21	0.41
1:A:554:G:H2'	1:A:555:U:C6	2.55	0.41
7:G:155:ARG:H	7:G:155:ARG:HG3	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:56:GLN:HG2	7:G:56:GLN:H	1.64	0.41
1:A:1022:C:C5	1:A:1023:U:C5	3.09	0.41
9:I:114:TYR:HE2	10:J:59:SER:HA	1.80	0.41
20:T:74:LYS:HB2	20:T:75:ASN:H	1.66	0.41
3:C:11:ARG:HD3	3:C:178:LEU:O	2.20	0.41
10:J:22:LYS:C	10:J:24:VAL:H	2.24	0.41
1:A:1453:G:H5''	1:A:1453:G:C8	2.56	0.41
2:B:76:GLN:NE2	2:B:76:GLN:H	2.18	0.41
1:A:1160:G:N2	1:A:1162:A:H3'	2.35	0.41
1:A:1001:G:H3'	1:A:1002:G:H8	1.86	0.41
1:A:1068:U:H3'	1:A:1069:U:C6	2.56	0.41
1:A:1068:U:H2'	1:A:1068:U:O5'	2.21	0.41
11:K:29:ILE:HD11	11:K:31:THR:HG23	2.01	0.41
13:M:15:VAL:HA	13:M:18:ALA:HB3	2.02	0.41
1:A:1125:G:H5''	1:A:1126:G:OP2	2.21	0.41
1:A:803:A:C8	1:A:803:A:C5'	3.01	0.41
20:T:86:ARG:O	20:T:87:LYS:C	2.59	0.41
4:D:14:ARG:C	4:D:16:GLY:N	2.73	0.41
1:A:353:G:H2'	1:A:354:U:H6	1.86	0.41
8:H:1:MET:O	8:H:2:LEU:CB	2.68	0.41
7:G:113:GLU:OE1	7:G:122:HIS:HD2	2.04	0.41
1:A:1259:C:H2'	1:A:1261:A:C8	2.54	0.41
18:R:32:ARG:CA	18:R:69:THR:HG21	2.41	0.41
1:A:1355:U:H2'	1:A:1356:G:C5'	2.50	0.41
1:A:9:A:C5	4:D:209:ARG:HB3	2.56	0.41
4:D:63:LYS:HD2	4:D:198:VAL:HG22	2.03	0.41
1:A:535:U:H2'	1:A:536:U:C6	2.55	0.41
1:A:1431:U:H2'	1:A:1433:C:C5	2.56	0.41
1:A:389:A:O2'	1:A:390:G:H5'	2.21	0.41
1:A:1349:C:C2	1:A:1350:C:C5	3.09	0.41
1:A:1233:A:O2'	1:A:1352:C:O2'	2.39	0.41
14:N:53:LEU:HA	14:N:54:PRO:HD3	1.90	0.41
1:A:1337:G:O2'	1:A:1338:G:H5'	2.21	0.41
5:E:90:VAL:O	5:E:120:THR:HA	2.21	0.41
1:A:1031:G:OP1	14:N:4:LYS:HB2	2.21	0.41
1:A:258:A:H5'	20:T:74:LYS:HD3	2.01	0.41
16:P:74:LEU:HA	16:P:74:LEU:HD23	1.75	0.41
5:E:68:GLU:CG	5:E:68:GLU:O	2.61	0.41
7:G:127:ALA:O	7:G:130:GLY:N	2.54	0.41
1:A:400:U:H2'	1:A:401:U:C6	2.56	0.41
1:A:401:U:O2	1:A:482:U:O2'	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:173:TRP:HB2	4:D:187:ARG:HG3	2.03	0.41
1:A:163:G:C2	1:A:164:C:C5	3.09	0.41
3:C:134:ILE:CD1	3:C:153:VAL:HG23	2.51	0.41
5:E:36:ASP:OD2	5:E:40:ARG:HB2	2.21	0.41
1:A:1274:U:P	7:G:41:ARG:NH2	2.94	0.41
2:B:90:MET:HE2	2:B:90:MET:HA	2.03	0.41
1:A:822:G:O5'	1:A:822:G:H8	2.04	0.41
1:A:900:G:N3	1:A:1381:A:H2	2.19	0.41
1:A:200:C:H2'	1:A:201:C:C6	2.56	0.41
1:A:636:U:C2	1:A:736:G:N2	2.89	0.41
1:A:1487:C:H2'	1:A:1488:U:O4'	2.21	0.41
1:A:927:A:C2	1:A:1215:G:C4	3.08	0.41
1:A:1164:G:H4'	1:A:1165:A:H5''	2.02	0.41
1:A:1518:U:H3'	1:A:1518:U:C6	2.56	0.41
1:A:328:G:H2'	1:A:329:G:O5'	2.20	0.41
1:A:118:G:C6	1:A:119:U:C4	3.09	0.41
1:A:951:G:O5'	1:A:951:G:H8	2.03	0.41
1:A:394:C:H6	1:A:394:C:O5'	2.04	0.41
1:A:1382:C:C4	1:A:1384:G:C2	3.09	0.41
1:A:1474:C:H5''	1:A:1475:G:OP2	2.21	0.41
8:H:10:LEU:HD22	8:H:83:ILE:HD11	2.03	0.41
15:O:2:PRO:HB2	15:O:3:ILE:H	1.56	0.41
4:D:110:PHE:CD1	4:D:110:PHE:N	2.88	0.41
1:A:1348:G:C6	1:A:1349:C:C4	3.10	0.40
5:E:80:ILE:HA	8:H:104:ARG:NH2	2.36	0.40
3:C:70:VAL:O	3:C:105:GLU:HA	2.21	0.40
13:M:4:ILE:CD1	13:M:56:LEU:HD13	2.51	0.40
1:A:53:G:H2'	1:A:54:A:H5'	2.03	0.40
2:B:161:ALA:HB1	2:B:185:ILE:HD11	2.02	0.40
1:A:101:G:C2'	1:A:102:G:H5'	2.50	0.40
1:A:390:G:H2'	1:A:391:C:C6	2.56	0.40
1:A:329:G:H4'	20:T:16:HIS:CE1	2.56	0.40
3:C:157:ILE:HG21	3:C:164:ARG:NH2	2.36	0.40
1:A:1093:A:H8	1:A:1093:A:O5'	2.04	0.40
9:I:37:PHE:HB3	9:I:43:ALA:HB2	2.02	0.40
1:A:1263:U:O4'	1:A:1263:U:O2	2.39	0.40
7:G:17:VAL:O	7:G:17:VAL:HG12	2.21	0.40
1:A:199:U:C4'	20:T:103:GLY:HA2	2.50	0.40
2:B:108:ILE:O	2:B:108:ILE:CG2	2.69	0.40
6:F:3:ARG:NH1	6:F:64:GLN:HE21	2.20	0.40
1:A:536:U:O2'	1:A:537:A:H5'	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:980:G:C6	1:A:981:G:C6	3.10	0.40
1:A:982:G:C2	1:A:983:A:H1'	2.57	0.40
1:A:1252:C:H4'	1:A:1295:U:O2'	2.21	0.40
4:D:33:MET:HG3	4:D:33:MET:O	2.21	0.40
1:A:1077:G:O5'	1:A:1078:U:H5	2.04	0.40
1:A:1302:C:O2'	1:A:1303:C:H5'	2.21	0.40
1:A:1389:U:H2'	1:A:1390:C:H5'	2.04	0.40
1:A:168:U:H5''	1:A:204:A:O4'	2.22	0.40
1:A:1327:U:N3	1:A:1360:A:C2	2.90	0.40
11:K:13:GLN:HA	11:K:13:GLN:OE1	2.20	0.40
1:A:984:A:H5'	1:A:984:A:N3	2.37	0.40
1:A:1107:G:O2'	1:A:1128:C:N4	2.50	0.40
19:S:22:LEU:CD1	19:S:26:GLY:HA3	2.48	0.40
2:B:48:MET:HA	2:B:51:LEU:HD12	2.02	0.40
4:D:5:ILE:O	4:D:5:ILE:CG2	2.69	0.40
1:A:733:C:OP2	1:A:734:G:OP2	2.39	0.40
1:A:416:U:O2	1:A:420:G:N1	2.53	0.40
11:K:85:ARG:NH1	11:K:111:ASP:OD2	2.55	0.40
7:G:58:PRO:O	7:G:59:LEU:C	2.60	0.40
20:T:53:LEU:HD22	20:T:102:GLY:HA3	2.03	0.40
10:J:99:LYS:HD3	10:J:99:LYS:HA	1.96	0.40
1:A:1314:A:C2	1:A:1315:A:C4	3.09	0.40
1:A:772:U:H2'	1:A:773:U:O4'	2.22	0.40
13:M:87:TYR:O	13:M:89:GLY:N	2.55	0.40
1:A:1005:G:H1	1:A:1018:A:H61	1.70	0.40
2:B:54:THR:HG23	2:B:199:TYR:HB3	2.03	0.40
1:A:1092:C:O5'	1:A:1092:C:H6	2.04	0.40
20:T:24:LEU:HD22	20:T:24:LEU:HA	1.86	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	232/234 (99%)	168 (72%)	44 (19%)	20 (9%)	1	5
3	C	204/206 (99%)	137 (67%)	44 (22%)	23 (11%)	0	2
4	D	206/208 (99%)	163 (79%)	25 (12%)	18 (9%)	1	5
5	E	148/150 (99%)	126 (85%)	17 (12%)	5 (3%)	5	25
6	F	99/101 (98%)	79 (80%)	15 (15%)	5 (5%)	2	15
7	G	153/155 (99%)	122 (80%)	22 (14%)	9 (6%)	2	12
8	H	136/138 (99%)	120 (88%)	13 (10%)	3 (2%)	8	36
9	I	125/127 (98%)	86 (69%)	25 (20%)	14 (11%)	0	3
10	J	96/98 (98%)	69 (72%)	20 (21%)	7 (7%)	1	7
11	K	117/119 (98%)	101 (86%)	10 (8%)	6 (5%)	2	15
12	L	123/125 (98%)	93 (76%)	21 (17%)	9 (7%)	1	7
13	M	118/120 (98%)	83 (70%)	21 (18%)	14 (12%)	0	2
14	N	58/60 (97%)	37 (64%)	12 (21%)	9 (16%)	0	0
15	O	86/88 (98%)	75 (87%)	9 (10%)	2 (2%)	8	35
16	P	81/83 (98%)	73 (90%)	8 (10%)	0	100	100
17	Q	97/99 (98%)	81 (84%)	14 (14%)	2 (2%)	9	37
18	R	68/70 (97%)	62 (91%)	5 (7%)	1 (2%)	13	46
19	S	76/78 (97%)	54 (71%)	12 (16%)	10 (13%)	0	1
20	T	97/99 (98%)	74 (76%)	15 (16%)	8 (8%)	1	6
21	U	22/24 (92%)	17 (77%)	5 (23%)	0	100	100
All	All	2342/2382 (98%)	1820 (78%)	357 (15%)	165 (7%)	1	8

All (165) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	15	VAL
2	B	17	PHE
2	B	78	GLN
2	B	87	ARG
2	B	130	ARG
2	B	131	PRO
2	B	132	LYS
2	B	195	ASP
2	B	237	ALA
2	B	239	VAL
3	C	53	ALA

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Mol	Chain	Res	Type
3	C	127	ARG
3	C	154	SER
3	C	156	ARG
3	C	189	ALA
3	C	206	GLU
4	D	3	ARG
4	D	14	ARG
4	D	26	CYS
4	D	29	PRO
4	D	30	LYS
6	F	39	LYS
7	G	33	ASP
7	G	52	GLU
8	H	70	GLN
8	H	105	ARG
9	I	58	ARG
9	I	118	LYS
11	K	57	THR
11	K	127	LYS
12	L	27	LEU
12	L	28	LYS
12	L	30	ALA
12	L	47	LYS
12	L	79	GLU
13	M	4	ILE
13	M	12	ASN
13	M	83	ASP
13	M	91	ARG
13	M	113	PRO
14	N	3	ARG
14	N	41	ARG
14	N	44	LEU
17	Q	49	GLU
17	Q	81	ARG
18	R	87	ARG
19	S	6	LYS
19	S	10	PHE
19	S	46	GLY
20	T	9	ASN
20	T	74	LYS
20	T	97	ALA
20	T	98	PRO

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Mol	Chain	Res	Type
2	B	20	GLU
2	B	99	GLY
2	B	155	LEU
3	C	24	ALA
3	C	26	LYS
3	C	32	LEU
3	C	36	ASP
3	C	55	VAL
3	C	68	VAL
3	C	74	GLY
4	D	9	CYS
4	D	10	ARG
4	D	42	GLN
5	E	21	ALA
5	E	22	GLY
6	F	38	GLU
7	G	7	ALA
7	G	17	VAL
7	G	59	LEU
7	G	138	LYS
9	I	68	GLY
9	I	80	GLY
9	I	81	ILE
9	I	94	ALA
10	J	23	ILE
10	J	36	GLY
10	J	59	SER
11	K	103	LEU
11	K	117	ASN
13	M	3	ARG
13	M	6	GLY
13	M	46	LYS
13	M	71	ARG
13	M	89	GLY
14	N	5	ALA
14	N	16	PHE
14	N	27	CYS
15	O	88	ARG
19	S	30	LEU
19	S	42	PRO
19	S	67	VAL
19	S	68	GLY

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Mol	Chain	Res	Type
19	S	80	TYR
20	T	49	ALA
2	B	83	MET
3	C	15	THR
3	C	16	ARG
3	C	39	ILE
3	C	47	LEU
3	C	81	GLY
4	D	4	TYR
4	D	12	CYS
4	D	13	ARG
4	D	32	ALA
4	D	164	ALA
4	D	171	GLY
5	E	68	GLU
6	F	32	ASN
6	F	100	ASN
7	G	81	GLY
9	I	44	VAL
9	I	89	ASN
9	I	119	ALA
11	K	56	GLY
11	K	107	SER
12	L	41	ARG
12	L	48	PRO
13	M	14	ARG
13	M	88	ARG
13	M	90	LEU
14	N	23	ARG
20	T	50	GLU
20	T	75	ASN
2	B	59	GLU
2	B	221	LEU
3	C	60	ALA
3	C	181	ASN
3	C	188	LEU
4	D	15	GLU
6	F	79	LEU
9	I	54	ASP
9	I	88	TYR
9	I	105	ASP
9	I	127	LYS

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Mol	Chain	Res	Type
10	J	82	ILE
10	J	83	GLU
10	J	90	LEU
10	J	91	PRO
12	L	26	ALA
14	N	28	GLY
19	S	59	PRO
20	T	27	LYS
2	B	233	SER
3	C	4	LYS
3	C	9	GLY
4	D	69	GLY
7	G	9	VAL
12	L	82	VAL
13	M	120	LYS
15	O	87	ILE
19	S	45	VAL
2	B	227	GLY
4	D	5	ILE
4	D	53	ASP
5	E	59	GLY
7	G	16	LEU
9	I	55	ALA
14	N	4	LYS
2	B	174	VAL
8	H	73	ASP
2	B	232	PRO
5	E	52	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	202/202 (100%)	150 (74%)	52 (26%)	0	2
3	C	160/160 (100%)	119 (74%)	41 (26%)	0	2
4	D	180/180 (100%)	145 (81%)	35 (19%)	2	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	115/115 (100%)	91 (79%)	24 (21%)	1	6
6	F	90/90 (100%)	73 (81%)	17 (19%)	2	8
7	G	126/126 (100%)	107 (85%)	19 (15%)	3	15
8	H	119/119 (100%)	98 (82%)	21 (18%)	2	10
9	I	98/98 (100%)	73 (74%)	25 (26%)	1	2
10	J	88/88 (100%)	65 (74%)	23 (26%)	0	2
11	K	90/90 (100%)	74 (82%)	16 (18%)	2	10
12	L	104/104 (100%)	87 (84%)	17 (16%)	3	12
13	M	96/96 (100%)	61 (64%)	35 (36%)	0	0
14	N	49/49 (100%)	34 (69%)	15 (31%)	0	1
15	O	79/79 (100%)	66 (84%)	13 (16%)	3	12
16	P	72/72 (100%)	57 (79%)	15 (21%)	1	6
17	Q	94/94 (100%)	77 (82%)	17 (18%)	2	9
18	R	61/61 (100%)	49 (80%)	12 (20%)	1	7
19	S	69/69 (100%)	54 (78%)	15 (22%)	1	5
20	T	76/76 (100%)	62 (82%)	14 (18%)	2	9
21	U	19/19 (100%)	12 (63%)	7 (37%)	0	0
All	All	1987/1987 (100%)	1554 (78%)	433 (22%)	1	5

All (433) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	7	VAL
2	B	8	LYS
2	B	9	GLU
2	B	11	LEU
2	B	15	VAL
2	B	17	PHE
2	B	21	ARG
2	B	23	ARG
2	B	24	TRP
2	B	27	LYS
2	B	35	GLU
2	B	39	ILE
2	B	42	ILE
2	B	48	MET

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Mol	Chain	Res	Type
2	B	60	ASP
2	B	69	LEU
2	B	75	LYS
2	B	76	GLN
2	B	80	ILE
2	B	86	GLU
2	B	87	ARG
2	B	96	ARG
2	B	97	TRP
2	B	98	LEU
2	B	102	LEU
2	B	111	ARG
2	B	113	HIS
2	B	115	LEU
2	B	119	GLU
2	B	129	GLU
2	B	132	LYS
2	B	133	LYS
2	B	135	GLN
2	B	140	HIS
2	B	145	LEU
2	B	155	LEU
2	B	156	LYS
2	B	157	ARG
2	B	158	LEU
2	B	160	ASP
2	B	170	GLU
2	B	172	ILE
2	B	187	LEU
2	B	196	LEU
2	B	209	ARG
2	B	210	SER
2	B	212	GLN
2	B	221	LEU
2	B	230	VAL
2	B	231	GLU
2	B	236	TYR
2	B	238	LEU
3	C	3	ASN
3	C	5	ILE
3	C	11	ARG
3	C	16	ARG

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Mol	Chain	Res	Type
3	C	17	ASP
3	C	26	LYS
3	C	27	LYS
3	C	28	GLN
3	C	31	HIS
3	C	32	LEU
3	C	33	LEU
3	C	40	ARG
3	C	47	LEU
3	C	52	LEU
3	C	54	ARG
3	C	56	ASP
3	C	58	GLU
3	C	62	ASP
3	C	72	LYS
3	C	83	ARG
3	C	88	ARG
3	C	93	LYS
3	C	94	LEU
3	C	97	LYS
3	C	99	VAL
3	C	107	GLN
3	C	111	LEU
3	C	127	ARG
3	C	128	PHE
3	C	144	SER
3	C	156	ARG
3	C	164	ARG
3	C	166	GLU
3	C	172	ARG
3	C	175	LEU
3	C	178	LEU
3	C	179	ARG
3	C	188	LEU
3	C	191	THR
3	C	192	THR
3	C	196	LEU
4	D	3	ARG
4	D	9	CYS
4	D	10	ARG
4	D	11	LEU
4	D	17	VAL

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Mol	Chain	Res	Type
4	D	19	LEU
4	D	30	LYS
4	D	33	MET
4	D	34	GLU
4	D	47	ARG
4	D	50	ARG
4	D	58	LEU
4	D	76	ARG
4	D	84	LYS
4	D	85	LYS
4	D	106	TYR
4	D	108	LEU
4	D	122	ARG
4	D	127	THR
4	D	135	LEU
4	D	139	ARG
4	D	145	GLU
4	D	150	GLU
4	D	151	LYS
4	D	155	LEU
4	D	162	LEU
4	D	166	LYS
4	D	170	VAL
4	D	177	ASP
4	D	178	VAL
4	D	182	LYS
4	D	184	LYS
4	D	187	ARG
4	D	188	LEU
4	D	209	ARG
5	E	9	LYS
5	E	10	MET
5	E	11	ILE
5	E	12	LEU
5	E	18	ARG
5	E	20	GLN
5	E	25	ARG
5	E	31	LEU
5	E	33	VAL
5	E	41	VAL
5	E	52	PRO
5	E	53	LEU

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Mol	Chain	Res	Type
5	E	64	ARG
5	E	68	GLU
5	E	73	ASN
5	E	80	ILE
5	E	83	GLU
5	E	90	VAL
5	E	91	LEU
5	E	92	LYS
5	E	101	ILE
5	E	125	SER
5	E	147	ASP
5	E	153	LYS
6	F	15	ASP
6	F	21	LEU
6	F	30	LEU
6	F	36	ARG
6	F	38	GLU
6	F	47	ARG
6	F	61	LEU
6	F	65	VAL
6	F	69	GLU
6	F	70	ASP
6	F	79	LEU
6	F	80	ARG
6	F	81	ILE
6	F	83	ASP
6	F	89	MET
6	F	92	LYS
6	F	98	LEU
7	G	8	GLU
7	G	27	ILE
7	G	32	ARG
7	G	33	ASP
7	G	38	LEU
7	G	48	LYS
7	G	50	ILE
7	G	64	GLN
7	G	77	SER
7	G	79	ARG
7	G	94	ARG
7	G	104	LEU
7	G	114	ARG

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Mol	Chain	Res	Type
7	G	131	LYS
7	G	135	VAL
7	G	136	LYS
7	G	144	MET
7	G	155	ARG
7	G	156	TRP
8	H	18	ARG
8	H	23	SER
8	H	24	THR
8	H	38	ILE
8	H	39	LEU
8	H	50	ARG
8	H	53	VAL
8	H	54	ASP
8	H	56	LYS
8	H	63	LEU
8	H	75	ARG
8	H	85	ARG
8	H	91	ARG
8	H	97	VAL
8	H	98	LYS
8	H	104	ARG
8	H	109	ILE
8	H	112	LEU
8	H	119	LEU
8	H	127	LEU
8	H	133	LEU
9	I	10	ARG
9	I	14	VAL
9	I	31	GLN
9	I	34	ASN
9	I	40	LEU
9	I	41	VAL
9	I	42	ARG
9	I	47	LEU
9	I	54	ASP
9	I	58	ARG
9	I	60	ASP
9	I	64	THR
9	I	66	ARG
9	I	79	LEU
9	I	85	LEU

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Mol	Chain	Res	Type
9	I	86	VAL
9	I	91	ASP
9	I	96	LEU
9	I	97	LYS
9	I	104	ARG
9	I	111	ARG
9	I	114	TYR
9	I	125	TYR
9	I	126	SER
9	I	128	ARG
10	J	4	ILE
10	J	13	HIS
10	J	14	LYS
10	J	22	LYS
10	J	38	ILE
10	J	45	ARG
10	J	49	VAL
10	J	55	LYS
10	J	59	SER
10	J	60	ARG
10	J	70	ARG
10	J	74	ILE
10	J	76	ASN
10	J	79	ARG
10	J	83	GLU
10	J	86	MET
10	J	87	THR
10	J	88	LEU
10	J	89	ASP
10	J	90	LEU
10	J	95	GLU
10	J	96	ILE
10	J	98	ILE
11	K	14	VAL
11	K	29	ILE
11	K	40	ILE
11	K	47	VAL
11	K	53	SER
11	K	54	ARG
11	K	70	LYS
11	K	80	VAL
11	K	84	VAL

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Mol	Chain	Res	Type
11	K	85	ARG
11	K	92	GLU
11	K	95	ILE
11	K	106	LYS
11	K	109	VAL
11	K	114	VAL
11	K	122	LYS
12	L	18	VAL
12	L	20	LYS
12	L	21	LYS
12	L	33	ARG
12	L	47	LYS
12	L	52	LEU
12	L	53	ARG
12	L	54	LYS
12	L	60	LEU
12	L	67	THR
12	L	73	GLU
12	L	78	GLN
12	L	81	SER
12	L	85	ILE
12	L	111	LYS
12	L	113	ARG
12	L	114	LYS
13	M	7	VAL
13	M	8	GLU
13	M	15	VAL
13	M	19	LEU
13	M	20	THR
13	M	27	LYS
13	M	31	LYS
13	M	46	LYS
13	M	47	ASP
13	M	48	LEU
13	M	49	THR
13	M	54	VAL
13	M	57	ARG
13	M	63	THR
13	M	64	TRP
13	M	65	LYS
13	M	66	LEU
13	M	69	GLU

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Mol	Chain	Res	Type
13	M	70	LEU
13	M	73	GLU
13	M	79	LYS
13	M	81	LEU
13	M	82	MET
13	M	84	ILE
13	M	90	LEU
13	M	93	ARG
13	M	94	ARG
13	M	101	GLN
13	M	104	ARG
13	M	105	THR
13	M	108	ARG
13	M	115	LYS
13	M	116	THR
13	M	117	VAL
13	M	120	LYS
14	N	3	ARG
14	N	4	LYS
14	N	6	LEU
14	N	16	PHE
14	N	18	VAL
14	N	22	THR
14	N	23	ARG
14	N	24	CYS
14	N	26	ARG
14	N	27	CYS
14	N	29	ARG
14	N	33	VAL
14	N	35	ARG
14	N	41	ARG
14	N	42	ILE
15	O	3	ILE
15	O	13	GLN
15	O	17	ARG
15	O	31	LEU
15	O	32	LEU
15	O	39	LEU
15	O	40	SER
15	O	44	LYS
15	O	65	ARG
15	O	66	LEU

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Mol	Chain	Res	Type
15	O	67	LEU
15	O	82	ILE
15	O	88	ARG
16	P	2	VAL
16	P	5	ARG
16	P	8	ARG
16	P	12	LYS
16	P	21	VAL
16	P	27	LYS
16	P	28	ARG
16	P	33	ILE
16	P	36	ILE
16	P	45	THR
16	P	50	LYS
16	P	54	GLU
16	P	65	GLN
16	P	69	THR
16	P	71	ARG
17	Q	4	LYS
17	Q	7	THR
17	Q	9	VAL
17	Q	16	GLN
17	Q	23	VAL
17	Q	34	LYS
17	Q	38	ARG
17	Q	49	GLU
17	Q	52	LYS
17	Q	53	LEU
17	Q	59	ILE
17	Q	65	ILE
17	Q	68	ARG
17	Q	79	SER
17	Q	87	LYS
17	Q	96	GLU
17	Q	100	LYS
18	R	19	LYS
18	R	25	THR
18	R	32	ARG
18	R	46	GLU
18	R	47	THR
18	R	65	ILE
18	R	72	ARG

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Mol	Chain	Res	Type
18	R	76	LEU
18	R	82	THR
18	R	83	GLU
18	R	84	LYS
18	R	88	LYS
19	S	4	SER
19	S	5	LEU
19	S	6	LYS
19	S	7	LYS
19	S	10	PHE
19	S	13	ASP
19	S	22	LEU
19	S	25	LYS
19	S	31	ILE
19	S	37	ARG
19	S	44	MET
19	S	58	VAL
19	S	62	ILE
19	S	78	ARG
19	S	80	TYR
20	T	10	LEU
20	T	13	LEU
20	T	24	LEU
20	T	41	ILE
20	T	54	LYS
20	T	55	ILE
20	T	70	SER
20	T	72	LEU
20	T	73	HIS
20	T	84	LEU
20	T	86	ARG
20	T	87	LYS
20	T	99	LEU
20	T	104	LEU
21	U	6	ARG
21	U	8	THR
21	U	10	ARG
21	U	12	LYS
21	U	15	ARG
21	U	24	ARG
21	U	25	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such

sidechains are listed below:

Mol	Chain	Res	Type
2	B	76	GLN
2	B	94	ASN
2	B	95	GLN
2	B	110	GLN
2	B	135	GLN
3	C	110	ASN
5	E	78	HIS
5	E	127	ASN
5	E	130	ASN
6	F	64	GLN
6	F	94	GLN
7	G	13	GLN
7	G	122	HIS
9	I	31	GLN
9	I	124	GLN
11	K	117	ASN
13	M	62	ASN
15	O	37	ASN
20	T	16	HIS
20	T	45	GLN
20	T	90	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1515/1516 (99%)	423 (27%)	87 (5%)
22	X	5/6 (83%)	5 (100%)	0
23	Y	9/10 (90%)	2 (22%)	0
All	All	1529/1532 (99%)	430 (28%)	87 (5%)

All (430) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	7	G
1	A	10	G
1	A	21	U
1	A	33	A
1	A	40	G
1	A	45	G
1	A	48	C
1	A	49	C

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Mol	Chain	Res	Type
1	A	51	A
1	A	52	A
1	A	55	C
1	A	60	A
1	A	70	G
1	A	74	G
1	A	77	G
1	A	78	G
1	A	80	U
1	A	81	U
1	A	82	U
1	A	83	U
1	A	84	A
1	A	92	G
1	A	95	A
1	A	99	G
1	A	102	G
1	A	103	A
1	A	110	A
1	A	114	A
1	A	115	C
1	A	126	C
1	A	137	G
1	A	138	A
1	A	139	G
1	A	141	G
1	A	147	A
1	A	151	G
1	A	157	A
1	A	158	C
1	A	166	A
1	A	174	A
1	A	175	U
1	A	193	G
1	A	197	U
1	A	202	A
1	A	204	A
1	A	209	U
1	A	210	U
1	A	212	G
1	A	213	C
1	A	216	G

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Mol	Chain	Res	Type
1	A	222	G
1	A	227	G
1	A	243	G
1	A	246	A
1	A	247	G
1	A	258	A
1	A	262	G
1	A	263	C
1	A	266	A
1	A	271	G
1	A	285	G
1	A	296	A
1	A	304	C
1	A	317	A
1	A	324	C
1	A	325	A
1	A	326	C
1	A	328	G
1	A	335	C
1	A	341	C
1	A	346	G
1	A	348	C
1	A	349	A
1	A	350	G
1	A	351	C
1	A	363	U
1	A	365	C
1	A	366	C
1	A	368	C
1	A	369	A
1	A	375	C
1	A	393	A
1	A	394	C
1	A	401	U
1	A	402	G
1	A	404	A
1	A	407	A
1	A	408	A
1	A	409	G
1	A	410	A
1	A	415	C
1	A	417	U

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Mol	Chain	Res	Type
1	A	418	C
1	A	419	G
1	A	420	G
1	A	421	G
1	A	425	U
1	A	426	A
1	A	430	U
1	A	431	C
1	A	435	A
1	A	447	A
1	A	448	A
1	A	450	C
1	A	452	C
1	A	455	A
1	A	456	C
1	A	469	G
1	A	470	G
1	A	481	A
1	A	482	U
1	A	483	A
1	A	484	G
1	A	489	G
1	A	493	A
1	A	494	A
1	A	495	C
1	A	498	C
1	A	501	G
1	A	502	C
1	A	505	G
1	A	508	G
1	A	511	G
1	A	515	U
1	A	516	A
1	A	517	A
1	A	524	G
1	A	529	C
1	A	531	A
1	A	543	A
1	A	545	U
1	A	550	G
1	A	551	G
1	A	554	G

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Mol	Chain	Res	Type
1	A	555	U
1	A	556	A
1	A	557	A
1	A	560	G
1	A	566	U
1	A	572	G
1	A	579	G
1	A	580	C
1	A	591	A
1	A	593	A
1	A	614	G
1	A	616	A
1	A	617	G
1	A	633	G
1	A	636	U
1	A	637	A
1	A	645	G
1	A	646	G
1	A	649	A
1	A	650	G
1	A	671	A
1	A	672	G
1	A	679	A
1	A	685	C
1	A	687	G
1	A	689	U
1	A	705	G
1	A	706	A
1	A	707	U
1	A	715	G
1	A	733	C
1	A	739	G
1	A	753	G
1	A	760	G
1	A	761	A
1	A	775	G
1	A	776	A
1	A	777	U
1	A	778	A
1	A	779	C
1	A	788	U
1	A	794	C

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Mol	Chain	Res	Type
1	A	799	A
1	A	800	A
1	A	801	C
1	A	802	G
1	A	803	A
1	A	804	U
1	A	812	A
1	A	820	G
1	A	823	U
1	A	824	C
1	A	825	U
1	A	826	C
1	A	836	G
1	A	837	A
1	A	844	C
1	A	869	U
1	A	870	A
1	A	880	G
1	A	892	A
1	A	897	A
1	A	900	G
1	A	904	G
1	A	905	G
1	A	908	C
1	A	911	G
1	A	912	C
1	A	913	A
1	A	915	A
1	A	920	G
1	A	921	U
1	A	922	G
1	A	936	A
1	A	938	U
1	A	939	U
1	A	940	C
1	A	941	G
1	A	943	A
1	A	944	G
1	A	947	A
1	A	949	G
1	A	950	C
1	A	952	A

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Mol	Chain	Res	Type
1	A	953	A
1	A	954	G
1	A	955	A
1	A	956	A
1	A	958	C
1	A	959	U
1	A	962	C
1	A	963	C
1	A	967	C
1	A	971	G
1	A	975	U
1	A	980	G
1	A	982	G
1	A	983	A
1	A	984	A
1	A	985	C
1	A	986	C
1	A	987	C
1	A	988	G
1	A	989	G
1	A	995	A
1	A	996	G
1	A	1000	G
1	A	1002	G
1	A	1003	G
1	A	1004	U
1	A	1005	G
1	A	1006	C
1	A	1008	C
1	A	1009	C
1	A	1010	G
1	A	1012	G
1	A	1013	A
1	A	1014	G
1	A	1015	G
1	A	1016	G
1	A	1017	G
1	A	1018	A
1	A	1022	C
1	A	1023	U
1	A	1029	A
1	A	1032	U

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Mol	Chain	Res	Type
1	A	1036	G
1	A	1037	C
1	A	1038	A
1	A	1039	U
1	A	1044	G
1	A	1048	U
1	A	1050	A
1	A	1051	G
1	A	1053	U
1	A	1055	G
1	A	1069	U
1	A	1074	U
1	A	1075	A
1	A	1077	G
1	A	1078	U
1	A	1079	C
1	A	1084	A
1	A	1088	A
1	A	1091	G
1	A	1096	C
1	A	1098	C
1	A	1100	G
1	A	1101	C
1	A	1102	C
1	A	1106	A
1	A	1107	G
1	A	1108	U
1	A	1109	U
1	A	1110	G
1	A	1111	C
1	A	1112	C
1	A	1113	A
1	A	1114	G
1	A	1115	C
1	A	1117	G
1	A	1119	U
1	A	1120	C
1	A	1121	G
1	A	1122	G
1	A	1123	C
1	A	1124	C
1	A	1125	G

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Mol	Chain	Res	Type
1	A	1129	A
1	A	1134	A
1	A	1135	A
1	A	1141	C
1	A	1142	U
1	A	1143	G
1	A	1153	G
1	A	1155	G
1	A	1161	A
1	A	1166	G
1	A	1173	A
1	A	1174	C
1	A	1178	U
1	A	1179	G
1	A	1180	G
1	A	1182	C
1	A	1184	G
1	A	1188	G
1	A	1190	C
1	A	1193	U
1	A	1194	U
1	A	1195	A
1	A	1196	C
1	A	1197	G
1	A	1199	C
1	A	1200	C
1	A	1209	A
1	A	1220	A
1	A	1222	U
1	A	1223	G
1	A	1226	C
1	A	1227	A
1	A	1230	A
1	A	1231	C
1	A	1232	A
1	A	1233	A
1	A	1234	A
1	A	1235	G
1	A	1238	A
1	A	1239	U
1	A	1242	C
1	A	1244	C

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Mol	Chain	Res	Type
1	A	1245	C
1	A	1252	C
1	A	1254	G
1	A	1255	G
1	A	1259	C
1	A	1261	A
1	A	1262	A
1	A	1263	U
1	A	1264	C
1	A	1267	A
1	A	1269	A
1	A	1270	A
1	A	1271	A
1	A	1279	C
1	A	1281	A
1	A	1282	G
1	A	1284	U
1	A	1293	G
1	A	1294	G
1	A	1298	G
1	A	1299	C
1	A	1301	A
1	A	1302	C
1	A	1311	A
1	A	1312	U
1	A	1313	G
1	A	1316	G
1	A	1317	C
1	A	1318	C
1	A	1320	G
1	A	1322	A
1	A	1328	A
1	A	1329	G
1	A	1330	U
1	A	1332	A
1	A	1334	C
1	A	1335	G
1	A	1336	C
1	A	1346	A
1	A	1350	C
1	A	1352	C
1	A	1353	G

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Mol	Chain	Res	Type
1	A	1356	G
1	A	1362	G
1	A	1365	C
1	A	1370	G
1	A	1380	C
1	A	1381	A
1	A	1383	C
1	A	1384	G
1	A	1387	C
1	A	1397	U
1	A	1402	G
1	A	1404	G
1	A	1410	U
1	A	1425	G
1	A	1426	G
1	A	1427	A
1	A	1443	C
1	A	1453	G
1	A	1459	U
1	A	1465	G
1	A	1470	A
1	A	1474	C
1	A	1475	G
1	A	1477	A
1	A	1478	A
1	A	1481	A
1	A	1482	G
1	A	1484	U
1	A	1485	A
1	A	1495	G
1	A	1499	G
1	A	1507	G
1	A	1508	G
1	A	1510	U
1	A	1511	C
1	A	1512	A
1	A	1516	C
22	X	2	G
22	X	3	A
22	X	4	PSU
22	X	5	G
22	X	6	A

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Mol	Chain	Res	Type
23	Y	36	A
23	Y	40	U

All (87) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	81	U
1	A	82	U
1	A	83	U
1	A	102	G
1	A	109	G
1	A	114	A
1	A	209	U
1	A	239	A
1	A	246	A
1	A	262	G
1	A	276	C
1	A	325	A
1	A	340	A
1	A	349	A
1	A	365	C
1	A	401	U
1	A	408	A
1	A	417	U
1	A	418	C
1	A	425	U
1	A	466	G
1	A	469	G
1	A	480	A
1	A	483	A
1	A	493	A
1	A	516	A
1	A	544	U
1	A	559	G
1	A	571	G
1	A	614	G
1	A	646	G
1	A	670	U
1	A	671	A
1	A	686	A
1	A	732	C
1	A	775	G

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Mol	Chain	Res	Type
1	A	777	U
1	A	824	C
1	A	867	A
1	A	891	A
1	A	908	C
1	A	938	U
1	A	939	U
1	A	940	C
1	A	943	A
1	A	949	G
1	A	954	G
1	A	958	C
1	A	970	U
1	A	982	G
1	A	1004	U
1	A	1007	C
1	A	1012	G
1	A	1027	A
1	A	1032	U
1	A	1037	C
1	A	1050	A
1	A	1068	U
1	A	1100	G
1	A	1107	G
1	A	1111	C
1	A	1122	G
1	A	1124	C
1	A	1128	C
1	A	1134	A
1	A	1165	A
1	A	1173	A
1	A	1183	A
1	A	1193	U
1	A	1230	A
1	A	1231	C
1	A	1233	A
1	A	1234	A
1	A	1238	A
1	A	1267	A
1	A	1279	C
1	A	1281	A
1	A	1301	A

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Mol	Chain	Res	Type
1	A	1317	C
1	A	1319	G
1	A	1328	A
1	A	1352	C
1	A	1477	A
1	A	1482	G
1	A	1483	G
1	A	1508	G
1	A	1510	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	PSU	X	1	22	14,18,22	1.66	3 (21%)	18,26,33	4.61	12 (66%)
22	PSU	X	4	22,23	13,21,22	1.89	2 (15%)	18,30,33	3.44	6 (33%)

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
22	PSU	X	1	22	-	0/6/22/26	0/2/2/2
22	PSU	X	4	22,23	-	0/7/25/26	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	X	4	PSU	C5-C1'	-5.49	1.47	1.52
22	X	1	PSU	C2'-C1'	-3.64	1.50	1.53
22	X	4	PSU	C2'-C1'	-3.22	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	X	1	PSU	C5-C1'	-2.64	1.49	1.52
22	X	1	PSU	O3'-C3'	2.11	1.48	1.43

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	X	1	PSU	N1-C2-N3	-10.53	121.61	128.33
22	X	4	PSU	N1-C2-N3	-9.46	122.30	128.33
22	X	1	PSU	C5-C1'-C2'	-8.05	101.23	115.52
22	X	4	PSU	C5-C1'-C2'	-6.30	104.33	115.52
22	X	1	PSU	C5-C6-N1	-5.40	116.77	124.39
22	X	1	PSU	O4'-C4'-C3'	-3.90	97.29	105.15
22	X	4	PSU	C5-C6-N1	-2.69	120.59	124.39
22	X	1	PSU	O3'-C3'-C2'	-2.28	104.41	111.83
22	X	1	PSU	C5'-C4'-C3'	2.43	120.84	115.08
22	X	4	PSU	C6-N1-C2	3.05	120.38	115.47
22	X	4	PSU	C4'-O4'-C1'	3.16	112.81	109.58
22	X	1	PSU	C4-N3-C2	3.44	118.22	115.25
22	X	1	PSU	C3'-C2'-C1'	3.79	106.19	101.79
22	X	1	PSU	O5'-C5'-C4'	4.99	127.81	111.33
22	X	1	PSU	C4'-O4'-C1'	5.34	115.03	109.58
22	X	1	PSU	C6-N1-C2	5.48	124.28	115.47
22	X	1	PSU	O3'-C3'-C4'	5.54	127.66	111.05
22	X	4	PSU	C4-N3-C2	6.96	121.26	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	X	1	PSU	1	0
22	X	4	PSU	4	0

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 15 ligands modelled in this entry, 14 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
25	PAR	A	1614	-	45,45,45	1.26	6 (13%)	59,67,67	2.02	16 (27%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	PAR	A	1614	-	-	0/18/94/94	0/4/4/4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	1614	PAR	C34-C24	-3.96	1.48	1.53
25	A	1614	PAR	C13-C23	-3.26	1.48	1.52
25	A	1614	PAR	C31-C21	-2.49	1.50	1.53
25	A	1614	PAR	C33-C43	-2.28	1.46	1.52
25	A	1614	PAR	C62-C12	-2.23	1.48	1.53
25	A	1614	PAR	O41-C41	-2.12	1.37	1.43

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	1614	PAR	O54-C54-C64	-8.88	88.74	106.10
25	A	1614	PAR	O33-C33-C43	-3.74	96.68	111.83
25	A	1614	PAR	O53-C53-C43	-3.40	100.08	111.33
25	A	1614	PAR	C11-O51-C51	-3.30	107.34	113.75
25	A	1614	PAR	O44-C44-C34	-2.99	103.61	110.34
25	A	1614	PAR	O41-C41-C31	-2.90	103.81	110.34
25	A	1614	PAR	O23-C23-C13	-2.62	104.36	111.67
25	A	1614	PAR	O41-C41-C51	-2.36	102.98	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	1614	PAR	C14-C24-C34	-2.31	103.38	109.95
25	A	1614	PAR	O33-C14-O54	-2.28	104.90	110.68
25	A	1614	PAR	O11-C42-C32	-2.20	103.58	108.92
25	A	1614	PAR	O43-C13-C23	-2.18	101.72	104.78
25	A	1614	PAR	C31-C21-N21	-2.18	106.82	110.86
25	A	1614	PAR	C22-C12-C62	-2.03	107.00	110.11
25	A	1614	PAR	O51-C51-C61	2.54	112.78	106.36
25	A	1614	PAR	C14-O54-C54	3.15	119.86	113.75

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	A	1614	PAR	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1516/1516 (100%)	-0.33	6 (0%) 93 85	42, 72, 141, 239	0
2	B	234/234 (100%)	-0.27	3 (1%) 79 62	58, 105, 160, 191	0
3	C	206/206 (100%)	-0.29	0 100 100	62, 92, 140, 162	0
4	D	208/208 (100%)	-0.34	0 100 100	50, 80, 120, 145	0
5	E	150/150 (100%)	-0.45	0 100 100	46, 66, 94, 137	0
6	F	101/101 (100%)	-0.30	1 (0%) 84 69	66, 98, 125, 150	0
7	G	155/155 (100%)	-0.49	0 100 100	63, 89, 145, 165	0
8	H	138/138 (100%)	-0.54	0 100 100	41, 64, 91, 123	0
9	I	127/127 (100%)	-0.03	2 (1%) 74 55	52, 104, 135, 154	0
10	J	98/98 (100%)	0.13	3 (3%) 52 28	57, 126, 180, 221	0
11	K	119/119 (100%)	-0.27	3 (2%) 61 37	44, 76, 113, 168	0
12	L	125/125 (100%)	-0.22	3 (2%) 62 39	39, 73, 116, 168	0
13	M	120/120 (100%)	0.11	6 (5%) 32 13	62, 90, 131, 159	0
14	N	60/60 (100%)	-0.34	0 100 100	69, 91, 114, 127	0
15	O	88/88 (100%)	-0.26	1 (1%) 82 66	51, 79, 116, 161	0
16	P	83/83 (100%)	-0.31	0 100 100	50, 65, 94, 126	0
17	Q	99/99 (100%)	-0.21	0 100 100	42, 67, 102, 126	0
18	R	70/70 (100%)	-0.35	0 100 100	62, 85, 116, 132	0
19	S	78/78 (100%)	0.04	2 (2%) 59 35	67, 107, 161, 176	0
20	T	99/99 (100%)	-0.11	0 100 100	45, 70, 113, 128	0
21	U	24/24 (100%)	0.00	0 100 100	59, 79, 106, 136	0
22	X	4/6 (66%)	0.21	0 100 100	66, 67, 85, 93	0
23	Y	10/10 (100%)	0.41	0 100 100	76, 96, 145, 188	0
All	All	3912/3914 (99%)	-0.28	30 (0%) 87 75	39, 79, 141, 239	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
11	K	129	SER	8.6
19	S	30	LEU	6.9
13	M	121	LYS	5.3
19	S	81	ARG	4.9
11	K	128	ALA	4.3
15	O	89	GLY	3.9
13	M	119	GLY	3.8
12	L	127	GLU	3.7
13	M	7	VAL	3.4
13	M	120	LYS	3.4
2	B	132	LYS	3.0
1	A	707	U	2.9
9	I	7	THR	2.8
9	I	15	ALA	2.6
10	J	87	THR	2.5
13	M	84	ILE	2.4
1	A	1006	C	2.4
1	A	1017	G	2.4
11	K	127	LYS	2.4
10	J	10	GLY	2.3
12	L	128	ALA	2.3
10	J	34	VAL	2.3
1	A	1232	A	2.3
12	L	28	LYS	2.2
1	A	1112	C	2.2
6	F	101	ALA	2.1
2	B	36	ARG	2.1
13	M	118	ALA	2.1
1	A	1009	C	2.0
2	B	127	ILE	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
22	PSU	X	1	17/21	0.90	0.18	-	29,58,70,82	0
22	PSU	X	4	20/21	0.96	0.15	-	58,67,81,83	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
24	MG	A	1610	1/1	0.98	0.44	41.13	43,43,43,43	0
24	MG	A	1604	1/1	0.97	0.32	11.04	57,57,57,57	0
24	MG	A	1603	1/1	0.98	0.33	8.24	60,60,60,60	0
24	MG	A	1605	1/1	0.94	0.28	5.91	42,42,42,42	0
25	PAR	A	1614	42/42	0.97	0.14	0.13	49,60,88,106	0
24	MG	A	1601	1/1	0.98	0.11	-3.81	49,49,49,49	0
24	MG	A	1606	1/1	0.98	0.10	-6.57	52,52,52,52	0
24	MG	X	101	1/1	0.93	0.25	-	55,55,55,55	0
24	MG	A	1607	1/1	0.97	0.52	-	46,46,46,46	0
24	MG	A	1608	1/1	0.94	0.53	-	52,52,52,52	0
24	MG	A	1612	1/1	0.94	0.39	-	44,44,44,44	0
24	MG	A	1609	1/1	0.97	0.26	-	47,47,47,47	0
24	MG	A	1611	1/1	0.94	0.61	-	51,51,51,51	0
24	MG	A	1602	1/1	0.97	0.29	-	48,48,48,48	0
24	MG	A	1613	1/1	0.98	0.32	-	41,41,41,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.