



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:35 AM UTC

PDB ID : 4JYA / pdb_00004jya
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

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

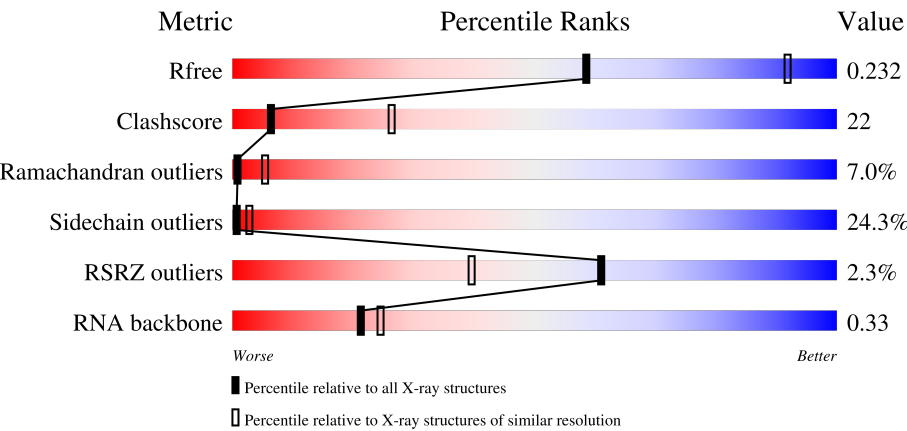
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.10 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}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)
RNA backbone	3983	1022 (3.32-2.88)

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

Mol	Chain	Length	Quality of chain
1	A	1516	37%37%20%5%
2	B	234	34%42%21%.3%
3	C	206	39%38%18%5%
4	D	208	47%35%13%5%4%

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Mol	Chain	Length	Quality of chain
5	E	150	 52% 37% 9%
6	F	101	 48% 41% 11%
7	G	155	 56% 31% 12%
8	H	138	 57% 36% 7%
9	I	127	 34% 43% 20%
10	J	98	 22% 49% 22% 10%
11	K	119	 56% 29% 13%
12	L	125	 47% 33% 17%
13	M	120	 38% 32% 24%
14	N	60	 42% 32% 18%
15	O	88	 55% 38% 7%
16	P	83	 54% 35% 11%
17	Q	99	 54% 32% 12%
18	R	70	 46% 43% 9%
19	S	78	 42% 35% 17%
20	T	99	 48% 35% 11%
21	U	24	 42% 38% 21%
22	X	6	 67% 33%
23	Y	10	 50% 40% 10%

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			

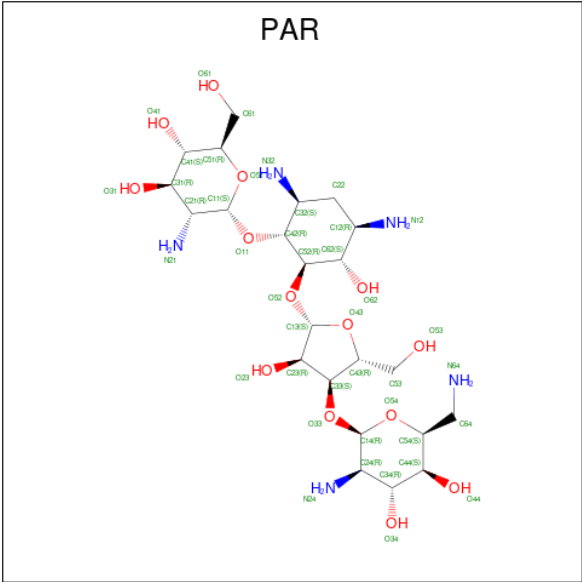
- Molecule 23 is a RNA chain called ASL-tRNA.

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 (CCD ID: MG) (formula: Mg).

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

- Molecule 25 is PAROMOMYCIN (CCD ID: PAR) (formula: C₂₃H₄₅N₅O₁₄).

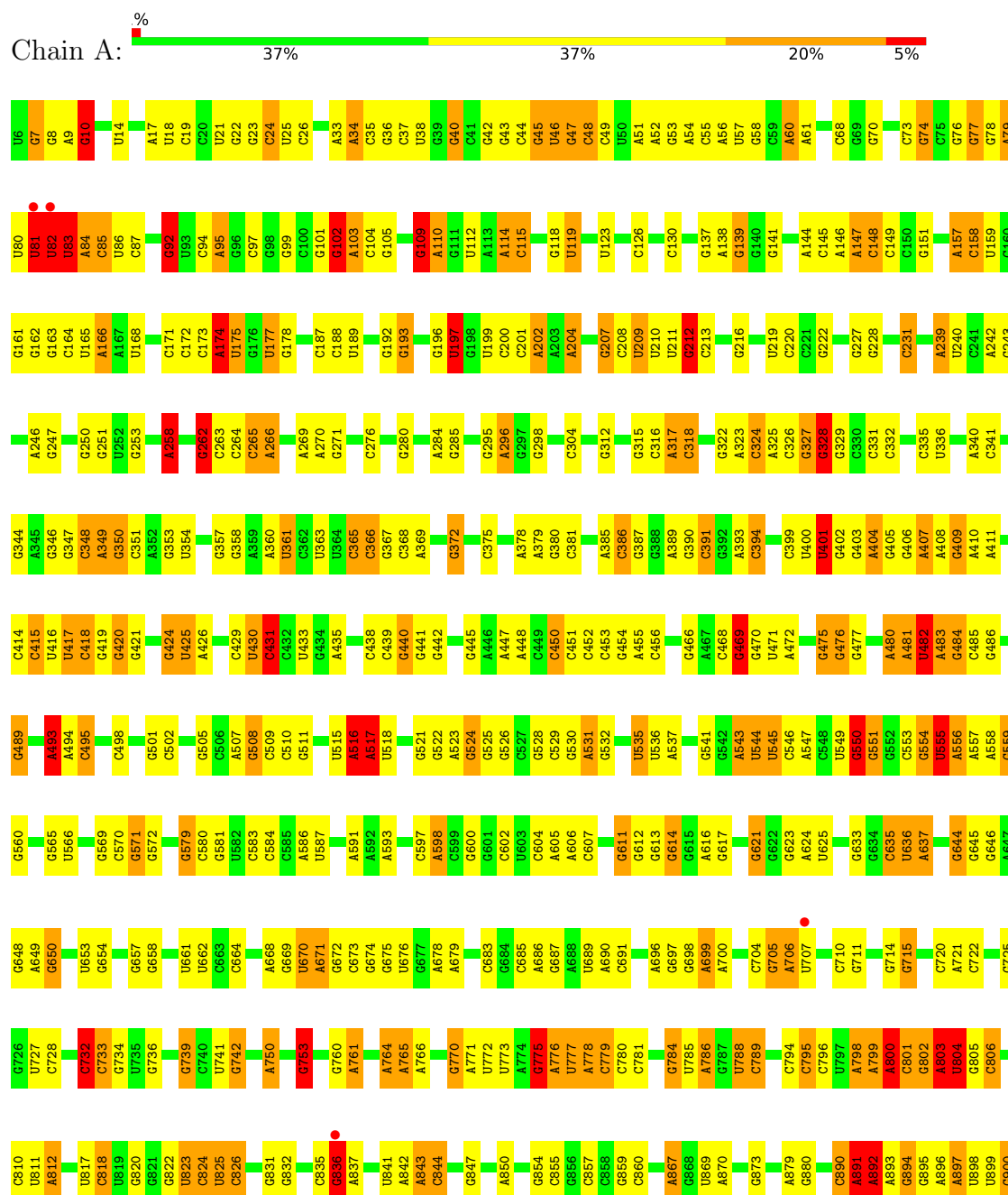


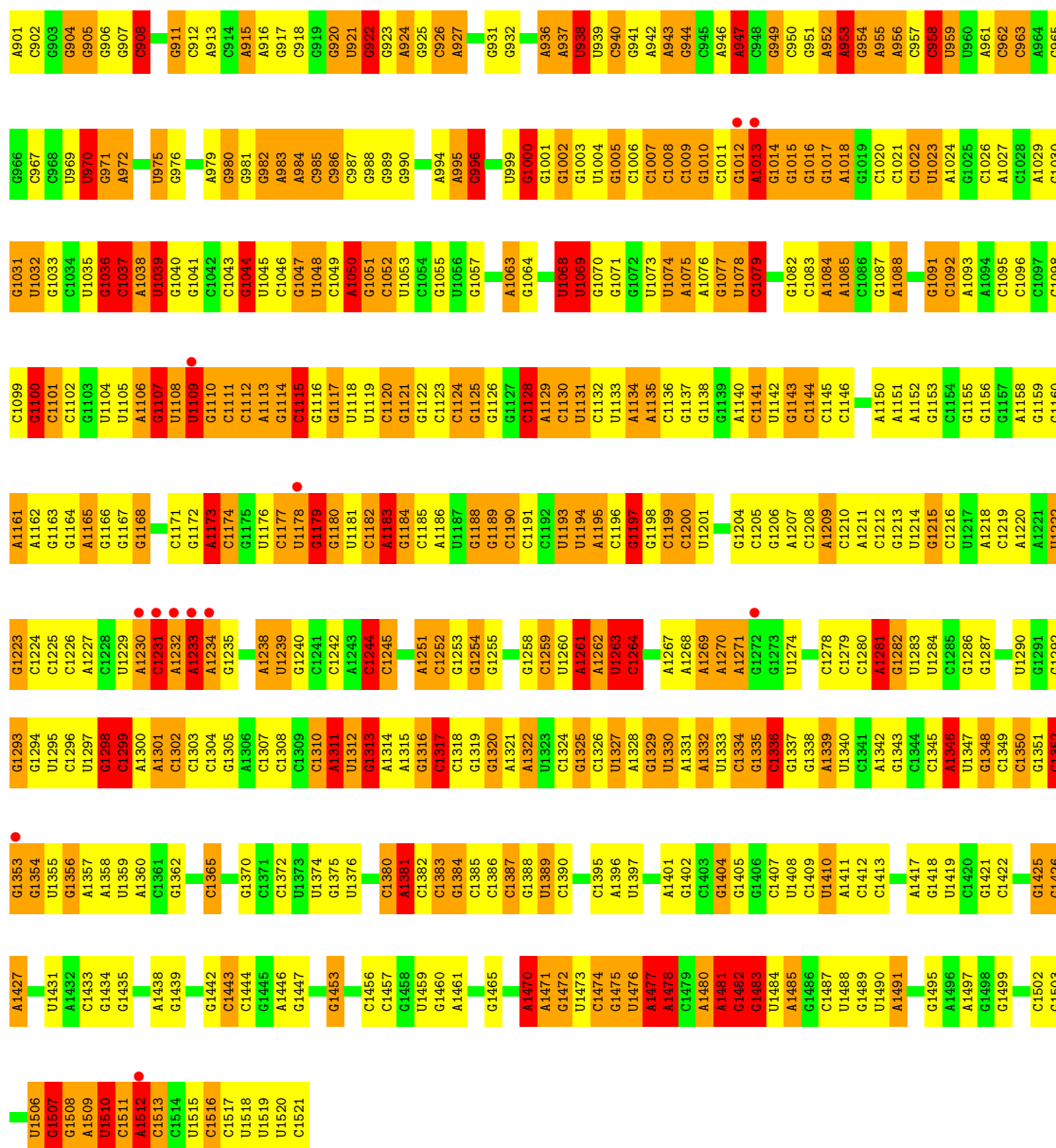
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	A	1	Total	C	N	O	0	0
			42	23	5	14		

3 Residue-property plots

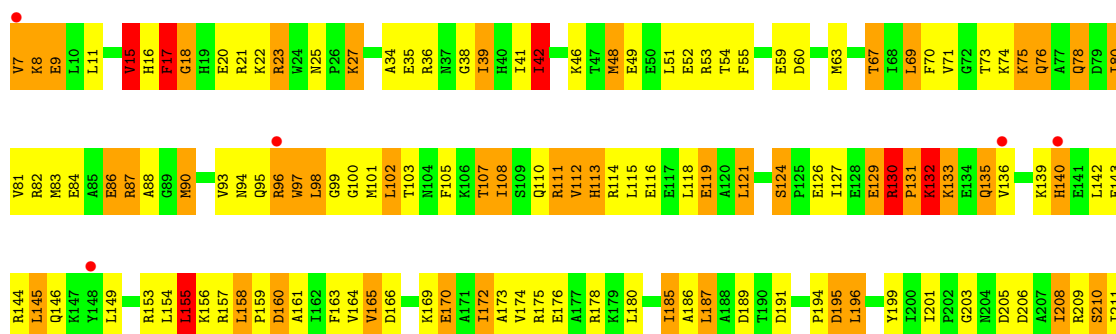
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

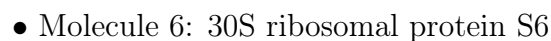
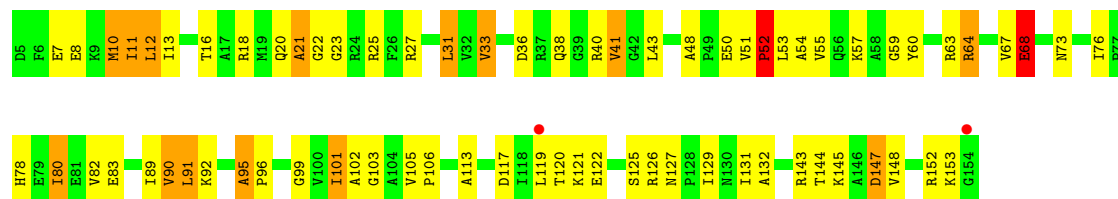
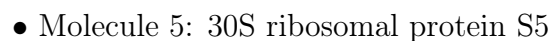
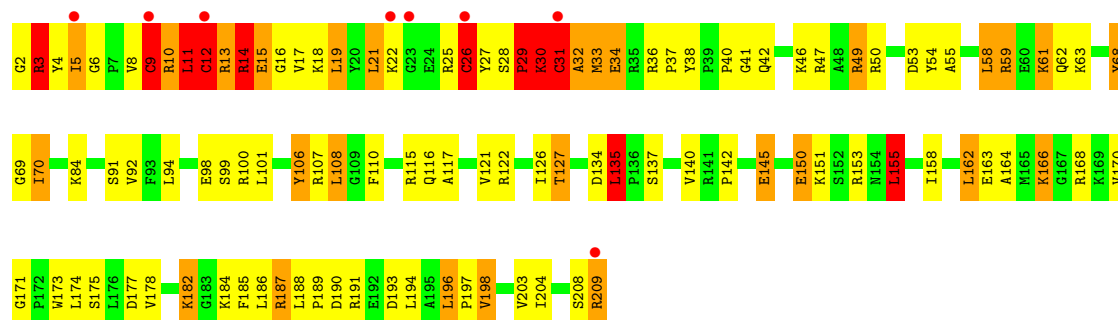
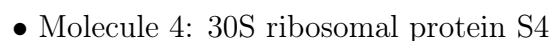
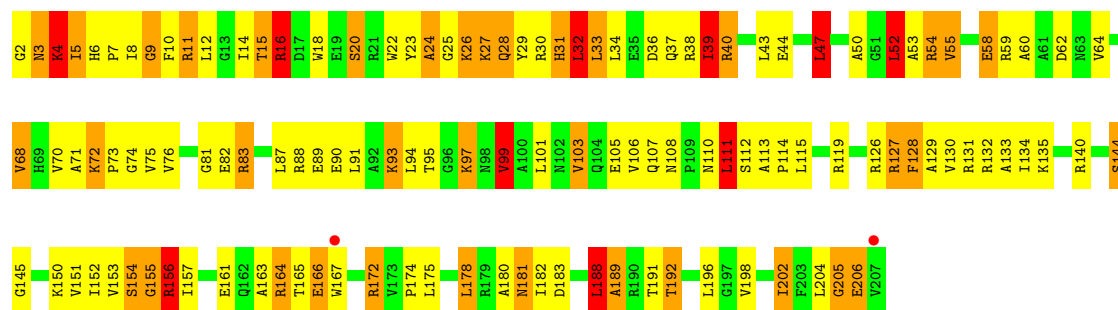
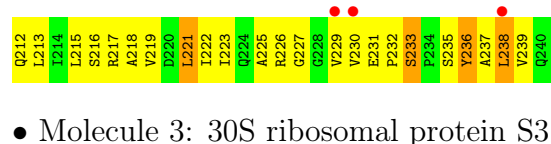
• Molecule 1: 16S ribosomal RNA





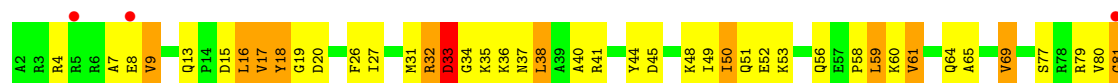
• Molecule 2: 30S ribosomal protein S2







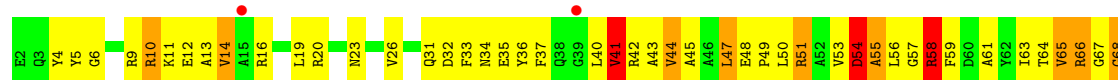
- Molecule 7: 30S ribosomal protein S7



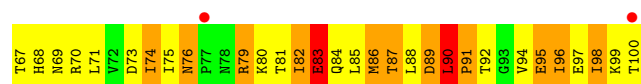
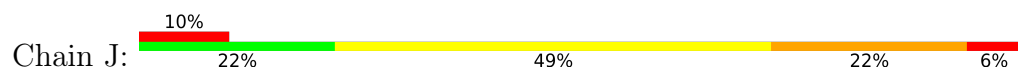
- Molecule 8: 30S ribosomal protein S8



- Molecule 9: 30S ribosomal protein S9

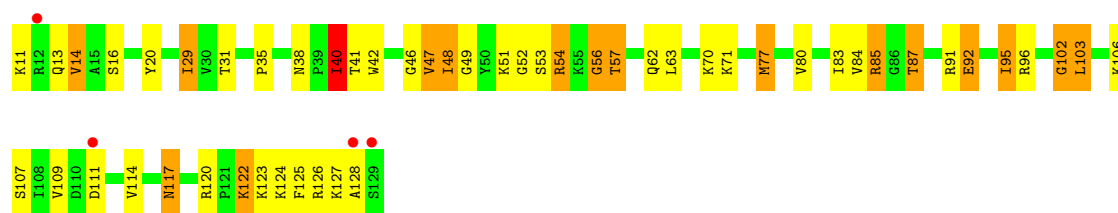


- Molecule 10: 30S ribosomal protein S10

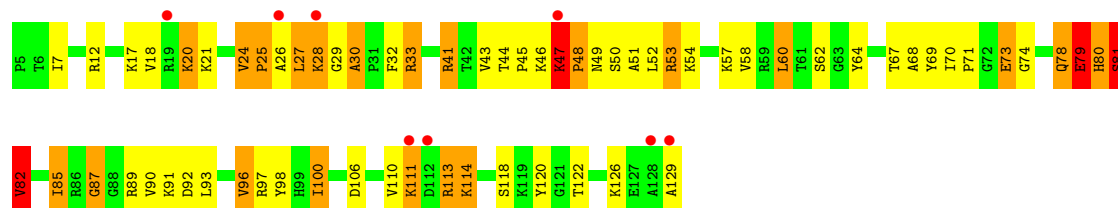


- Molecule 11: 30S ribosomal protein S11

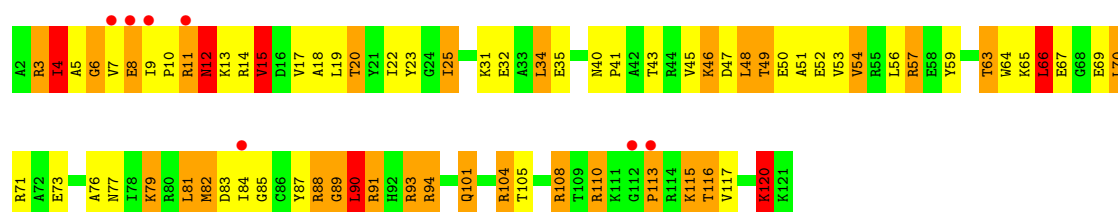




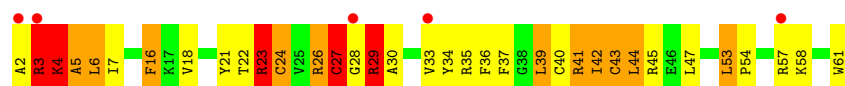
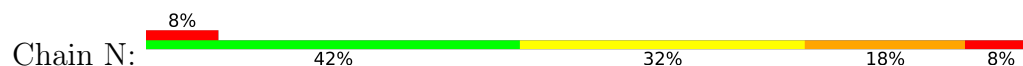
• Molecule 12: 30S ribosomal protein S12



• Molecule 13: 30S ribosomal protein S13



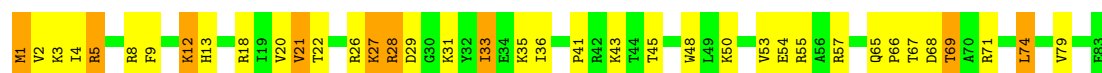
• Molecule 14: 30S ribosomal protein S14



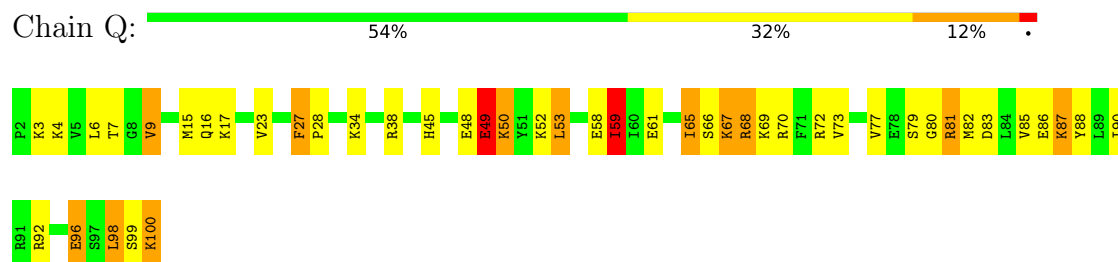
• Molecule 15: 30S ribosomal protein S15



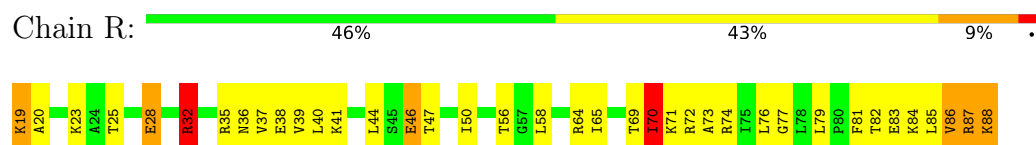
• Molecule 16: 30S ribosomal protein S16



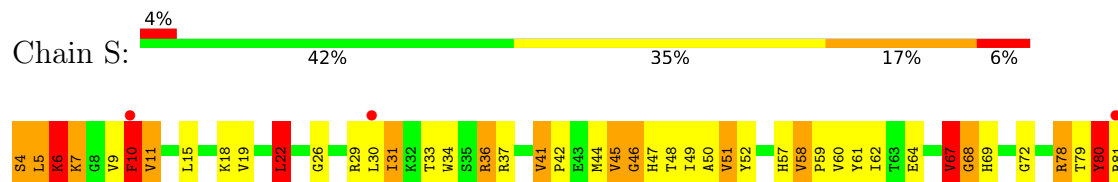
- Molecule 17: 30S ribosomal protein S17



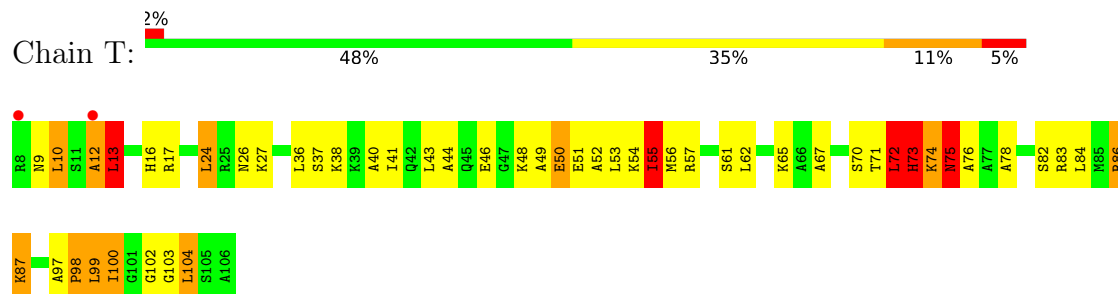
- Molecule 18: 30S ribosomal protein S18



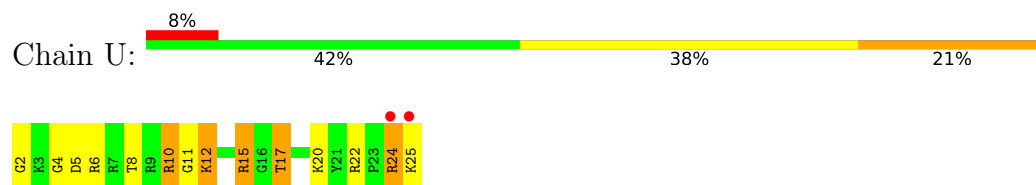
- Molecule 19: 30S ribosomal protein S19



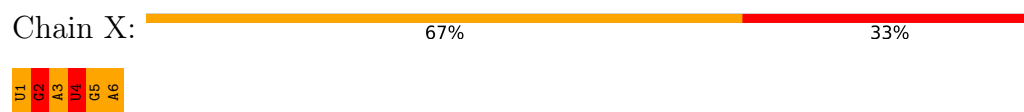
- Molecule 20: 30S ribosomal protein S20



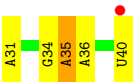
- Molecule 21: 30S ribosomal protein THX



- 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) 98.9 (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 (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	78.5	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 47.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.52	6/36456 (0.0%)	1.07	311/56897 (0.5%)
2	B	0.74	0/1935	1.19	14/2609 (0.5%)
3	C	0.87	1/1636 (0.1%)	1.18	9/2205 (0.4%)
4	D	0.88	5/1733 (0.3%)	1.30	18/2318 (0.8%)
5	E	0.87	1/1162 (0.1%)	1.38	13/1564 (0.8%)
6	F	0.70	0/856	1.11	3/1154 (0.3%)
7	G	0.70	0/1276	1.11	4/1709 (0.2%)
8	H	0.82	0/1136	1.21	6/1527 (0.4%)
9	I	0.73	0/1029	1.14	8/1378 (0.6%)
10	J	0.88	0/807	1.27	10/1085 (0.9%)
11	K	0.73	0/900	1.13	3/1213 (0.2%)
12	L	0.91	3/991 (0.3%)	1.34	7/1327 (0.5%)
13	M	0.80	0/965	1.24	4/1292 (0.3%)
14	N	1.04	0/501	1.41	6/664 (0.9%)
15	O	0.72	0/745	1.05	1/992 (0.1%)
16	P	0.78	0/716	1.17	0/963
17	Q	0.83	1/836 (0.1%)	1.36	11/1117 (1.0%)
18	R	0.70	0/579	1.16	3/768 (0.4%)
19	S	0.87	2/642 (0.3%)	1.33	8/865 (0.9%)
20	T	0.82	1/765 (0.1%)	1.31	4/1007 (0.4%)
21	U	0.78	0/212	1.17	1/277 (0.4%)
22	X	0.75	0/102	1.49	4/160 (2.5%)
23	Y	0.49	0/239	1.04	1/370 (0.3%)
All	All	0.64	20/56219 (0.0%)	1.12	449/83461 (0.5%)

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 (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	82	U	O3'-P	9.13	1.74	1.61
1	A	81	U	O3'-P	7.92	1.73	1.61
1	A	83	U	O3'-P	7.24	1.72	1.61
4	D	12	CYS	CA-CB	7.12	1.65	1.53
1	A	750	A	P-OP2	6.77	1.62	1.49
19	S	80	TYR	N-CA	5.80	1.53	1.46
4	D	30	LYS	N-CA	5.78	1.53	1.46
4	D	12	CYS	CA-C	5.73	1.60	1.52
19	S	79	THR	CA-C	5.67	1.59	1.52
12	L	25	PRO	CA-C	5.66	1.60	1.52
3	C	4	LYS	N-CA	5.55	1.53	1.46
20	T	12	ALA	CA-C	5.52	1.59	1.53
5	E	67	VAL	CA-C	5.47	1.59	1.52
12	L	25	PRO	N-CA	5.27	1.54	1.47
4	D	14	ARG	N-CA	5.24	1.52	1.46
4	D	26	CYS	CA-C	5.22	1.59	1.52
1	A	836	G	O3'-P	5.11	1.68	1.61
1	A	799	A	O3'-P	-5.11	1.53	1.61
12	L	82	VAL	N-CA	5.06	1.52	1.46
17	Q	6	LEU	CA-C	-5.03	1.46	1.52

All (449) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	891	A	C2'-C3'-O3'	13.74	130.10	109.50
1	A	109	G	C2'-C3'-O3'	12.51	128.26	109.50
1	A	1050	A	C2'-C3'-O3'	11.91	127.36	109.50
1	A	671	A	C2'-C3'-O3'	11.23	126.35	109.50
1	A	469	G	C2'-C3'-O3'	10.81	125.72	109.50
1	A	516	A	C2'-C3'-O3'	10.76	125.64	109.50
1	A	547	A	C4'-C3'-O3'	-10.72	96.92	113.00
1	A	82	U	C2'-C3'-O3'	10.61	125.41	109.50
5	E	105	VAL	CA-C-N	-10.48	108.97	119.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	105	VAL	C-N-CA	-10.48	108.97	119.87
1	A	1510	U	C2'-C3'-O3'	10.37	129.25	113.70
14	N	30	ALA	N-CA-C	9.80	121.56	111.07
20	T	13	LEU	N-CA-C	-9.67	101.15	113.72
1	A	775	G	C2'-C3'-O3'	9.64	128.16	113.70
1	A	873	G	C3'-C2'-O2'	9.62	125.13	110.70
1	A	1134	A	C2'-C3'-O3'	9.58	123.86	109.50
1	A	1348	G	C2'-C3'-O3'	-9.52	99.42	113.70
1	A	1215	G	C3'-C2'-O2'	9.43	124.85	110.70
1	A	1037	C	C4'-C3'-O3'	-9.37	95.35	109.40
1	A	262	G	C2'-C3'-O3'	9.29	127.63	113.70
1	A	1513	C	C4'-C3'-O3'	-9.10	95.75	109.40
1	A	1183	A	C2'-C3'-O3'	8.88	122.81	109.50
3	C	155	GLY	N-CA-C	8.87	124.17	110.96
1	A	803	A	C2'-C3'-O3'	8.73	122.60	109.50
1	A	704	C	C2'-C3'-O3'	-8.63	100.75	113.70
1	A	894	G	C4'-C3'-O3'	-8.51	100.23	113.00
1	A	1317	C	C2'-C3'-O3'	-8.51	100.93	113.70
1	A	795	C	C4'-C3'-O3'	-8.47	100.30	113.00
4	D	12	CYS	N-CA-C	-8.31	93.10	110.80
5	E	67	VAL	N-CA-C	8.26	120.77	108.46
1	A	401	U	C2'-C3'-O3'	8.23	126.05	113.70
1	A	803	A	C4'-C3'-O3'	-8.13	97.20	109.40
1	A	1233	A	C4'-C3'-O3'	8.12	121.58	109.40
1	A	1183	A	C1'-C2'-O2'	-8.08	99.68	111.80
1	A	228	G	C1'-C2'-O2'	-8.05	96.33	108.40
1	A	79	A	C4'-C3'-O3'	-8.05	100.93	113.00
1	A	1231	C	C4'-C3'-O3'	8.03	125.05	113.00
5	E	95	ALA	CA-C-N	8.02	128.08	119.90
5	E	95	ALA	C-N-CA	8.02	128.08	119.90
1	A	1389	U	C2'-C3'-O3'	-7.97	101.75	113.70
5	E	48	ALA	N-CA-C	7.90	115.33	108.22
1	A	1508	G	C2'-C3'-O3'	-7.85	101.93	113.70
1	A	258	A	C4'-C3'-O3'	-7.82	101.27	113.00
1	A	83	U	N1-C1'-C2'	7.80	125.71	114.00
17	Q	27	PHE	N-CA-C	7.80	115.24	108.22
2	B	160	ASP	N-CA-C	-7.78	103.36	113.17
1	A	670	U	C4'-C3'-O3'	-7.78	97.73	109.40
1	A	901	A	C2'-C3'-O3'	-7.77	102.04	113.70
5	E	23	GLY	N-CA-C	7.75	121.86	112.48
1	A	1310	C	C3'-C2'-O2'	7.67	122.21	110.70
7	G	18	TYR	N-CA-C	-7.65	105.11	114.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1044	G	C2'-C3'-O3'	-7.64	102.24	113.70
1	A	431	C	C1'-C2'-O2'	7.62	119.84	108.40
1	A	1381	A	C1'-C2'-O2'	7.61	119.82	108.40
12	L	81	SER	N-CA-C	7.61	120.65	111.82
1	A	764	A	C4'-C3'-O3'	-7.59	101.62	113.00
1	A	1380	C	C4'-C3'-O3'	-7.59	98.02	109.40
1	A	348	C	C1'-C2'-O2'	7.55	119.73	108.40
10	J	89	ASP	N-CA-C	7.55	121.65	110.48
11	K	87	THR	N-CA-C	-7.53	95.77	108.26
8	H	134	ILE	N-CA-C	7.52	117.49	110.42
1	A	1047	G	C4'-C3'-O3'	7.51	120.66	109.40
1	A	867	A	C4'-C3'-O3'	-7.43	98.26	109.40
10	J	55	LYS	CA-C-N	-7.42	113.09	123.03
10	J	55	LYS	C-N-CA	-7.42	113.09	123.03
1	A	970	U	C2'-C3'-O3'	7.36	120.54	109.50
1	A	1233	A	C1'-C2'-O2'	-7.36	100.76	111.80
1	A	940	C	C3'-C2'-O2'	7.34	121.71	110.70
1	A	1278	C	C4'-C3'-O3'	-7.31	102.03	113.00
1	A	784	G	C4'-C3'-O3'	-7.31	102.04	113.00
1	A	854	G	C3'-C2'-O2'	7.29	121.63	110.70
1	A	115	C	C1'-C2'-O2'	-7.24	100.94	111.80
22	X	2	G	C2'-C3'-O3'	-7.20	102.89	113.70
1	A	1107	G	C1'-C2'-O2'	7.20	122.60	111.80
1	A	1386	C	C2'-C3'-O3'	-7.19	102.92	113.70
1	A	843	A	C1'-C2'-O2'	-7.18	97.62	108.40
1	A	46	U	C3'-C2'-O2'	7.14	121.41	110.70
1	A	493	A	C2'-C3'-O3'	7.10	124.36	113.70
1	A	1039	U	C4'-C3'-O3'	-7.09	102.37	113.00
1	A	109	G	C1'-C2'-O2'	-7.08	101.19	111.80
13	M	66	LEU	N-CA-C	7.06	119.90	109.24
1	A	1313	G	C1'-C2'-O2'	-7.05	97.83	108.40
1	A	1085	A	C4'-C3'-O3'	-7.02	102.48	113.00
2	B	130	ARG	CA-C-N	7.01	128.60	119.84
2	B	130	ARG	C-N-CA	7.01	128.60	119.84
9	I	69	GLY	N-CA-C	6.98	123.71	111.14
1	A	468	C	C4'-C3'-O3'	-6.96	102.56	113.00
17	Q	27	PHE	CA-C-N	6.95	126.71	119.76
17	Q	27	PHE	C-N-CA	6.95	126.71	119.76
4	D	11	LEU	N-CA-C	-6.95	105.43	114.04
1	A	915	A	C3'-C2'-O2'	6.94	121.11	110.70
1	A	926	C	C3'-C2'-O2'	6.94	121.11	110.70
4	D	9	CYS	CA-C-N	6.93	134.78	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	9	CYS	C-N-CA	6.93	134.78	121.54
1	A	1083	C	C3'-C2'-O2'	6.91	121.06	110.70
1	A	1480	A	C3'-C2'-O2'	-6.91	104.24	114.60
1	A	1483	G	C2'-C3'-O3'	-6.90	103.35	113.70
1	A	530	G	C4'-C3'-O3'	-6.88	102.68	113.00
1	A	424	G	C4'-C3'-O3'	6.81	119.62	109.40
3	C	5	ILE	CB-CA-C	-6.71	102.02	111.28
1	A	174	A	C3'-C2'-O2'	6.70	120.75	110.70
1	A	1481	A	C4'-C3'-O3'	-6.70	99.35	109.40
1	A	799	A	C1'-C2'-O2'	-6.69	101.76	111.80
1	A	1417	A	C1'-C2'-O2'	6.69	118.43	108.40
2	B	34	ALA	N-CA-C	6.68	118.30	108.14
1	A	804	U	C2'-C3'-O3'	-6.67	99.49	109.50
1	A	911	G	C3'-C2'-O2'	6.67	120.71	110.70
9	I	63	ILE	N-CA-C	6.67	117.91	108.17
1	A	239	A	C1'-C2'-O2'	-6.67	101.80	111.80
10	J	58	ASP	N-CA-C	-6.64	100.69	110.52
1	A	510	C	C2'-C3'-O3'	-6.63	103.76	113.70
1	A	48	C	C1'-C2'-O2'	-6.63	101.86	111.80
1	A	1352	C	C2'-C3'-O3'	-6.62	103.77	113.70
1	A	895	G	C2'-C3'-O3'	-6.62	103.78	113.70
1	A	1477	A	C2'-C3'-O3'	-6.58	103.84	113.70
1	A	367	G	C1'-C2'-O2'	6.57	118.25	108.40
1	A	1507	G	C1'-C2'-O2'	-6.55	101.98	111.80
1	A	372	G	C1'-C2'-O2'	6.53	118.20	108.40
1	A	742	G	C4'-C3'-O3'	-6.53	103.21	113.00
1	A	855	C	C3'-C2'-O2'	6.52	120.48	110.70
2	B	124	SER	N-CA-C	6.51	114.08	108.22
14	N	29	ARG	N-CA-C	6.50	120.17	108.48
1	A	739	G	C3'-C2'-O2'	6.49	120.43	110.70
1	A	996	G	C3'-C2'-O2'	6.48	120.42	110.70
4	D	135	LEU	CA-C-N	6.48	126.70	119.32
4	D	135	LEU	C-N-CA	6.48	126.70	119.32
1	A	1130	C	C3'-C2'-O2'	6.43	120.35	110.70
17	Q	68	ARG	N-CA-C	6.42	124.47	110.80
1	A	26	C	C3'-C2'-O2'	6.40	120.30	110.70
1	A	1031	G	C3'-C2'-O2'	6.39	120.29	110.70
1	A	683	C	C3'-C2'-O2'	6.38	120.28	110.70
1	A	556	A	C4'-C3'-O3'	-6.38	103.43	113.00
1	A	1131	U	C1'-C2'-O2'	6.37	117.95	108.40
1	A	34	A	C3'-C2'-O2'	6.36	120.24	110.70
1	A	662	U	C1'-C2'-O2'	-6.35	98.87	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	197	U	C1'-C2'-O2'	6.35	117.92	108.40
4	D	168	ARG	N-CA-C	6.33	119.43	110.50
1	A	1281	A	C3'-C2'-O2'	-6.33	105.10	114.60
1	A	1482	G	C1'-C2'-O2'	-6.33	102.30	111.80
1	A	360	A	C4'-C3'-O3'	-6.33	103.51	113.00
1	A	115	C	C4'-C3'-O3'	-6.32	99.92	109.40
1	A	102	G	O4'-C4'-C3'	-6.31	97.69	104.00
1	A	937	A	C3'-C2'-O2'	6.30	120.15	110.70
1	A	1167	G	C1'-C2'-O2'	6.30	117.84	108.40
1	A	1168	G	C3'-C2'-O2'	6.30	120.14	110.70
10	J	66	ARG	N-CA-C	6.29	119.45	107.75
1	A	1197	G	C4'-C3'-O3'	-6.29	103.57	113.00
17	Q	67	LYS	N-CA-C	-6.25	100.78	110.10
1	A	1346	A	C3'-C2'-O2'	-6.25	105.23	114.60
1	A	553	C	C4'-C3'-O3'	-6.24	103.64	113.00
1	A	602	C	C4'-C3'-O3'	-6.23	103.65	113.00
1	A	541	G	C4'-C3'-O3'	-6.23	103.66	113.00
22	X	6	A	C4'-C3'-O3'	6.22	122.34	113.00
1	A	551	G	C2'-C3'-O3'	-6.22	104.36	113.70
1	A	1189	G	C1'-C2'-O2'	6.21	117.72	108.40
4	D	196	LEU	CA-C-N	6.21	127.61	119.84
4	D	196	LEU	C-N-CA	6.21	127.61	119.84
1	A	1193	U	C1'-C2'-O2'	-6.20	102.50	111.80
1	A	1325	G	C1'-C2'-O2'	6.20	117.70	108.40
1	A	24	C	C1'-C2'-O2'	6.20	117.69	108.40
1	A	1413	C	C3'-C2'-O2'	6.19	119.99	110.70
1	A	25	U	C3'-C2'-O2'	6.19	119.98	110.70
1	A	1336	C	C2'-C3'-O3'	-6.19	104.42	113.70
1	A	212	G	C4'-C3'-O3'	-6.18	100.13	109.40
1	A	1128	C	C2'-C3'-O3'	-6.17	104.44	113.70
20	T	72	LEU	N-CA-C	-6.17	103.05	112.99
1	A	327	G	C2'-C3'-O3'	-6.16	104.46	113.70
19	S	41	VAL	CA-C-N	6.16	127.53	119.84
19	S	41	VAL	C-N-CA	6.16	127.53	119.84
1	A	114	A	C2'-C3'-O3'	-6.15	104.47	113.70
1	A	570	C	C3'-C2'-O2'	6.15	119.93	110.70
1	A	323	A	C1'-C2'-O2'	-6.12	102.61	111.80
2	B	132	LYS	N-CA-C	6.12	123.84	110.80
1	A	1339	A	C2'-C3'-O3'	-6.11	104.54	113.70
5	E	48	ALA	CA-C-N	6.10	126.55	119.47
5	E	48	ALA	C-N-CA	6.10	126.55	119.47
2	B	42	ILE	N-CA-C	6.10	116.59	107.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	12	CYS	N-CA-CB	6.08	120.76	110.49
1	A	535	U	C3'-C2'-O2'	6.07	119.80	110.70
1	A	493	A	C4'-C3'-O3'	6.06	122.09	113.00
17	Q	98	LEU	CA-C-N	-6.04	116.66	123.13
17	Q	98	LEU	C-N-CA	-6.04	116.66	123.13
1	A	1079	C	C1'-C2'-O2'	6.04	117.46	108.40
4	D	155	LEU	N-CA-C	6.04	118.09	110.24
9	I	70	LYS	N-CA-C	6.04	117.53	111.07
4	D	9	CYS	N-CA-C	-6.03	97.95	110.80
14	N	39	LEU	N-CA-C	6.03	118.35	108.52
17	Q	9	VAL	CB-CA-C	-6.02	101.72	110.63
1	A	1251	A	C3'-C2'-O2'	6.02	119.73	110.70
18	R	86	VAL	N-CA-C	5.99	116.44	107.51
1	A	177	U	C3'-C2'-O2'	5.99	119.68	110.70
1	A	1100	G	C1'-C2'-O2'	5.98	117.38	108.40
1	A	804	U	C4'-C3'-O3'	5.98	118.37	109.40
20	T	55	ILE	N-CA-C	5.94	116.12	110.53
1	A	1031	G	C2'-C3'-O3'	5.94	122.61	113.70
1	A	1064	G	C1'-C2'-O2'	5.94	117.31	108.40
1	A	972	A	C1'-C2'-O2'	5.93	117.30	108.40
1	A	892	A	C2'-C3'-O3'	-5.93	104.81	113.70
1	A	965	G	C3'-C2'-O2'	5.93	119.59	110.70
1	A	1068	U	C4'-C3'-O3'	5.93	118.29	109.40
2	B	206	ASP	N-CA-C	5.92	120.16	111.34
1	A	82	U	C3'-C2'-O2'	5.92	123.47	114.60
1	A	1144	C	C3'-C2'-O2'	5.90	119.56	110.70
1	A	850	A	C2'-C3'-O3'	-5.90	100.65	109.50
19	S	22	LEU	N-CA-C	-5.90	105.91	113.23
2	B	25	ASN	CA-C-N	-5.90	113.73	119.87
2	B	25	ASN	C-N-CA	-5.90	113.73	119.87
1	A	587	U	C3'-C2'-O2'	5.88	119.51	110.70
1	A	123	U	C4'-C3'-O3'	-5.87	104.19	113.00
1	A	936	A	C3'-C2'-O2'	5.87	119.51	110.70
1	A	440	G	C3'-C2'-O2'	5.87	119.50	110.70
1	A	1365	C	C1'-C2'-O2'	5.85	117.17	108.40
1	A	1261	A	C4'-C3'-O3'	-5.84	104.24	113.00
1	A	761	A	C2'-C3'-O3'	-5.83	104.96	113.70
9	I	23	ASN	N-CA-C	5.82	123.20	110.80
1	A	336	U	C3'-C2'-O2'	5.82	119.43	110.70
7	G	111	ARG	CA-C-N	5.82	127.11	119.84
7	G	111	ARG	C-N-CA	5.82	127.11	119.84
1	A	549	U	C4'-C3'-O3'	-5.81	104.28	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	860	C	C2'-C3'-O3'	-5.81	104.98	113.70
12	L	24	VAL	CA-C-N	-5.81	112.58	119.84
12	L	24	VAL	C-N-CA	-5.81	112.58	119.84
11	K	40	ILE	N-CA-C	-5.80	106.57	111.56
1	A	764	A	C3'-C2'-O2'	5.79	119.38	110.70
1	A	1442	G	C1'-C2'-O2'	5.79	117.08	108.40
1	A	372	G	C3'-C2'-O2'	-5.78	102.02	110.70
1	A	908	C	O4'-C4'-C3'	-5.78	98.22	104.00
6	F	94	GLN	N-CA-C	5.77	117.79	108.32
2	B	238	LEU	N-CA-C	-5.77	106.14	112.72
1	A	1173	A	C2'-C3'-O3'	-5.76	105.06	113.70
1	A	1109	U	C3'-C2'-O2'	5.74	119.31	110.70
1	A	789	C	C1'-C2'-O2'	-5.73	99.80	108.40
1	A	1177	C	C2'-C3'-O3'	-5.73	105.11	113.70
1	A	1470	A	C2'-C3'-O3'	-5.69	105.16	113.70
1	A	495	C	C4'-C3'-O3'	-5.69	100.86	109.40
1	A	1321	A	C3'-C2'-O2'	5.69	119.23	110.70
1	A	1490	U	C4'-C3'-O3'	-5.69	104.47	113.00
1	A	786	A	C2'-C3'-O3'	-5.68	105.17	113.70
1	A	1000	G	C4'-C3'-O3'	5.68	121.53	113.00
5	E	76	ILE	CA-C-N	5.68	125.15	119.24
5	E	76	ILE	C-N-CA	5.68	125.15	119.24
1	A	399	C	C3'-C2'-O2'	5.68	119.22	110.70
1	A	798	A	C3'-C2'-O2'	5.67	119.21	110.70
10	J	22	LYS	N-CA-C	-5.66	105.10	112.23
3	C	205	GLY	N-CA-C	5.66	123.45	112.64
18	R	32	ARG	N-CA-C	-5.65	106.26	114.12
1	A	1052	C	C2'-C3'-O3'	-5.65	105.23	113.70
1	A	949	G	C3'-C2'-O2'	5.64	123.06	114.60
5	E	127	ASN	CA-C-N	5.64	126.90	119.84
5	E	127	ASN	C-N-CA	5.64	126.90	119.84
1	A	1013	A	C3'-C2'-O2'	5.64	119.16	110.70
4	D	29	PRO	CA-C-N	5.63	132.30	121.54
4	D	29	PRO	C-N-CA	5.63	132.30	121.54
17	Q	59	ILE	CB-CA-C	5.63	119.17	110.50
1	A	207	G	C4'-C3'-O3'	-5.63	104.56	113.00
1	A	1085	A	C2'-C3'-O3'	-5.62	105.26	113.70
1	A	1506	U	C1'-C2'-O2'	-5.62	103.36	111.80
1	A	47	G	C1'-C2'-O2'	5.62	116.83	108.40
1	A	621	G	C3'-C2'-O2'	5.62	119.12	110.70
1	A	1313	G	N9-C1'-C2'	5.61	120.42	112.00
3	C	52	LEU	N-CA-C	5.61	117.80	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1372	C	C4'-C3'-O3'	5.61	121.41	113.00
4	D	28	SER	CA-C-N	5.60	126.84	119.84
4	D	28	SER	C-N-CA	5.60	126.84	119.84
1	A	890	C	C4'-C3'-O3'	-5.59	104.61	113.00
13	M	15	VAL	N-CA-C	5.59	118.04	111.05
1	A	938	U	C4'-C3'-O3'	5.59	117.78	109.40
1	A	920	G	C4'-C3'-O3'	-5.59	104.62	113.00
1	A	83	U	O4'-C1'-C2'	-5.58	100.22	105.80
1	A	644	G	C3'-C2'-O2'	5.57	119.05	110.70
1	A	82	U	P-O3'-C3'	5.56	128.55	120.20
1	A	391	C	C2'-C3'-O3'	-5.56	105.36	113.70
1	A	1244	C	C3'-C2'-O2'	5.56	119.04	110.70
9	I	124	GLN	CA-C-N	5.55	128.73	120.90
9	I	124	GLN	C-N-CA	5.55	128.73	120.90
1	A	73	C	C3'-C2'-O2'	5.55	119.02	110.70
1	A	553	C	C1'-C2'-O2'	-5.55	100.08	108.40
23	Y	35	A	C4'-C3'-O3'	-5.52	104.72	113.00
1	A	732	C	C2'-C3'-O3'	-5.51	101.24	109.50
1	A	583	C	C1'-C2'-O2'	-5.50	100.14	108.40
7	G	116	ALA	N-CA-C	5.50	117.72	111.11
14	N	45	ARG	N-CA-C	-5.50	105.38	111.71
1	A	85	C	C3'-C2'-O2'	5.50	118.94	110.70
1	A	796	C	C4'-C3'-O3'	-5.50	101.15	109.40
1	A	947	A	C3'-C2'-O2'	5.50	118.94	110.70
1	A	372	G	C2'-C3'-O3'	-5.49	105.47	113.70
1	A	1327	U	C1'-C2'-O2'	-5.49	103.57	111.80
1	A	202	A	C4'-C3'-O3'	-5.48	104.78	113.00
1	A	1036	G	C4'-C3'-O3'	-5.48	101.18	109.40
1	A	10	G	C2'-C3'-O3'	-5.48	105.48	113.70
1	A	771	A	C4'-C3'-O3'	-5.48	104.78	113.00
1	A	1299	C	C3'-C2'-O2'	5.47	118.90	110.70
1	A	664	C	C3'-C2'-O2'	5.46	118.89	110.70
1	A	1229	U	C3'-C2'-O2'	5.46	118.89	110.70
1	A	242	A	C2'-C3'-O3'	-5.45	101.33	109.50
1	A	482	U	C4'-C3'-O3'	5.45	117.57	109.40
12	L	80	HIS	N-CA-C	5.45	118.74	112.97
1	A	841	U	C4'-C3'-O3'	-5.44	104.84	113.00
22	X	6	A	C2'-C3'-O3'	5.44	121.86	113.70
10	J	6	ILE	N-CA-C	5.44	115.95	108.12
1	A	476	G	C1'-C2'-O2'	5.42	116.53	108.40
1	A	1298	G	C1'-C2'-O2'	5.41	116.52	108.40
20	T	76	ALA	N-CA-C	-5.41	105.55	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	202	A	C3'-C2'-O2'	5.41	118.81	110.70
1	A	1069	U	C3'-C2'-O2'	5.41	118.81	110.70
1	A	280	G	C2'-C3'-O3'	-5.40	105.60	113.70
17	Q	59	ILE	CA-CB-CG2	5.40	119.68	110.50
14	N	27	CYS	CA-CB-SG	-5.39	102.00	114.40
1	A	472	A	C1'-C2'-O2'	5.39	116.48	108.40
1	A	927	A	C2'-C3'-O3'	-5.39	105.61	113.70
1	A	953	A	C2'-C3'-O3'	5.39	117.58	109.50
18	R	70	ILE	CB-CA-C	-5.39	104.98	111.88
1	A	902	C	C3'-C2'-O2'	5.39	118.78	110.70
1	A	242	A	C1'-C2'-O2'	-5.38	103.73	111.80
13	M	12	ASN	N-CA-C	5.38	122.25	110.80
1	A	1037	C	C2'-C3'-O3'	5.37	117.56	109.50
1	A	1264	C	C3'-C2'-O2'	5.37	118.76	110.70
1	A	753	G	C1'-C2'-O2'	-5.36	100.36	108.40
1	A	328	G	C2'-C3'-O3'	-5.36	105.66	113.70
10	J	51	ARG	N-CA-C	5.36	117.81	111.33
1	A	584	C	C3'-C2'-O2'	5.35	118.73	110.70
1	A	1063	A	C4'-C3'-O3'	-5.35	104.97	113.00
1	A	61	A	C1'-C2'-O2'	-5.35	103.78	111.80
1	A	558	A	C4'-C3'-O3'	-5.35	104.98	113.00
1	A	806	C	C3'-C2'-O2'	5.35	118.72	110.70
1	A	411	A	C1'-C2'-O2'	5.34	116.42	108.40
4	D	12	CYS	CA-CB-SG	5.34	126.69	114.40
8	H	136	GLU	N-CA-C	-5.34	102.10	110.17
1	A	611	G	C2'-C3'-O3'	-5.34	105.69	113.70
1	A	231	C	C2'-C3'-O3'	-5.34	105.69	113.70
1	A	581	G	C2'-C3'-O3'	-5.34	105.70	113.70
1	A	1478	A	C4'-C3'-O3'	-5.34	105.00	113.00
1	A	1483	G	C1'-C2'-O2'	-5.33	100.40	108.40
1	A	990	G	C1'-C2'-O2'	5.33	116.39	108.40
1	A	1478	A	C1'-C2'-O2'	-5.33	100.41	108.40
1	A	699	A	C4'-C3'-O3'	-5.33	105.01	113.00
1	A	843	A	C4'-C3'-O3'	-5.33	105.01	113.00
3	C	145	GLY	N-CA-C	5.33	122.43	115.40
1	A	1357	A	C4'-C3'-O3'	-5.32	105.02	113.00
1	A	119	U	O4'-C4'-C3'	-5.32	98.68	104.00
1	A	555	U	C4'-C3'-O3'	-5.32	105.02	113.00
8	H	24	THR	CB-CA-C	-5.32	100.34	109.65
19	S	10	PHE	CA-C-N	5.32	127.71	120.63
19	S	10	PHE	C-N-CA	5.32	127.71	120.63
1	A	489	G	C4'-C3'-O3'	-5.31	105.04	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J	62	HIS	N-CA-C	5.30	117.16	108.52
1	A	518	U	C2'-C3'-O3'	-5.30	105.75	113.70
1	A	1354	G	C2'-C3'-O3'	-5.30	105.75	113.70
9	I	41	VAL	CB-CA-C	-5.30	104.31	112.05
1	A	361	U	C3'-C2'-O2'	5.30	118.64	110.70
11	K	102	GLY	N-CA-C	-5.30	100.63	113.18
1	A	800	A	C2'-C3'-O3'	-5.29	105.77	113.70
21	U	17	THR	N-CA-C	5.29	122.06	110.80
1	A	1044	G	C1'-C2'-O2'	5.29	116.33	108.40
9	I	101	PHE	N-CA-C	-5.28	106.87	113.15
12	L	70	ILE	CA-C-N	5.28	125.48	120.31
12	L	70	ILE	C-N-CA	5.28	125.48	120.31
3	C	20	SER	N-CA-C	-5.27	99.56	110.80
1	A	924	A	C2'-C3'-O3'	-5.27	105.79	113.70
14	N	43	CYS	N-CA-C	-5.27	98.99	108.58
1	A	1261	A	N9-C1'-C2'	5.26	119.90	112.00
17	Q	81	ARG	N-CA-C	5.26	122.02	110.80
1	A	1032	U	C2'-C3'-O3'	5.26	117.39	109.50
13	M	11	ARG	N-CA-C	5.26	116.98	109.14
1	A	1317	C	C4'-C3'-O3'	-5.25	105.12	113.00
1	A	441	G	C1'-C2'-O2'	5.25	116.27	108.40
1	A	1352	C	C4'-C3'-O3'	-5.25	105.13	113.00
1	A	895	G	C4'-C3'-O3'	-5.25	105.13	113.00
19	S	10	PHE	N-CA-C	5.25	121.97	110.80
1	A	1115	C	C3'-C2'-O2'	5.24	118.56	110.70
1	A	908	C	C4'-C3'-O3'	5.23	120.85	113.00
22	X	6	A	C3'-C2'-O2'	5.23	118.55	110.70
1	A	1088	A	C1'-C2'-O2'	5.23	116.24	108.40
1	A	850	A	C1'-C2'-O2'	-5.22	103.96	111.80
1	A	92	G	C3'-C2'-O2'	5.22	118.52	110.70
1	A	1283	U	C1'-C2'-O2'	-5.21	103.98	111.80
2	B	18	GLY	N-CA-C	5.21	117.92	111.93
1	A	148	C	C2'-C3'-O3'	-5.21	105.89	113.70
1	A	550	G	C1'-C2'-O2'	-5.21	103.99	111.80
1	A	770	G	C2'-C3'-O3'	-5.20	105.89	113.70
12	L	20	LYS	N-CA-C	5.20	117.32	109.41
1	A	1047	G	C2'-C3'-O3'	-5.20	101.70	109.50
1	A	386	C	C4'-C3'-O3'	-5.20	105.20	113.00
1	A	1183	A	C4'-C3'-O3'	5.19	117.19	109.40
1	A	1305	G	C3'-C2'-O2'	5.18	118.47	110.70
1	A	579	G	C1'-C2'-O2'	-5.18	104.03	111.80
1	A	598	A	C4'-C3'-O3'	-5.18	105.22	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	802	G	C2'-C3'-O3'	-5.18	101.73	109.50
1	A	209	U	C2'-C3'-O3'	5.17	117.26	109.50
6	F	60	PHE	N-CA-C	5.17	117.04	108.20
8	H	73	ASP	CA-C-N	5.16	126.29	119.84
8	H	73	ASP	C-N-CA	5.16	126.29	119.84
1	A	598	A	C2'-C3'-O3'	5.16	121.44	113.70
1	A	1293	G	C3'-C2'-O2'	5.16	118.44	110.70
1	A	318	C	C2'-C3'-O3'	-5.16	105.96	113.70
1	A	475	G	C1'-C2'-O2'	5.16	116.14	108.40
1	A	1092	C	C3'-C2'-O2'	5.15	118.42	110.70
1	A	1134	A	C4'-C3'-O3'	-5.15	101.68	109.40
1	A	35	C	C3'-C2'-O2'	5.15	118.42	110.70
1	A	600	G	C1'-C2'-O2'	5.14	116.11	108.40
1	A	74	G	C3'-C2'-O2'	5.13	118.40	110.70
1	A	1491	A	C3'-C2'-O2'	5.13	118.39	110.70
1	A	975	U	C4'-C3'-O3'	5.13	120.69	113.00
19	S	41	VAL	N-CA-C	5.13	114.10	108.05
1	A	535	U	C1'-C2'-O2'	-5.13	100.71	108.40
1	A	265	C	C1'-C2'-O2'	5.12	116.09	108.40
1	A	602	C	C1'-C2'-O2'	5.12	116.08	108.40
1	A	635	C	C2'-C3'-O3'	-5.12	106.02	113.70
1	A	1512	A	C4'-C3'-O3'	5.12	120.68	113.00
1	A	1099	C	C4'-C3'-O3'	5.12	120.67	113.00
4	D	31	CYS	N-CA-C	-5.11	105.77	112.72
1	A	1298	G	C3'-C2'-O2'	5.11	118.36	110.70
1	A	922	G	C4'-C3'-O3'	-5.11	105.34	113.00
19	S	36	ARG	N-CA-C	-5.10	107.00	113.18
1	A	7	G	C1'-C2'-O2'	5.10	116.06	108.40
1	A	187	C	C2'-C3'-O3'	-5.10	106.05	113.70
1	A	958	C	C3'-C2'-O2'	5.10	118.36	110.70
1	A	1225	C	C1'-C2'-O2'	-5.10	100.75	108.40
1	A	1472	G	C1'-C2'-O2'	5.10	116.05	108.40
1	A	76	G	C1'-C2'-O2'	5.09	116.04	108.40
1	A	765	A	C1'-C2'-O2'	-5.09	100.76	108.40
1	A	1476	U	C2'-C3'-O3'	5.09	117.13	109.50
8	H	100	ILE	CB-CA-C	-5.09	104.83	110.68
1	A	711	G	C2'-C3'-O3'	5.08	121.33	113.70
3	C	99	VAL	N-CA-C	5.08	114.92	107.15
3	C	111	LEU	N-CA-C	-5.08	105.13	113.50
1	A	1281	A	N9-C1'-C2'	5.07	121.61	114.00
6	F	80	ARG	N-CA-C	5.07	119.16	112.92
1	A	517	A	C1'-C2'-O2'	-5.06	104.21	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	92	G	C4'-C3'-O3'	-5.06	105.41	113.00
1	A	546	C	C4'-C3'-O3'	5.06	116.98	109.40
1	A	1471	A	N9-C1'-C2'	5.06	119.58	112.00
2	B	73	THR	N-CA-C	-5.06	107.11	113.28
1	A	1009	C	C2'-C3'-O3'	5.05	117.08	109.50
3	C	4	LYS	N-CA-C	5.05	121.56	110.80
1	A	905	G	C2'-C3'-O3'	-5.04	106.14	113.70
1	A	1178	U	C2'-C3'-O3'	5.04	117.06	109.50
10	J	44	VAL	N-CA-C	5.04	114.86	107.15
1	A	1320	G	C2'-C3'-O3'	-5.03	106.15	113.70
1	A	842	A	C2'-C3'-O3'	-5.03	106.15	113.70
2	B	165	VAL	N-CA-C	5.03	115.70	110.82
1	A	818	C	C2'-C3'-O3'	-5.03	106.16	113.70
1	A	1206	G	C1'-C2'-O2'	-5.03	104.26	111.80
1	A	1263	U	C1'-C2'-O2'	5.03	119.34	111.80
1	A	1179	G	C2'-C3'-O3'	-5.02	106.17	113.70
1	A	1311	A	C3'-C2'-O2'	5.02	118.23	110.70
1	A	315	G	C3'-C2'-O2'	5.02	118.22	110.70
1	A	1216	C	C3'-C2'-O2'	5.01	118.21	110.70
15	O	44	LYS	N-CA-C	-5.00	106.69	112.89

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
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	884	0
2	B	1900	0	1951	151	0
3	C	1612	0	1677	139	0
4	D	1703	0	1763	101	0
5	E	1146	0	1207	54	0
6	F	843	0	857	37	0
7	G	1257	0	1296	56	0
8	H	1116	0	1177	41	0
9	I	1011	0	1043	88	0
10	J	794	0	840	98	0
11	K	885	0	904	38	0
12	L	975	0	1062	68	0
13	M	955	0	1021	60	0
14	N	492	0	529	68	0
15	O	734	0	771	24	0
16	P	700	0	720	29	0
17	Q	823	0	891	35	0
18	R	574	0	644	39	0
19	S	629	0	652	59	0
20	T	763	0	861	41	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
25	A	42	0	45	3	0
All	All	52087	0	36749	1951	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 (1951) 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:HB3	10:J:45:ARG:NH1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H6	1:A:197:U:H5''	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
4:D:33:MET:HE2	4:D:37:PRO:HA	1.40	1.01
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:1108:U:H5''	1:A:1108:U:H6	1.16	1.01
1:A:1230:A:O2'	1:A:1231:C:C5'	2.09	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:298:G:H5''	12:L:17:LYS:HE2	1.45	0.99
1:A:1108:U:O4	10:J:5:ARG:HD3	1.61	0.99
21:U:10:ARG:HG3	21:U:10:ARG:NH1	1.61	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:HB3	10:J:45:ARG:HH11	0.81	0.98
21:U:10:ARG:HH11	21:U:10:ARG:HG3	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:HG2	16:P:28:ARG:HH11	1.28	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O4'	1:A:1232:A:OP1	1.86	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
12:L:47:LYS:CB	12:L:48:PRO:HD3	1.97	0.93
10:J:8:LEU:CD1	10:J:20:ALA:HB1	1.98	0.93
10:J:8:LEU:CD1	10:J:20:ALA:CB	2.45	0.93
3:C:70:VAL:HG12	3:C:72:LYS:H	1.32	0.93
14:N:27:CYS:HB3	14:N:43:CYS:HB3	1.47	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
18:R:46:GLU:H	18:R:46:GLU:CD	1.77	0.92
1:A:197:U:H5''	1:A:197:U:C6	2.06	0.91
1:A:1239:U:OP2	1:A:1239:U:H4'	1.68	0.90
1:A:1135:A:H5'	10:J:13:HIS:CD2	2.06	0.90
14:N:24:CYS:CB	14:N:40:CYS:HB3	2.02	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:1233:A:HO2'	1:A:1234:A:H8	1.20	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
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:N3	23:Y:31:A:H2'	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
1:A:648:G:H22	1:A:725:G:H1	1.18	0.88
10:J:5:ARG:HG3	10:J:73:ASP:OD1	1.73	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
5:E:91:LEU:HD12	5:E:120:THR:HG22	1.56	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1515:U:O2'	1:A:1516:C:OP2	1.93	0.87
15:O:17:ARG:HG3	15:O:17:ARG:HH11	1.39	0.86
3:C:108:ASN:HD21	3:C:144:SER:HB3	1.39	0.86
4:D:11:LEU:C	4:D:13:ARG:N	2.30	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
3:C:110:ASN:O	3:C:111:LEU:HD23	1.75	0.84
10:J:50:ILE:H	10:J:50:ILE:HD12	1.39	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
3:C:23:TYR:CE1	3:C:24:ALA:O	2.30	0.83
14:N:24:CYS:HB2	14:N:40:CYS:N	1.92	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:430:U:H2'	1:A:431:C:C6	2.14	0.83
1:A:1307:C:O3'	21:U:17:THR:HG21	1.78	0.83
1:A:1334:C:H2'	1:A:1335:G:C8	2.14	0.83
18:R:32:ARG:HA	18:R:69:THR:HG21	1.61	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
12:L:24:VAL:O	12:L:24:VAL:HG12	1.77	0.82
18:R:85:LEU:HD23	18:R:88:LYS:HG3	1.62	0.82
16:P:74:LEU:O	16:P:79:VAL:HG23	1.80	0.82
1:A:1130:C:H4'	9:I:5:TYR:HE2	1.44	0.82
1:A:1351:G:H2'	1:A:1352:C:H5'	1.61	0.82
9:I:9:ARG:HG3	9:I:14:VAL:HG13	1.62	0.81
13:M:67:GLU:O	13:M:67:GLU:HG3	1.79	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:571:G:H1'	8:H:1:MET:HE1	1.63	0.81
1:A:906:G:O2'	1:A:1511:C:OP1	1.97	0.81
2:B:88:ALA:HB2	2:B:219:VAL:CG1	2.09	0.81
17:Q:67:LYS:HA	17:Q:70:ARG:HH12	1.45	0.81
1:A:614:G:H8	1:A:614:G:H5''	1.45	0.81
5:E:80:ILE:CD1	5:E:91:LEU:CB	2.59	0.81
1:A:1322:A:H5''	1:A:1322:A:H8	1.45	0.80
1:A:81:U:OP2	1:A:81:U:H6	1.64	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
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:O	2:B:23:ARG:HG2	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
3:C:95:THR:HG22	3:C:97:LYS:HB2	1.62	0.79
4:D:30:LYS:HB2	4:D:32:ALA:CA	2.11	0.79
1:A:1014:G:N3	1:A:1015:G:O6	2.16	0.79
1:A:1287:G:H22	1:A:1313:G:H2'	1.45	0.79
19:S:45:VAL:O	19:S:47:HIS:N	2.15	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
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
1:A:779:C:H5''	1:A:780:C:OP2	1.84	0.77
22:X:4:PSU:H2'	22:X:5:G:H5''	1.64	0.77
1:A:972:A:H2'	1:A:972:A:N3	1.99	0.77
1:A:1296:C:OP2	19:S:6:LYS:HE2	1.84	0.77
1:A:1008:C:H6	1:A:1008:C:H3'	1.50	0.77
1:A:1313:G:OP1	1:A:1313:G:H4'	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:961:A:H5'	1:A:962:C:OP2	1.85	0.76
1:A:1512:A:H2'	1:A:1513:C:H5'	1.65	0.76
23:Y:34:G:H2'	23:Y:35:A:C8	2.20	0.76
1:A:953:A:C5'	1:A:953:A:H8	1.99	0.76
9:I:88:TYR:O	9:I:89:ASN:HB2	1.86	0.76
18:R:36:ASN:OD1	18:R:39:VAL:HB	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
2:B:90:MET:HE2	2:B:90:MET:HA	1.65	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:1104:U:H2'	1:A:1105:U:H6	1.51	0.75
1:A:1230:A:H4'	1:A:1231:C:OP1	1.86	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
3:C:11:ARG:O	3:C:14:ILE:O	2.04	0.75
6:F:69:GLU:O	6:F:72:VAL:HG12	1.86	0.75
1:A:1351:G:C2'	1:A:1352:C:H5'	2.17	0.75
1:A:924:A:H2'	1:A:925:G:C8	2.22	0.75
3:C:76:VAL:HG21	3:C:103:VAL:HG21	1.69	0.75
10:J:90:LEU:N	10:J:91:PRO:HD3	1.99	0.75
19:S:6:LYS:O	19:S:7:LYS:HD3	1.86	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:O	5:E:68:GLU:HG3	1.84	0.74
1:A:1208:C:N4	13:M:104:ARG:HG2	2.03	0.74
3:C:15:THR:O	3:C:15:THR:HG22	1.85	0.74
16:P:28:ARG:HG2	16:P:28:ARG:NH1	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
12:L:25:PRO:C	12:L:27:LEU:H	1.94	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:1049:C:C2'	1:A:1050:A:H5'	2.17	0.73
1:A:1480:A:H2	1:A:1483:G:H1	1.34	0.73
7:G:138:LYS:HD3	7:G:138:LYS:C	2.13	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:4:ILE:HG22	10:J:74:ILE:HG13	1.68	0.73
1:A:957:C:C3'	1:A:958:C:H5''	2.17	0.73
14:N:24:CYS:HB2	14:N:40:CYS:HB3	1.69	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
1:A:79:A:H61	1:A:85:C:H42	1.36	0.73
1:A:1011:C:H2'	1:A:1012:G:H5'	1.71	0.73
8:H:89:PRO:HA	8:H:92:ARG:NH1	2.04	0.73
1:A:969:U:C5	1:A:1194:U:H1'	2.24	0.73
1:A:1049:C:H2'	1:A:1050:A:H5'	1.69	0.73
1:A:1334:C:H2'	1:A:1335:G:H8	1.53	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:836:G:N7	1:A:847:G:N7	2.37	0.72
1:A:961:A:H3'	1:A:961:A:N3	2.03	0.72
7:G:65:ALA:O	7:G:69:VAL:HG23	1.90	0.72
8:H:112:LEU:C	8:H:112:LEU:HD12	2.14	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:HD12	17:Q:65:ILE:N	2.04	0.72
1:A:859:G:P	12:L:12:ARG:HH22	2.13	0.72
10:J:79:ARG:HH11	10:J:82:ILE:CD1	2.02	0.72
5:E:101:ILE:CD1	5:E:119:LEU:HD23	2.19	0.71
1:A:250:G:OP1	17:Q:67:LYS:O	2.09	0.71
1:A:1184:G:C4	14:N:42:ILE:HD12	2.25	0.71
1:A:1408:U:H3	1:A:1453:G:H1	1.34	0.71
14:N:4:LYS:C	14:N:6:LEU:H	1.95	0.71
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
2:B:80:ILE:CD1	2:B:212:GLN:HA	2.20	0.71
1:A:1183:A:H4'	1:A:1184:G:O5'	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1231:C:H2'	1:A:1232:A:OP1	1.91	0.70
3:C:30:ARG:HB2	3:C:30:ARG:HH11	1.56	0.70
3:C:55:VAL:O	3:C:55:VAL:HG12	1.90	0.70
2:B:208:ILE:H	2:B:208:ILE:HD12	1.56	0.70
10:J:8:LEU:HD13	10:J:20:ALA:HB3	1.73	0.70
4:D:25:ARG:C	4:D:27:TYR:H	1.98	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:H5''	22:X:3:A:H8	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
1:A:211:U:H4'	1:A:212:G:O5'	1.92	0.70
2:B:74:LYS:HG2	2:B:75:LYS:HE3	1.72	0.70
19:S:22:LEU:HD12	19:S:26:GLY:HA3	1.74	0.69
1:A:953:A:H8	1:A:953:A:H5'	1.58	0.69
1:A:1120:C:O2'	1:A:1121:G:N2	2.24	0.69
1:A:1329:G:H22	1:A:1356:G:H2'	1.56	0.69
1:A:779:C:C5'	1:A:780:C:OP2	2.39	0.69
1:A:957:C:H3'	1:A:958:C:C5'	2.18	0.69
1:A:1232:A:O4'	1:A:1232:A:P	2.50	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:9:A:N7	4:D:208:SER:HB3	2.08	0.69
1:A:1231:C:H41	1:A:1270:A:H62	1.39	0.69
1:A:1322:A:H5''	1:A:1322:A:C8	2.27	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
1:A:1108:U:O4	10:J:5:ARG:CD	2.40	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
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:1198:G:H5''	14:N:5:ALA:CB	2.23	0.69
4:D:173:TRP:O	4:D:186:LEU:HB2	1.92	0.69
5:E:10:MET:HG3	5:E:10:MET:O	1.90	0.69
1:A:9:A:N7	4:D:208:SER:CB	2.56	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1244:C:H2'	1:A:1245:C:H6	1.58	0.68
12:L:110:VAL:O	12:L:122:THR:HG21	1.93	0.68
22:X:3:A:H5''	22:X:3:A:C8	2.28	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:51:VAL:HG11	8:H:60:ARG:NH1	2.07	0.68
8:H:112:LEU:HD12	8:H:113:SER:N	2.08	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
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
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:614:G:H5''	1:A:614:G:C8	2.27	0.68
1:A:197:U:H6	1:A:197:U:C5'	2.00	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
1:A:1185:C:OP1	14:N:3:ARG:HD3	1.94	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
1:A:971:G:H4'	1:A:972:A:OP2	1.94	0.67
3:C:150:LYS:HD3	3:C:152:ILE:HD11	1.75	0.67
9:I:104:ARG:O	9:I:105:ASP:HB3	1.94	0.67
13:M:11:ARG:O	13:M:13:LYS:N	2.22	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:1171:C:P	10:J:51:ARG:HH22	2.17	0.67
1:A:1310:C:OP1	21:U:20:LYS:NZ	2.28	0.67
1:A:803:A:C8	1:A:803:A:H5''	2.30	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
4:D:11:LEU:O	4:D:12:CYS:C	2.37	0.67
18:R:46:GLU:CD	18:R:46:GLU:N	2.53	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
17:Q:27:PHE:HB2	17:Q:28:PRO:HD2	1.76	0.66
20:T:87:LYS:HA	20:T:87:LYS:HE3	1.78	0.66
1:A:349:A:H5'	1:A:349:A:C8	2.31	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
1:A:1300:A:H5''	19:S:10:PHE:HD2	1.61	0.66
4:D:163:GLU:HG3	4:D:166:LYS:HE2	1.77	0.66
1:A:1111:C:H4'	9:I:16:ARG:HH12	1.59	0.66
10:J:49:VAL:C	10:J:60:ARG:HB3	2.21	0.66
1:A:148:C:H42	1:A:163:G:H1	1.43	0.66
3:C:30:ARG:HB2	3:C:30:ARG:NH1	2.11	0.66
8:H:103:VAL:HG21	8:H:109:ILE:O	1.95	0.66
14:N:24:CYS:HB2	14:N:40:CYS:CB	2.26	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
6:F:21:LEU:O	6:F:25:ILE:HG13	1.96	0.66
8:H:122:ARG:NH1	8:H:122:ARG:HB2	2.11	0.66
13:M:40:ASN:OD1	13:M:41:PRO:HD2	1.96	0.66
1:A:353:G:C2	1:A:354:U:C5	2.83	0.66
1:A:430:U:H2'	1:A:431:C:H6	1.61	0.66
1:A:722:C:OP2	6:F:92:LYS:NZ	2.25	0.66
1:A:1068:U:H3'	1:A:1069:U:C5	2.30	0.66
1:A:1144:C:H2'	1:A:1145:C:C6	2.31	0.66
1:A:1355:U:H2'	1:A:1356:G:O5'	1.95	0.66
3:C:62:ASP:HA	3:C:97:LYS:HG2	1.78	0.66
17:Q:66:SER:OG	17:Q:69:LYS:HB2	1.95	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1130:C:H4'	9:I:5:TYR:CE2	2.29	0.65
7:G:38:LEU:C	7:G:38:LEU:HD12	2.22	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
1:A:1223:G:H2'	1:A:1224:C:H6	1.61	0.65
1:A:1473:U:H2'	1:A:1474:C:H6	1.61	0.65
14:N:4:LYS:C	14:N:6:LEU:N	2.55	0.65
14:N:36:PHE:CD2	14:N:36:PHE:O	2.49	0.65
1:A:1008:C:H3'	1:A:1008:C:C6	2.31	0.65
1:A:1078:U:P	1:A:1091:G:H1	2.19	0.65
1:A:1118:U:O2	1:A:1118:U:H2'	1.97	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: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
1:A:1117:G:H8	1:A:1117:G:O5'	1.80	0.65
2:B:21:ARG:HH21	2:B:38:GLY:HA3	1.61	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
1:A:1325:G:H2'	1:A:1326:C:C6	2.32	0.65
2:B:111:ARG:HD3	2:B:145:LEU:HD11	1.79	0.65
10:J:23:ILE:O	10:J:23:ILE:HG22	1.97	0.65
11:K:48:ILE:HD13	11:K:48:ILE:N	2.11	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
1:A:1133:U:H4'	10:J:41:PRO:HG3	1.79	0.64
14:N:24:CYS:CB	14:N:40:CYS:CB	2.75	0.64
17:Q:86:GLU:O	17:Q:90:ILE:HG12	1.96	0.64
1:A:349:A:H5'	1:A:349:A:H8	1.62	0.64
1:A:199:U:O4'	20:T:103:GLY:HA2	1.97	0.64
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
2:B:96:ARG:O	2:B:98:LEU:HD23	1.98	0.64
3:C:70:VAL:CG1	3:C:71:ALA:N	2.61	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
8:H:35:ILE:HG23	8:H:111:ILE:HG21	1.80	0.64
17:Q:45:HIS:HB3	17:Q:72:ARG:HG2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:G:HO2'	4:D:116:GLN:HG3	1.61	0.64
5:E:8:GLU:HA	5:E:33:VAL:O	1.97	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
1:A:400:U:O2'	1:A:401:U:H5'	1.97	0.64
1:A:836:G:C6	1:A:847:G:C8	2.86	0.64
1:A:1472:G:O2'	1:A:1473:U:H5'	1.98	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
15:O:70:LEU:HD23	15:O:78:TYR:HA	1.78	0.64
1:A:295:G:H2'	1:A:296:A:C8	2.33	0.64
1:A:1316:G:H5''	1:A:1317:C:OP2	1.98	0.64
12:L:25:PRO:C	12:L:27:LEU:N	2.56	0.64
19:S:67:VAL:HG12	19:S:68:GLY:H	1.63	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
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
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:68:C:O2'	1:A:166:A:H1'	1.99	0.63
1:A:1375:G:N2	1:A:1480:A:H8	1.96	0.63
8:H:73:ASP:OD1	8:H:75:ARG:HD3	1.99	0.63
12:L:41:ARG:HH22	12:L:57:LYS:HE2	1.62	0.63
1:A:1052:C:O2'	1:A:1174:C:H1'	1.98	0.63
9:I:88:TYR:O	9:I:88:TYR:CD1	2.52	0.63
12:L:46:LYS:NZ	12:L:47:LYS:HE3	2.13	0.63
1:A:1521:C:N4	2:B:23:ARG:NH2	2.42	0.63
2:B:69:LEU:HD12	2:B:70:PHE:N	2.13	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
3:C:59:ARG:HG2	3:C:64:VAL:HG12	1.80	0.63
21:U:10:ARG:CG	21:U:10:ARG:NH1	2.38	0.63
3:C:6:HIS:CE1	3:C:8:ILE:HB	2.34	0.63
11:K:92:GLU:HA	11:K:95:ILE:HG13	1.80	0.63
17:Q:80:GLY:O	17:Q:82:MET:N	2.32	0.63
19:S:22:LEU:HD12	19:S:26:GLY:CA	2.29	0.63
20:T:73:HIS:O	20:T:74:LYS:CG	2.47	0.63
1:A:1207:A:H2'	1:A:1208:C:C5	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:158:LEU:H	2:B:158:LEU:CD1	2.11	0.62
3:C:188:LEU:O	3:C:189:ALA:HB2	1.99	0.62
1:A:81:U:OP2	1:A:81:U:C6	2.50	0.62
1:A:1261:A:H5''	1:A:1262:A:OP1	1.99	0.62
1:A:1384:G:C2	1:A:1385:C:H1'	2.33	0.62
2:B:158:LEU:HD12	2:B:158:LEU:N	2.12	0.62
1:A:1515:U:O2'	1:A:1516:C:P	2.57	0.62
20:T:73:HIS:C	20:T:74:LYS:CG	2.71	0.62
1:A:1232:A:H1'	1:A:1233:A:N7	2.14	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
19:S:5:LEU:HA	19:S:6:LYS:NZ	2.14	0.62
1:A:231:C:H5'	17:Q:70:ARG:HG2	1.81	0.62
1:A:429:C:H2'	1:A:430:U:H5'	1.80	0.62
1:A:1128:C:H4'	1:A:1129:A:O5'	1.99	0.62
1:A:1198:G:O2'	1:A:1199:C:H5'	2.00	0.62
3:C:7:PRO:O	3:C:11:ARG:HG3	2.00	0.62
1:A:668:A:O2'	11:K:38:ASN:HB3	1.99	0.62
1:A:1300:A:H5''	19:S:10:PHE:CD2	2.35	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
10:J:50:ILE:H	10:J:50:ILE:CD1	2.08	0.62
7:G:51:GLN:O	7:G:53:LYS:N	2.33	0.62
9:I:53:VAL:HG11	9:I:85:LEU:HD11	1.82	0.62
1:A:144:A:H2'	1:A:145:C:C6	2.34	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
18:R:85:LEU:HD23	18:R:88:LYS:CG	2.28	0.61
1:A:207:G:H2'	1:A:208:C:O4'	1.99	0.61
1:A:1313:G:OP1	1:A:1313:G:C4'	2.47	0.61
22:X:2:G:H2'	22:X:3:A:O5'	2.00	0.61
5:E:51:VAL:HB	5:E:52:PRO:HD3	1.83	0.61
5:E:144:THR:O	5:E:148:VAL:HG23	2.00	0.61
6:F:23:LYS:NZ	6:F:42:GLU:OE2	2.33	0.61
8:H:6:ILE:O	8:H:10:LEU:HG	2.01	0.61
1:A:644:G:OP1	15:O:5:LYS:HD2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:22:THR:HA	16:P:33:ILE:HG13	1.80	0.61
1:A:1078:U:H2'	1:A:1079:C:C6	2.35	0.61
2:B:96:ARG:HB2	2:B:96:ARG:NH1	2.16	0.61
10:J:94:VAL:HG12	10:J:95:GLU:N	2.15	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
19:S:6:LYS:CG	19:S:7:LYS:HE3	2.30	0.61
1:A:482:U:O2'	1:A:483:A:P	2.58	0.61
2:B:67:THR:HG22	2:B:90:MET:HE1	1.81	0.61
3:C:70:VAL:CG1	3:C:72:LYS:H	2.09	0.61
1:A:1108:U:H5'	1:A:1109:U:O4	1.99	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
9:I:4:TYR:CZ	9:I:88:TYR:HD2	2.19	0.61
13:M:94:ARG:HA	13:M:94:ARG:HH11	1.64	0.61
1:A:765:A:H5'	1:A:766:A:OP2	2.01	0.61
1:A:952:A:H8	1:A:952:A:OP1	1.83	0.61
1:A:193:G:H8	1:A:193:G:H5''	1.65	0.60
1:A:265:C:H2'	1:A:266:A:C8	2.35	0.60
10:J:45:ARG:NH1	10:J:45:ARG:CB	2.49	0.60
10:J:96:ILE:CD1	10:J:96:ILE:H	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
1:A:344:G:H2'	1:A:344:G:N3	2.16	0.60
1:A:1184:G:C2'	1:A:1185:C:H5'	2.31	0.60
3:C:34:LEU:O	3:C:38:ARG:HG2	2.01	0.60
4:D:11:LEU:C	4:D:13:ARG:H	2.08	0.60
20:T:67:ALA:O	20:T:73:HIS:CE1	2.54	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
2:B:22:LYS:HD2	2:B:22:LYS:N	2.16	0.60
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
1:A:1043:C:H5	3:C:2:GLY:CA	2.04	0.60
1:A:1137:G:H2'	1:A:1138:G:C8	2.37	0.60
20:T:10:LEU:O	20:T:13:LEU:HG	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:73:ALA:HB3	18:R:79:LEU:HD12	1.83	0.60
1:A:1137:G:H2'	1:A:1138:G:H8	1.67	0.60
2:B:111:ARG:HB3	2:B:149:LEU:HD11	1.84	0.60
7:G:51:GLN:C	7:G:53:LYS:H	2.08	0.60
9:I:114:TYR:CE2	10:J:59:SER:HA	2.37	0.60
1:A:1037:C:OP2	1:A:1179:G:OP2	2.20	0.59
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:438:C:H2'	1:A:439:C:H6	1.67	0.59
1:A:516:A:O2'	1:A:517:A:OP1	2.14	0.59
1:A:835:C:H2'	1:A:836:G:O4'	2.02	0.59
3:C:155:GLY:O	3:C:156:ARG:HB2	2.01	0.59
1:A:544:U:H5'	1:A:550:G:N2	2.17	0.59
3:C:15:THR:O	3:C:15:THR:CG2	2.49	0.59
16:P:26:ARG:HD2	16:P:31:LYS:O	2.01	0.59
19:S:29:ARG:C	19:S:31:ILE:H	2.10	0.59
1:A:778:A:H2'	1:A:779:C:C6	2.38	0.59
1:A:1039:U:O2'	1:A:1040:G:H5'	2.02	0.59
1:A:1043:C:O2	1:A:1180:G:C2	2.55	0.59
1:A:1333:U:C2'	1:A:1334:C:H5'	2.33	0.59
2:B:80:ILE:HD13	2:B:212:GLN:HA	1.84	0.59
12:L:28:LYS:O	12:L:30:ALA:N	2.32	0.59
1:A:82:U:C6	1:A:83:U:O2	2.56	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
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
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
2:B:86:GLU:C	2:B:88:ALA:H	2.11	0.59
4:D:18:LYS:CD	4:D:31:CYS:HB2	2.32	0.59
1:A:1057:G:O3'	2:B:103:THR:HG22	2.02	0.59
4:D:150:GLU:HA	4:D:153:ARG:CD	2.19	0.59
9:I:54:ASP:C	9:I:56:LEU:H	2.11	0.59
10:J:38:ILE:HD11	10:J:71:LEU:HD23	1.83	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
1:A:637:A:OP1	8:H:56:LYS:NZ	2.27	0.58
3:C:70:VAL:CG1	3:C:71:ALA:H	2.15	0.58
5:E:147:ASP:OD1	5:E:147:ASP:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:26:ARG:NH1	14:N:47:LEU:CD2	2.66	0.58
19:S:10:PHE:HD1	19:S:10:PHE:H	1.46	0.58
1:A:1074:U:H5''	1:A:1075:A:OP2	2.03	0.58
2:B:71:VAL:HG12	2:B:93:VAL:HB	1.85	0.58
2:B:74:LYS:HE3	2:B:205:ASP:O	2.03	0.58
7:G:16:LEU:H	7:G:16:LEU:HD23	1.69	0.58
8:H:122:ARG:HB2	8:H:122:ARG:CZ	2.33	0.58
1:A:691:C:H4'	11:K:20:TYR:CD2	2.38	0.58
1:A:798:A:H2'	1:A:800:A:H5''	1.84	0.58
3:C:52:LEU:HD23	3:C:52:LEU:H	1.68	0.58
4:D:15:GLU:OE2	4:D:59:ARG:NH1	2.37	0.58
8:H:119:LEU:HD12	8:H:124:ALA:HB2	1.84	0.58
15:O:74:ASP:C	15:O:76:GLU:H	2.11	0.58
1:A:1184:G:H21	14:N:43:CYS:HB3	1.69	0.58
10:J:96:ILE:CD1	10:J:96:ILE:N	2.66	0.58
20:T:73:HIS:C	20:T:74:LYS:HG3	2.28	0.58
1:A:197:U:C6	1:A:197:U:C5'	2.80	0.58
1:A:251:G:O6	1:A:262:G:O6	2.20	0.58
1:A:324:C:O2	1:A:324:C:C2'	2.50	0.58
1:A:483:A:H4'	1:A:484:G:OP1	2.03	0.58
13:M:90:LEU:O	13:M:91:ARG:HB2	2.02	0.58
1:A:469:G:H5'	1:A:471:U:O4'	2.03	0.58
1:A:923:G:H2'	1:A:923:G:N3	2.17	0.58
1:A:1114:G:C6	1:A:1115:C:N4	2.72	0.58
3:C:10:PHE:CE2	3:C:178:LEU:HD13	2.39	0.58
1:A:1355:U:C2'	1:A:1356:G:O5'	2.51	0.58
2:B:136:VAL:O	2:B:140:HIS:HB2	2.03	0.58
4:D:25:ARG:C	4:D:27:TYR:N	2.61	0.58
9:I:44:VAL:O	9:I:51:ARG:NH2	2.35	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:165:U:O2'	1:A:166:A:H5'	2.04	0.58
1:A:1084:A:H4'	1:A:1085:A:O5'	2.04	0.58
1:A:1158:A:H3'	1:A:1159:G:C8	2.39	0.58
1:A:1310:C:H2'	1:A:1311:A:O4'	2.04	0.58
1:A:1351:G:C2	1:A:1352:C:C5	2.92	0.58
2:B:80:ILE:HG13	2:B:80:ILE:O	2.01	0.58
15:O:74:ASP:O	15:O:76:GLU:N	2.36	0.58
1:A:937:A:H5''	1:A:938:U:OP2	2.04	0.58
5:E:43:LEU:HD21	5:E:132:ALA:HB1	1.85	0.58
1:A:898:U:H2'	1:A:899:U:C6	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:10:LEU:HB2	6:F:59:TYR:HB3	1.86	0.57
16:P:67:THR:HG22	16:P:68:ASP:N	2.19	0.57
1:A:1014:G:H1'	1:A:1015:G:N1	2.19	0.57
1:A:1068:U:H3'	1:A:1069:U:H5	1.69	0.57
2:B:15:VAL:H	2:B:16:HIS:CE1	2.22	0.57
3:C:16:ARG:HH11	3:C:16:ARG:HB2	1.68	0.57
7:G:156:TRP:CD1	7:G:156:TRP:H	2.22	0.57
9:I:114:TYR:H	9:I:114:TYR:HD1	1.52	0.57
1:A:648:G:OP1	18:R:64:ARG:NE	2.32	0.57
1:A:1043:C:C2'	1:A:1044:G:H5'	2.35	0.57
1:A:1329:G:C6	9:I:107:ARG:NH2	2.73	0.57
1:A:103:A:H2'	1:A:322:G:N2	2.19	0.57
1:A:1145:C:H2'	1:A:1146:C:H6	1.68	0.57
1:A:1470:A:OP1	12:L:46:LYS:HB2	2.05	0.57
3:C:130:VAL:O	3:C:134:ILE:HG12	2.04	0.57
3:C:188:LEU:O	3:C:189:ALA:CB	2.53	0.57
14:N:43:CYS:O	14:N:43:CYS:SG	2.62	0.57
22:X:5:G:H5''	22:X:5:G:N3	2.19	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
1:A:1184:G:H2'	1:A:1185:C:H5'	1.87	0.57
1:A:1351:G:C2	1:A:1352:C:C6	2.92	0.57
17:Q:99:SER:OG	17:Q:100:LYS:N	2.38	0.57
1:A:171:C:H2'	1:A:172:C:H6	1.69	0.57
1:A:262:G:H5''	1:A:264:C:H41	1.69	0.57
1:A:1172:G:OP1	3:C:4:LYS:HA	2.04	0.57
1:A:1190:C:H2'	1:A:1191:C:H6	1.69	0.57
1:A:1421:G:H2'	1:A:1422:C:C6	2.39	0.57
4:D:175:SER:HB3	4:D:186:LEU:HD11	1.86	0.57
2:B:75:LYS:HB2	2:B:76:GLN:HE21	1.70	0.57
7:G:31:MET:SD	7:G:34:GLY:HA2	2.43	0.57
19:S:50:ALA:HB1	19:S:57:HIS:HB3	1.86	0.57
20:T:48:LYS:HB3	20:T:51:GLU:CD	2.30	0.57
1:A:1022:C:C6	1:A:1023:U:C5	2.92	0.57
1:A:1135:A:O2'	1:A:1136:C:H5'	2.05	0.57
1:A:1200:C:H2'	1:A:1201:U:C6	2.40	0.57
1:A:1297:U:H2'	1:A:1298:G:O4'	2.05	0.57
1:A:1354:G:O2'	1:A:1355:U:H5'	2.05	0.57
2:B:35:GLU:HG3	2:B:35:GLU:O	2.05	0.57
4:D:63:LYS:HD2	4:D:198:VAL:CG2	2.35	0.57
9:I:79:LEU:HD23	9:I:101:PHE:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:4:ILE:HA	10:J:100:THR:HG22	1.87	0.57
18:R:86:VAL:O	18:R:87:ARG:HG2	2.04	0.57
19:S:5:LEU:HA	19:S:6:LYS:HZ1	1.69	0.57
20:T:36:LEU:HD12	20:T:62:LEU:HD12	1.87	0.57
5:E:102:ALA:HA	5:E:120:THR:OG1	2.04	0.57
22:X:4:PSU:H6	22:X:4:PSU:O5'	1.87	0.57
1:A:528:G:OP1	4:D:59:ARG:NH2	2.38	0.57
1:A:1106:A:H4'	10:J:37:PRO:HD2	1.87	0.57
1:A:1188:G:C6	1:A:1189:G:C5	2.93	0.57
10:J:96:ILE:H	10:J:96:ILE:HD12	1.70	0.57
1:A:1395:C:H2'	1:A:1396:A:C8	2.39	0.56
3:C:29:TYR:OH	14:N:54:PRO:HD2	2.04	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:604:C:C2	4:D:135:LEU:HG	2.41	0.56
1:A:1116:G:H2'	1:A:1117:G:C8	2.40	0.56
1:A:1295:U:O4	19:S:4:SER:N	2.39	0.56
2:B:71:VAL:CG2	2:B:164:VAL:HG22	2.36	0.56
3:C:22:TRP:CZ2	3:C:32:LEU:O	2.58	0.56
11:K:126:ARG:O	11:K:128:ALA:N	2.38	0.56
12:L:82:VAL:HB	12:L:106:ASP:OD2	2.04	0.56
13:M:34:LEU:CD1	13:M:41:PRO:HA	2.35	0.56
1:A:890:C:O2'	1:A:891:A:H5'	2.06	0.56
1:A:943:A:H4'	1:A:944:G:O5'	2.04	0.56
1:A:1502:C:OP1	11:K:120:ARG:NH1	2.39	0.56
2:B:78:GLN:O	2:B:94:ASN:OD1	2.23	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
1:A:1482:G:OP1	1:A:1485:A:H4'	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
1:A:1330:U:O2'	1:A:1331:A:H5'	2.05	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
12:L:68:ALA:HB1	12:L:100:ILE:HD12	1.88	0.56
18:R:37:VAL:O	18:R:41:LYS:HB3	2.06	0.56
1:A:606:A:C8	1:A:607:C:C5	2.93	0.56
1:A:1231:C:O2	1:A:1231:C:H3'	2.05	0.56
3:C:15:THR:O	3:C:16:ARG:HB2	2.06	0.56
6:F:47:ARG:HA	6:F:57:GLN:HG2	1.86	0.56
13:M:108:ARG:HG3	13:M:108:ARG:NH1	2.13	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
1:A:36:G:H2'	1:A:37:C:C6	2.41	0.56
1:A:1073:U:H2'	1:A:1074:U:H6	1.71	0.56
3:C:8:ILE:HG23	3:C:16:ARG:HG2	1.88	0.56
1:A:144:A:H2'	1:A:145:C:H6	1.69	0.56
2:B:18:GLY:CA	2:B:42:ILE:HG23	2.30	0.56
10:J:94:VAL:CG1	10:J:95:GLU:N	2.69	0.56
1:A:378:A:H2'	1:A:379:A:C8	2.41	0.55
1:A:801:C:N3	1:A:1507:G:O6	2.38	0.55
2:B:105:PHE:HE1	2:B:155:LEU:CD1	2.18	0.55
10:J:38:ILE:HD12	10:J:71:LEU:HD23	1.87	0.55
1:A:953:A:C8	1:A:953:A:H5''	2.41	0.55
1:A:1132:C:O5'	1:A:1132:C:H6	1.89	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:36:TYR:HD2	9:I:37:PHE:CE1	2.24	0.55
9:I:48:GLU:N	9:I:49:PRO:CD	2.69	0.55
1:A:262:G:C8	1:A:262:G:H5'	2.41	0.55
1:A:365:C:H2'	1:A:366:C:O5'	2.06	0.55
9:I:47:LEU:C	9:I:49:PRO:HD2	2.32	0.55
12:L:126:LYS:HA	12:L:129:ALA:O	2.06	0.55
1:A:9:A:N7	4:D:208:SER:HB2	2.21	0.55
1:A:825:U:H3'	1:A:826:C:O4'	2.05	0.55
2:B:139:LYS:O	2:B:143:GLU:HG2	2.06	0.55
2:B:153:ARG:HG3	2:B:154:LEU:HD23	1.89	0.55
4:D:2:GLY:O	4:D:3:ARG:O	2.24	0.55
5:E:36:ASP:OD1	5:E:38:GLN:N	2.28	0.55
6:F:97:PHE:CB	18:R:32:ARG:HH21	2.18	0.55
11:K:56:GLY:O	11:K:57:THR:O	2.25	0.55
18:R:73:ALA:CB	18:R:79:LEU:HD12	2.37	0.55
19:S:5:LEU:HG	19:S:10:PHE:CE1	2.41	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
2:B:164:VAL:HB	2:B:186:ALA:HB2	1.88	0.55
9:I:89:ASN:HB3	9:I:92:TYR:CD2	2.42	0.55
1:A:162:G:H2'	1:A:163:G:C8	2.41	0.55
1:A:734:G:N3	15:O:23:GLY:HA3	2.22	0.55
1:A:1014:G:N3	1:A:1015:G:C6	2.75	0.55
1:A:1477:A:O2'	1:A:1478:A:H5'	2.06	0.55
3:C:31:HIS:C	3:C:33:LEU:H	2.13	0.55
11:K:48:ILE:HG22	11:K:49:GLY:N	2.19	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:C:O2	1:A:324:C:H2'	2.05	0.55
1:A:386:C:O3'	16:P:28:ARG:NH2	2.40	0.55
1:A:831:G:C2'	1:A:832:G:H5'	2.36	0.55
1:A:1140:A:H4'	1:A:1141:C:O5'	2.06	0.55
2:B:15:VAL:C	2:B:16:HIS:CG	2.84	0.55
7:G:45:ASP:O	7:G:49:ILE:HG12	2.06	0.55
2:B:78:GLN:NE2	2:B:94:ASN:O	2.39	0.55
11:K:31:THR:HG22	11:K:42:TRP:HB3	1.89	0.55
1:A:650:G:H5'	1:A:710:C:H1'	1.89	0.55
1:A:859:G:OP2	12:L:12:ARG:NH2	2.40	0.55
1:A:1108:U:O2'	1:A:1263:U:O2	2.17	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
20:T:57:ARG:HH11	20:T:102:GLY:HA2	1.70	0.55
1:A:485:C:H2'	1:A:486:G:H8	1.72	0.55
1:A:1473:U:H2'	1:A:1474:C:C6	2.41	0.55
9:I:65:VAL:O	9:I:66:ARG:HG3	2.06	0.55
10:J:38:ILE:HG13	10:J:71:LEU:HB3	1.88	0.55
1:A:331:C:H2'	1:A:332:C:C6	2.43	0.54
1:A:1210:C:H4'	13:M:116:THR:HA	1.88	0.54
3:C:126:ARG:O	3:C:128:PHE:N	2.40	0.54
12:L:68:ALA:HB3	12:L:100:ILE:CD1	2.38	0.54
22:X:5:G:N3	22:X:5:G:C5'	2.70	0.54
1:A:962:C:H2'	1:A:963:C:H6	1.72	0.54
1:A:417:U:H3'	1:A:417:U:OP2	2.08	0.54
1:A:1109:U:C6	1:A:1262:A:N7	2.74	0.54
1:A:1270:A:C2	1:A:1334:C:H1'	2.42	0.54
2:B:35:GLU:HA	2:B:39:ILE:O	2.06	0.54
4:D:196:LEU:CD2	4:D:197:PRO:HD2	2.38	0.54
5:E:80:ILE:HD12	5:E:91:LEU:CB	2.33	0.54
9:I:99:LEU:HB2	9:I:101:PHE:HE1	1.70	0.54
19:S:6:LYS:HD2	19:S:6:LYS:N	2.22	0.54
20:T:56:MET:HE1	20:T:104:LEU:HD13	1.90	0.54
1:A:954:G:OP2	1:A:1340:U:O2'	2.25	0.54
10:J:96:ILE:N	10:J:96:ILE:HD12	2.22	0.54
12:L:73:GLU:OE2	12:L:73:GLU:HA	2.07	0.54
13:M:25:ILE:HD11	13:M:66:LEU:HD21	1.90	0.54
1:A:429:C:C2'	1:A:430:U:H5'	2.37	0.54
1:A:485:C:H2'	1:A:486:G:C8	2.42	0.54
2:B:78:GLN:HE22	2:B:95:GLN:NE2	2.05	0.54
10:J:50:ILE:HD13	14:N:41:ARG:HD3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:4:SER:C	19:S:5:LEU:HD13	2.32	0.54
1:A:438:C:H2'	1:A:439:C:C6	2.42	0.54
1:A:721:A:H1'	6:F:73:ASN:HD21	1.73	0.54
1:A:1100:G:H5''	1:A:1100:G:H8	1.72	0.54
2:B:55:PHE:HE1	2:B:218:ALA:HA	1.73	0.54
12:L:68:ALA:CB	12:L:100:ILE:HD12	2.37	0.54
8:H:80:ILE:O	8:H:80:ILE:HG22	2.07	0.54
8:H:119:LEU:CD1	8:H:124:ALA:HA	2.37	0.54
1:A:406:G:H5''	1:A:407:A:OP1	2.07	0.54
2:B:105:PHE:CE1	2:B:155:LEU:CD1	2.91	0.54
9:I:100:GLY:C	9:I:102:LEU:H	2.14	0.54
19:S:6:LYS:HD2	19:S:6:LYS:C	2.32	0.54
21:U:5:ASP:O	21:U:11:GLY:HA3	2.08	0.54
1:A:53:G:O2'	1:A:54:A:H5'	2.08	0.54
1:A:1374:U:H2'	1:A:1375:G:H8	1.68	0.54
3:C:28:GLN:HA	3:C:31:HIS:CE1	2.43	0.54
13:M:59:TYR:O	13:M:63:THR:OG1	2.20	0.54
17:Q:67:LYS:HA	17:Q:70:ARG:NH1	2.20	0.54
18:R:50:ILE:HG12	18:R:70:ILE:HD13	1.89	0.54
1:A:1404:G:N2	1:A:1457:C:N3	2.51	0.54
5:E:53:LEU:O	5:E:57:LYS:HB2	2.07	0.54
13:M:4:ILE:HG22	13:M:5:ALA:N	2.22	0.54
13:M:45:VAL:O	13:M:48:LEU:HD22	2.08	0.54
20:T:37:SER:O	20:T:38:LYS:C	2.50	0.54
1:A:955:A:C2'	1:A:956:A:H5'	2.37	0.53
1:A:970:U:H4'	1:A:971:G:O5'	2.08	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:41:ARG:HH22	12:L:57:LYS:CE	2.21	0.53
1:A:946:A:H4'	1:A:947:A:OP2	2.08	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
9:I:43:ALA:C	9:I:45:ALA:H	2.16	0.53
10:J:6:ILE:HG22	10:J:98:ILE:HA	1.90	0.53
12:L:47:LYS:CB	12:L:48:PRO:CD	2.58	0.53
1:A:612:G:O2'	1:A:613:G:H5'	2.08	0.53
1:A:657:G:H2'	1:A:658:G:C8	2.42	0.53
4:D:14:ARG:HG3	4:D:15:GLU:N	2.23	0.53
6:F:62:TRP:CG	18:R:35:ARG:NH1	2.76	0.53
12:L:81:SER:O	12:L:106:ASP:CB	2.51	0.53
19:S:4:SER:O	19:S:5:LEU:HD22	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:637:A:P	8:H:56:LYS:HZ1	2.30	0.53
1:A:675:G:O6	11:K:52:GLY:HA2	2.09	0.53
1:A:994:A:H2'	1:A:995:A:C8	2.43	0.53
1:A:1008:C:C6	1:A:1008:C:C3'	2.91	0.53
1:A:1030:G:O5'	1:A:1030:G:H8	1.90	0.53
1:A:1057:G:O3'	2:B:103:THR:CG2	2.56	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:921:U:C3'	1:A:922:G:H5'	2.38	0.53
3:C:90:GLU:O	3:C:93:LYS:HB3	2.08	0.53
4:D:18:LYS:HG3	4:D:31:CYS:CB	2.38	0.53
12:L:47:LYS:HB3	12:L:48:PRO:HD2	1.80	0.53
2:B:187:LEU:HD23	2:B:201:ILE:O	2.09	0.53
3:C:152:ILE:HG13	3:C:167:TRP:HB2	1.91	0.53
9:I:54:ASP:HA	9:I:56:LEU:HD12	1.91	0.53
3:C:70:VAL:HG12	3:C:72:LYS:N	2.13	0.53
12:L:29:GLY:O	12:L:30:ALA:O	2.25	0.53
1:A:971:G:H2'	1:A:971:G:N3	2.23	0.53
1:A:1044:G:O2'	1:A:1045:U:H5'	2.08	0.53
1:A:1101:C:H1'	1:A:1161:A:C4	2.44	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
7:G:38:LEU:HD12	7:G:38:LEU:O	2.08	0.53
14:N:37:PHE:O	14:N:39:LEU:HG	2.09	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:18:TRP:CD1	14:N:54:PRO:HA	2.44	0.53
3:C:22:TRP:CE3	3:C:22:TRP:O	2.62	0.53
17:Q:87:LYS:HA	17:Q:87:LYS:HE3	1.91	0.53
1:A:938:U:O2	1:A:938:U:H2'	2.08	0.53
3:C:87:LEU:HD23	3:C:90:GLU:OE2	2.09	0.53
1:A:38:U:O2'	1:A:484:G:H4'	2.09	0.52
1:A:429:C:O2'	1:A:430:U:H5''	2.09	0.52
1:A:1253:G:O5'	1:A:1253:G:H8	1.92	0.52
1:A:1426:G:H4'	1:A:1427:A:O5'	2.10	0.52
2:B:101:MET:O	2:B:105:PHE:HA	2.09	0.52
10:J:27:ALA:HB2	10:J:85:LEU:HD11	1.90	0.52
12:L:87:GLY:HA2	12:L:98:TYR:HA	1.91	0.52
14:N:41:ARG:HA	14:N:44:LEU:HD13	1.90	0.52
18:R:56:THR:CB	18:R:58:LEU:HD13	2.37	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:C:O2'	1:A:430:U:C5'	2.56	0.52
1:A:623:G:O2'	1:A:624:A:H5'	2.09	0.52
1:A:896:A:H2'	1:A:897:A:C8	2.43	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: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
6:F:80:ARG:HB3	6:F:88:VAL:HG21	1.91	0.52
9:I:26:VAL:HG13	9:I:61:ALA:HB3	1.90	0.52
12:L:47:LYS:CG	12:L:48:PRO:HD3	2.40	0.52
12:L:78:GLN:O	12:L:79:GLU:C	2.53	0.52
13:M:45:VAL:O	13:M:46:LYS:C	2.53	0.52
14:N:4:LYS:O	14:N:6:LEU:N	2.42	0.52
20:T:72:LEU:O	20:T:73:HIS:C	2.52	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
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
7:G:51:GLN:C	7:G:53:LYS:N	2.68	0.52
10:J:81:THR:C	10:J:83:GLU:H	2.16	0.52
11:K:16:SER:O	11:K:35:PRO:HD3	2.09	0.52
15:O:74:ASP:C	15:O:76:GLU:N	2.66	0.52
17:Q:68:ARG:H	17:Q:70:ARG:NH1	2.07	0.52
7:G:16:LEU:O	7:G:17:VAL:HG23	2.08	0.52
7:G:26:PHE:HB2	7:G:101:LEU:HD22	1.92	0.52
9:I:65:VAL:C	9:I:66:ARG:HG3	2.34	0.52
9:I:88:TYR:O	9:I:88:TYR:CG	2.63	0.52
13:M:56:LEU:O	13:M:57:ARG:C	2.52	0.52
18:R:19:LYS:HD3	18:R:20:ALA:H	1.75	0.52
1:A:1332:A:C6	1:A:1333:U:N3	2.78	0.52
9:I:9:ARG:HB3	9:I:104:ARG:NH1	2.25	0.52
9:I:36:TYR:CD2	9:I:37:PHE:CE1	2.98	0.52
1:A:741:U:H2'	1:A:742:G:O4'	2.10	0.52
1:A:1131:U:H2'	1:A:1132:C:O4'	2.09	0.52
1:A:1324:C:O2'	1:A:1325:G:H5'	2.09	0.52
2:B:140:HIS:HA	2:B:143:GLU:CG	2.35	0.52
4:D:8:VAL:CG1	4:D:21:LEU:HB3	2.40	0.52
4:D:8:VAL:HG21	4:D:115:ARG:NH1	2.24	0.52
13:M:49:THR:HG22	13:M:51:ALA:H	1.75	0.52
1:A:56:A:O2'	1:A:57:U:H5'	2.09	0.52
1:A:193:G:H8	1:A:193:G:C5'	2.22	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:G:H2'	1:A:197:U:C6	2.44	0.52
1:A:386:C:H2'	1:A:387:G:H8	1.74	0.52
1:A:938:U:H1'	1:A:1205:C:H5'	1.91	0.52
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:1190:C:H2'	1:A:1191:C:C6	2.43	0.52
1:A:1352:C:H2'	1:A:1353:G:O4'	2.09	0.52
4:D:8:VAL:HG11	4:D:21:LEU:HB3	1.92	0.52
7:G:15:ASP:OD2	7:G:18:TYR:HB2	2.10	0.52
10:J:45:ARG:NH2	14:N:36:PHE:CD1	2.78	0.52
13:M:66:LEU:C	13:M:70:LEU:HB2	2.34	0.52
14:N:29:ARG:HD3	14:N:40:CYS:CB	2.40	0.52
4:D:142:PRO:HA	4:D:185:PHE:HD2	1.73	0.52
9:I:118:LYS:O	9:I:119:ALA:CB	2.57	0.52
18:R:38:GLU:H	18:R:38:GLU:CD	2.17	0.52
1:A:954:G:C8	1:A:1340:U:C2	2.98	0.52
1:A:1117:G:N1	1:A:1124:C:C4	2.78	0.52
1:A:1254:G:H5''	1:A:1254:G:H8	1.75	0.52
1:A:1287:G:H5''	21:U:4:GLY:HA3	1.93	0.52
2:B:142:LEU:O	2:B:146:GLN:HB2	2.09	0.52
3:C:31:HIS:C	3:C:33:LEU:N	2.66	0.52
3:C:172:ARG:HD2	3:C:174:PRO:HG3	1.92	0.52
8:H:119:LEU:HD12	8:H:124:ALA:CB	2.40	0.52
14:N:44:LEU:O	14:N:44:LEU:HD23	2.10	0.52
1:A:18:U:H2'	1:A:19:C:C6	2.45	0.51
1:A:1040:G:C4	1:A:1186:A:C2	2.98	0.51
1:A:1352:C:H2'	1:A:1352:C:O2	2.10	0.51
4:D:108:LEU:HD13	4:D:174:LEU:HD13	1.91	0.51
1:A:958:C:H5'	1:A:958:C:C6	2.44	0.51
1:A:1078:U:OP1	1:A:1091:G:N2	2.42	0.51
1:A:1087:G:OP1	2:B:144:ARG:NH1	2.43	0.51
1:A:1107:G:N2	1:A:1110:G:N2	2.57	0.51
1:A:1238:A:N6	1:A:1260:U:OP2	2.43	0.51
1:A:1446:A:H2'	1:A:1447:G:O4'	2.10	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
8:H:1:MET:O	8:H:1:MET:HG2	2.09	0.51
1:A:1177:C:O2	1:A:1177:C:H2'	2.11	0.51
1:A:1472:G:N7	25:A:1614:PAR:N32	2.58	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:40:CYS:O	14:N:42:ILE:N	2.44	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
2:B:105:PHE:CE1	2:B:155:LEU:HD12	2.42	0.51
4:D:8:VAL:HG13	4:D:21:LEU:HD13	1.92	0.51
9:I:104:ARG:HD2	9:I:104:ARG:C	2.35	0.51
12:L:54:LYS:N	12:L:54:LYS:HD3	2.26	0.51
1:A:1214:U:H5''	9:I:124:GLN:O	2.11	0.51
2:B:212:GLN:O	2:B:213:LEU:C	2.52	0.51
13:M:15:VAL:HG22	13:M:43:THR:O	2.11	0.51
13:M:76:ALA:HA	13:M:79:LYS:HG2	1.91	0.51
14:N:26:ARG:HH11	14:N:47:LEU:CG	2.23	0.51
1:A:53:G:C2'	1:A:54:A:H5'	2.40	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
4:D:31:CYS:N	4:D:33:MET:H	2.08	0.51
20:T:48:LYS:HB3	20:T:51:GLU:HG2	1.92	0.51
1:A:22:G:H2'	1:A:23:G:C8	2.46	0.51
1:A:951:G:OP1	10:J:57:LYS:NZ	2.35	0.51
1:A:953:A:H8	1:A:953:A:H5''	1.74	0.51
1:A:1292:G:H5'	13:M:77:ASN:ND2	2.25	0.51
2:B:52:GLU:HG2	2:B:53:ARG:N	2.26	0.51
2:B:194:PRO:O	2:B:196:LEU:N	2.44	0.51
16:P:9:PHE:CD1	16:P:18:ARG:HG3	2.46	0.51
1:A:598:A:C2	1:A:611:G:C2	2.99	0.51
1:A:1205:C:P	19:S:78:ARG:HH21	2.33	0.51
1:A:1234:A:H2'	1:A:1234:A:N3	2.26	0.51
1:A:995:A:H2'	1:A:996:G:O4'	2.11	0.51
1:A:1251:A:C2	1:A:1295:U:O4'	2.64	0.51
1:A:1345:C:H5'	1:A:1346:A:O5'	2.11	0.51
3:C:23:TYR:CD1	3:C:23:TYR:C	2.89	0.51
10:J:82:ILE:HG22	10:J:82:ILE:O	2.11	0.51
14:N:3:ARG:NE	14:N:3:ARG:O	2.44	0.51
15:O:70:LEU:CD2	15:O:78:TYR:HA	2.41	0.51
1:A:507:A:H61	12:L:92:ASP:HB2	1.76	0.51
1:A:715:G:OP1	1:A:750:A:H1'	2.10	0.51
1:A:1010:G:N1	1:A:1015:G:N7	2.59	0.51
1:A:1358:A:C5	1:A:1359:U:C5	2.99	0.51
2:B:102:LEU:O	2:B:105:PHE:HB2	2.11	0.51
4:D:13:ARG:HA	4:D:33:MET:HE1	1.92	0.51
19:S:51:VAL:O	19:S:57:HIS:HA	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
11:K:102:GLY:O	11:K:103:LEU:C	2.54	0.50
1:A:316:C:H2'	1:A:317:A:C8	2.47	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
1:A:172:C:OP1	20:T:65:LYS:NZ	2.43	0.50
1:A:1063:A:H5''	5:E:16:THR:HG21	1.93	0.50
1:A:1117:G:N2	1:A:1125:G:C4	2.79	0.50
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
4:D:14:ARG:C	4:D:16:GLY:H	2.19	0.50
5:E:60:TYR:CE1	5:E:64:ARG:NH2	2.79	0.50
10:J:8:LEU:CD1	10:J:20:ALA:HB2	2.37	0.50
19:S:51:VAL:O	19:S:58:VAL:HG22	2.11	0.50
1:A:219:U:H2'	1:A:220:C:O4'	2.11	0.50
1:A:450:C:H2'	1:A:451:C:C6	2.47	0.50
1:A:1443:C:H2'	1:A:1444:C:O4'	2.11	0.50
2:B:116:GLU:HA	2:B:119:GLU:HB2	1.94	0.50
3:C:11:ARG:HG3	3:C:11:ARG:HH11	1.76	0.50
3:C:72:LYS:HB3	3:C:75:VAL:HG23	1.93	0.50
6:F:3:ARG:HH11	6:F:64:GLN:HE21	1.60	0.50
8:H:20:TYR:CE2	8:H:75:ARG:HG2	2.46	0.50
10:J:23:ILE:O	10:J:23:ILE:CG2	2.59	0.50
1:A:36:G:O2'	12:L:118:SER:O	2.23	0.50
1:A:531:A:OP2	4:D:2:GLY:CA	2.50	0.50
1:A:698:G:H2'	1:A:699:A:C8	2.47	0.50
1:A:952:A:OP2	14:N:29:ARG:NH2	2.45	0.50
1:A:1335:G:O2'	1:A:1336:C:H5'	2.12	0.50
2:B:218:ALA:O	2:B:222:ILE:HG13	2.12	0.50
9:I:93:ARG:O	9:I:95:LYS:N	2.45	0.50
10:J:8:LEU:HD23	10:J:95:GLU:O	2.12	0.50
1:A:1008:C:O2	1:A:1016:G:O6	2.30	0.50
1:A:1074:U:O2	1:A:1076:A:C8	2.65	0.50
1:A:1118:U:O2	1:A:1120:C:H1'	2.12	0.50
3:C:70:VAL:O	3:C:106:VAL:HG23	2.11	0.50
4:D:49:ARG:CZ	4:D:49:ARG:HA	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:69:TYR:CE2	12:L:71:PRO:HA	2.47	0.50
15:O:56:LEU:HA	15:O:59:MET:HE2	1.92	0.50
1:A:83:U:H1'	1:A:84:A:OP2	2.12	0.50
1:A:822:G:H2'	1:A:823:U:H5''	1.93	0.50
1:A:900:G:H5''	1:A:900:G:H8	1.76	0.50
1:A:963:C:O2	1:A:963:C:H2'	2.12	0.50
1:A:1144:C:H2'	1:A:1145:C:H6	1.76	0.50
9:I:51:ARG:HA	9:I:56:LEU:HG	1.93	0.50
1:A:349:A:H8	1:A:349:A:C5'	2.25	0.50
1:A:439:C:H2'	1:A:440:G:H8	1.77	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
3:C:58:GLU:OE1	10:J:92:THR:HG21	2.10	0.50
6:F:80:ARG:NH1	6:F:88:VAL:HB	2.27	0.50
9:I:33:PHE:CE2	9:I:47:LEU:HD21	2.47	0.50
9:I:43:ALA:HA	9:I:74:ILE:HD13	1.94	0.50
1:A:480:A:H4'	1:A:481:A:OP1	2.12	0.50
1:A:953:A:H5'	1:A:953:A:C8	2.44	0.50
1:A:976:G:N2	1:A:1026:C:O2	2.40	0.50
3:C:172:ARG:HB3	3:C:174:PRO:HD3	1.94	0.50
5:E:51:VAL:O	5:E:54:ALA:HB3	2.11	0.50
7:G:40:ALA:O	7:G:41:ARG:C	2.53	0.50
13:M:5:ALA:O	13:M:6:GLY:C	2.54	0.50
17:Q:67:LYS:O	17:Q:68:ARG:HG2	2.12	0.50
1:A:130:C:O2	16:P:1:MET:HB2	2.12	0.49
1:A:296:A:O5'	1:A:296:A:H8	1.95	0.49
1:A:612:G:H2'	1:A:613:G:C8	2.47	0.49
1:A:1173:A:OP2	3:C:3:ASN:OD1	2.30	0.49
1:A:1259:C:H2'	1:A:1261:A:H8	1.77	0.49
1:A:1301:A:OP2	19:S:5:LEU:HD11	2.11	0.49
1:A:1516:C:H2'	1:A:1517:C:O4'	2.12	0.49
2:B:35:GLU:O	2:B:35:GLU:CG	2.60	0.49
2:B:173:ALA:O	2:B:176:GLU:N	2.45	0.49
3:C:75:VAL:O	3:C:83:ARG:HD2	2.12	0.49
13:M:9:ILE:HG21	13:M:11:ARG:HH21	1.76	0.49
13:M:82:MET:O	13:M:85:GLY:HA2	2.12	0.49
14:N:37:PHE:CE1	14:N:53:LEU:HD13	2.46	0.49
14:N:57:ARG:HG2	14:N:58:LYS:H	1.77	0.49
15:O:26:GLU:OE2	15:O:77:ARG:NH1	2.45	0.49
18:R:44:LEU:HD11	18:R:79:LEU:HD22	1.92	0.49
1:A:83:U:H4'	1:A:84:A:C8	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1002:G:H2'	1:A:1002:G:N3	2.27	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
13:M:20:THR:C	13:M:22:ILE:H	2.19	0.49
1:A:923:G:C2	1:A:924:A:C8	2.99	0.49
1:A:952:A:P	14:N:41:ARG:HH12	2.35	0.49
1:A:1107:G:N2	1:A:1110:G:H21	2.09	0.49
1:A:1109:U:H6	1:A:1262:A:N7	2.10	0.49
1:A:1231:C:H41	1:A:1270:A:N6	2.08	0.49
2:B:97:TRP:CH2	2:B:176:GLU:CD	2.90	0.49
2:B:98:LEU:HG	2:B:101:MET:HE3	1.93	0.49
3:C:15:THR:HG23	3:C:181:ASN:CA	2.43	0.49
3:C:30:ARG:NH1	3:C:30:ARG:CB	2.75	0.49
5:E:20:GLN:O	5:E:21:ALA:C	2.55	0.49
9:I:5:TYR:CD1	9:I:6:GLY:N	2.80	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
13:M:108:ARG:NH1	13:M:113:PRO:O	2.45	0.49
14:N:24:CYS:CB	14:N:40:CYS:H	2.11	0.49
1:A:1350:C:H4'	10:J:48:THR:HG21	1.93	0.49
14:N:26:ARG:HD3	14:N:47:LEU:HD11	1.94	0.49
19:S:67:VAL:O	19:S:69:HIS:N	2.41	0.49
1:A:87:C:O2	1:A:87:C:O4'	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
17:Q:48:GLU:O	17:Q:49:GLU:C	2.55	0.49
1:A:614:G:C8	1:A:614:G:C5'	2.95	0.49
1:A:1233:A:N6	1:A:1269:A:C5	2.81	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:211:U:H6	1:A:211:U:H5'	1.78	0.49
1:A:1350:C:C2	1:A:1351:G:C8	3.00	0.49
1:A:1438:A:H2'	1:A:1439:G:O4'	2.12	0.49
1:A:1481:A:H5'	1:A:1509:A:O4'	2.12	0.49
5:E:12:LEU:HB3	5:E:31:LEU:HB2	1.95	0.49
19:S:10:PHE:CD1	19:S:10:PHE:N	2.72	0.49
19:S:15:LEU:O	19:S:19:VAL:HG23	2.12	0.49
1:A:932:G:H4'	13:M:120:LYS:CD	2.42	0.49
1:A:1300:A:OP1	19:S:10:PHE:CE2	2.66	0.49
6:F:80:ARG:HB3	6:F:88:VAL:CG2	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:18:ARG:HD3	16:P:35:LYS:HD2	1.94	0.49
1:A:803:A:H5''	1:A:803:A:H8	1.74	0.49
1:A:1302:C:O2	19:S:72:GLY:HA3	2.13	0.49
3:C:15:THR:HG21	3:C:181:ASN:H	1.77	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: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
1:A:955:A:H2'	1:A:956:A:H5'	1.95	0.48
1:A:1425:G:C8	1:A:1425:G:H3'	2.48	0.48
5:E:51:VAL:O	5:E:55:VAL:HG23	2.12	0.48
8:H:11:THR:HA	8:H:14:ARG:NH1	2.28	0.48
9:I:43:ALA:C	9:I:45:ALA:N	2.71	0.48
11:K:124:LYS:HD2	11:K:125:PHE:CZ	2.48	0.48
12:L:46:LYS:HE3	12:L:47:LYS:HG2	1.94	0.48
1:A:1136:C:P	10:J:13:HIS:HE2	2.36	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
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:81:U:O2	1:A:82:U:O2	2.31	0.48
1:A:727:U:H2'	1:A:728:C:C6	2.48	0.48
1:A:1037:C:C6	1:A:1037:C:H5''	2.48	0.48
8:H:4:ASP:CG	8:H:85:ARG:HH11	2.20	0.48
16:P:67:THR:HG22	16:P:69:THR:N	2.26	0.48
1:A:103:A:H4'	1:A:104:C:OP2	2.13	0.48
1:A:188:C:H2'	1:A:189:U:O4'	2.12	0.48
1:A:836:G:OP2	1:A:836:G:H8	1.96	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
3:C:132:ARG:O	3:C:135:LYS:HB2	2.14	0.48
9:I:5:TYR:HD1	9:I:6:GLY:N	2.10	0.48
9:I:9:ARG:CG	9:I:14:VAL:HG13	2.40	0.48
12:L:27:LEU:C	12:L:29:GLY:N	2.70	0.48
1:A:23:G:C6	1:A:24:C:C4	3.02	0.48
1:A:57:U:H2'	1:A:58:G:C8	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1172:G:O2'	3:C:3:ASN:HB3	2.11	0.48
2:B:178:ARG:HH12	8:H:68:ARG:HH22	1.61	0.48
3:C:129:ALA:HB3	3:C:132:ARG:HG2	1.95	0.48
4:D:8:VAL:C	4:D:10:ARG:N	2.71	0.48
7:G:16:LEU:H	7:G:16:LEU:CD2	2.26	0.48
14:N:36:PHE:O	14:N:36:PHE:CG	2.66	0.48
1:A:778:A:C2'	1:A:779:C:O5'	2.61	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
1:A:1519:U:H2'	1:A:1520:U:C1'	2.43	0.48
2:B:110:GLN:HA	2:B:113:HIS:HB2	1.96	0.48
2:B:121:LEU:HA	2:B:124:SER:HB2	1.95	0.48
13:M:49:THR:HB	13:M:52:GLU:H	1.79	0.48
14:N:2:ALA:O	14:N:4:LYS:N	2.46	0.48
16:P:43:LYS:HG2	16:P:48:TRP:CE2	2.49	0.48
1:A:959:U:H5'	14:N:21:TYR:CE1	2.48	0.48
1:A:1070:G:H2'	1:A:1071:G:C8	2.49	0.48
7:G:17:VAL:O	7:G:17:VAL:CG1	2.61	0.48
7:G:32:ARG:O	7:G:33:ASP:C	2.56	0.48
13:M:34:LEU:HD13	13:M:41:PRO:HA	1.95	0.48
20:T:82:SER:O	20:T:83:ARG:C	2.56	0.48
1:A:9:A:C6	4:D:209:ARG:HB3	2.49	0.48
1:A:442:G:H8	1:A:442:G:O5'	1.96	0.48
1:A:516:A:H5'	1:A:516:A:N3	2.29	0.48
1:A:1195:A:O2'	1:A:1197:G:N7	2.40	0.48
4:D:91:SER:O	4:D:94:LEU:N	2.47	0.48
10:J:86:MET:HE2	10:J:86:MET:HB3	1.76	0.48
10:J:94:VAL:CG1	10:J:95:GLU:H	2.26	0.48
11:K:87:THR:HA	11:K:91:ARG:HH11	1.78	0.48
1:A:201:C:OP1	20:T:61:SER:OG	2.31	0.48
1:A:265:C:H2'	1:A:266:A:H8	1.78	0.48
1:A:1300:A:OP1	19:S:10:PHE:HE2	1.97	0.48
1:A:1331:A:H2'	1:A:1332:A:C8	2.48	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
19:S:22:LEU:HD12	19:S:26:GLY:C	2.39	0.48
19:S:22:LEU:O	19:S:26:GLY:HA3	2.13	0.48
1:A:8:G:H21	5:E:121:LYS:HG2	1.79	0.48
1:A:741:U:H5''	1:A:806:C:O2	2.14	0.48
1:A:1311:A:C3'	1:A:1312:U:H5'	2.44	0.48
3:C:43:LEU:HD23	3:C:47:LEU:HD13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:180:ALA:O	3:C:181:ASN:HB3	2.13	0.48
4:D:158:ILE:O	4:D:162:LEU:HB2	2.14	0.48
4:D:190:ASP:O	4:D:191:ARG:C	2.56	0.48
5:E:51:VAL:CB	5:E:52:PRO:CD	2.91	0.48
8:H:86:ILE:HG21	8:H:133:LEU:HD13	1.95	0.48
20:T:44:ALA:C	20:T:46:GLU:H	2.22	0.48
1:A:653:U:H2'	1:A:654:G:H8	1.79	0.47
1:A:961:A:C5'	1:A:962:C:OP2	2.60	0.47
1:A:1135:A:H2'	1:A:1136:C:C6	2.49	0.47
10:J:47:PHE:CZ	14:N:37:PHE:HE2	2.32	0.47
12:L:53:ARG:NH1	12:L:92:ASP:OD2	2.45	0.47
22:X:4:PSU:C2'	22:X:5:G:H5''	2.38	0.47
1:A:365:C:O2'	1:A:366:C:O5'	2.32	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
12:L:74:GLY:O	12:L:111:LYS:NZ	2.47	0.47
14:N:44:LEU:HD23	14:N:44:LEU:C	2.39	0.47
1:A:174:A:H2'	1:A:175:U:C6	2.50	0.47
1:A:349:A:C8	1:A:349:A:C5'	2.98	0.47
1:A:526:G:H5'	4:D:41:GLY:HA3	1.95	0.47
1:A:954:G:N7	1:A:1340:U:C2	2.82	0.47
1:A:1124:C:O2'	1:A:1125:G:C8	2.58	0.47
1:A:1290:U:H5'	13:M:110:ARG:HH11	1.80	0.47
1:A:1506:U:O3'	1:A:1507:G:H3'	2.15	0.47
3:C:150:LYS:HG2	3:C:151:VAL:N	2.30	0.47
6:F:91:VAL:HG13	18:R:72:ARG:NH2	2.30	0.47
7:G:58:PRO:O	7:G:60:LYS:N	2.48	0.47
9:I:13:ALA:HA	9:I:67:GLY:HA3	1.96	0.47
14:N:36:PHE:HD2	14:N:37:PHE:CD2	2.31	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
1:A:1118:U:O2	1:A:1118:U:C2'	2.63	0.47
2:B:9:GLU:CD	2:B:9:GLU:C	2.82	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
9:I:111:ARG:O	9:I:113:LYS:HD2	2.15	0.47
10:J:24:VAL:HG13	10:J:34:VAL:HG11	1.95	0.47
11:K:54:ARG:O	11:K:57:THR:OG1	2.30	0.47
22:X:3:A:H8	22:X:3:A:C5'	2.27	0.47
1:A:1407:C:H2'	1:A:1408:U:O4'	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
17:Q:3:LYS:HB3	17:Q:61:GLU:HB3	1.95	0.47
22:X:5:G:O6	23:Y:35:A:N1	2.47	0.47
1:A:101:G:H2'	1:A:102:G:H5'	1.97	0.47
1:A:1401:A:N6	1:A:1460:G:HO2'	2.12	0.47
1:A:1421:G:H2'	1:A:1422:C:H6	1.78	0.47
1:A:1476:U:H4'	1:A:1497:A:C2	2.50	0.47
2:B:21:ARG:NH1	2:B:39:ILE:HG12	2.29	0.47
3:C:22:TRP:HB3	3:C:59:ARG:HB2	1.96	0.47
3:C:113:ALA:HB2	3:C:202:ILE:HG13	1.96	0.47
12:L:46:LYS:HZ1	12:L:47:LYS:HE3	1.77	0.47
17:Q:68:ARG:H	17:Q:70:ARG:HH11	1.62	0.47
19:S:49:ILE:O	19:S:60:VAL:HG12	2.15	0.47
1:A:157:A:C5	1:A:158:C:H1'	2.50	0.47
1:A:486:G:OP1	12:L:118:SER:CB	2.63	0.47
1:A:522:G:H5''	12:L:114:LYS:HB2	1.96	0.47
1:A:817:U:H2'	1:A:818:C:C6	2.49	0.47
1:A:916:A:C6	1:A:917:G:C5	3.03	0.47
1:A:981:G:N2	1:A:1022:C:C6	2.81	0.47
1:A:982:G:H8	1:A:982:G:O5'	1.98	0.47
1:A:1188:G:C4	1:A:1189:G:C8	3.03	0.47
1:A:1245:C:N3	1:A:1254:G:O6	2.47	0.47
1:A:1300:A:H5''	19:S:10:PHE:HB3	1.97	0.47
1:A:1347:U:O2'	1:A:1348:G:H5'	2.15	0.47
1:A:1405:G:N2	1:A:1456:C:O2	2.48	0.47
4:D:29:PRO:O	4:D:30:LYS:CD	2.53	0.47
7:G:18:TYR:CD2	7:G:59:LEU:HB2	2.48	0.47
8:H:29:SER:OG	8:H:32:LYS:HD2	2.14	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
19:S:33:THR:OG1	19:S:34:TRP:N	2.48	0.47
3:C:112:SER:HB3	3:C:115:LEU:HD12	1.95	0.47
7:G:60:LYS:HA	7:G:60:LYS:HE2	1.97	0.47
10:J:46:ARG:HB3	10:J:46:ARG:HH11	1.79	0.47
14:N:27:CYS:CB	14:N:43:CYS:CB	2.89	0.47
17:Q:65:ILE:N	17:Q:65:ILE:CD1	2.74	0.47
1:A:676:U:H2'	1:A:678:A:OP2	2.15	0.47
1:A:705:G:H4'	1:A:706:A:H5''	1.97	0.47
1:A:831:G:H2'	1:A:832:G:H5'	1.96	0.47
1:A:1039:U:H5'	3:C:163:ALA:HB3	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1135:A:OP1	10:J:68:HIS:ND1	2.47	0.47
1:A:1188:G:H4'	3:C:192:THR:O	2.15	0.47
1:A:1290:U:H5'	13:M:110:ARG:NH1	2.30	0.47
1:A:1329:G:N7	9:I:10:ARG:NH2	2.62	0.47
21:U:2:GLY:O	21:U:4:GLY:N	2.48	0.47
22:X:2:G:C2'	22:X:3:A:O5'	2.63	0.47
1:A:606:A:C8	1:A:607:C:C6	3.03	0.47
1:A:753:G:H4'	1:A:1491:A:H4'	1.96	0.47
1:A:981:G:H2'	1:A:982:G:C8	2.50	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
4:D:30:LYS:HB2	4:D:32:ALA:C	2.40	0.47
5:E:11:ILE:HG22	5:E:12:LEU:N	2.30	0.47
5:E:78:HIS:C	5:E:78:HIS:CD2	2.93	0.47
8:H:77:GLU:HG2	8:H:78:GLN:O	2.14	0.47
13:M:67:GLU:O	13:M:67:GLU:CG	2.51	0.47
1:A:92:G:H5''	1:A:92:G:H8	1.79	0.46
1:A:1128:C:O2'	1:A:1129:A:H5''	2.15	0.46
1:A:1231:C:HO2'	9:I:73:GLN:NE2	2.13	0.46
1:A:1515:U:H2'	1:A:1515:U:O5'	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:1302:C:C2	19:S:72:GLY:HA3	2.50	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
4:D:101:LEU:HD23	4:D:121:VAL:CG1	2.45	0.46
7:G:41:ARG:HG2	7:G:41:ARG:HH11	1.80	0.46
17:Q:83:ASP:OD1	17:Q:83:ASP:N	2.49	0.46
18:R:36:ASN:C	18:R:40:LEU:HD12	2.40	0.46
1:A:10:G:OP1	5:E:122:GLU:HG3	2.16	0.46
1:A:764:A:C2	1:A:785:U:C5	3.03	0.46
1:A:907:G:H2'	1:A:908:C:O4'	2.16	0.46
1:A:956:A:O2'	1:A:1304:C:N3	2.43	0.46
9:I:32:ASP:HB3	9:I:35:GLU:HB2	1.97	0.46
12:L:69:TYR:HE2	12:L:71:PRO:HA	1.80	0.46
1:A:403:G:H2'	1:A:404:A:C8	2.51	0.46
1:A:483:A:H4'	1:A:484:G:H5'	1.98	0.46
1:A:536:U:C2'	1:A:537:A:H5'	2.46	0.46
1:A:959:U:H6	1:A:959:U:O5'	1.98	0.46
1:A:1015:G:H1'	1:A:1016:G:H5'	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:87:LEU:C	3:C:89:GLU:H	2.24	0.46
3:C:119:ARG:HG2	3:C:140:ARG:HH21	1.81	0.46
4:D:62:GLN:OE1	4:D:62:GLN:HA	2.14	0.46
10:J:3:LYS:HA	10:J:75:ILE:HA	1.96	0.46
12:L:92:ASP:C	12:L:93:LEU:HD23	2.41	0.46
16:P:1:MET:HE3	16:P:1:MET:HB3	1.74	0.46
1:A:253:G:H8	1:A:253:G:O5'	1.99	0.46
1:A:414:C:H2'	1:A:415:C:H6	1.80	0.46
1:A:843:A:C2'	1:A:844:C:H5'	2.46	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: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
9:I:80:GLY:O	9:I:81:ILE:C	2.58	0.46
16:P:4:ILE:O	16:P:66:PRO:HA	2.15	0.46
21:U:12:LYS:HB3	21:U:22:ARG:HD2	1.97	0.46
1:A:312:G:OP2	1:A:347:G:O2'	2.33	0.46
1:A:523:A:H2'	1:A:524:G:H8	1.76	0.46
1:A:770:G:C2	1:A:781:C:C2	3.04	0.46
1:A:1007:C:C2'	1:A:1008:C:O4'	2.63	0.46
1:A:1173:A:H2'	1:A:1174:C:C6	2.51	0.46
1:A:1411:A:H2'	1:A:1412:C:C6	2.50	0.46
1:A:1434:G:H2'	1:A:1435:G:O4'	2.15	0.46
2:B:129:GLU:O	2:B:130:ARG:HB2	2.15	0.46
3:C:180:ALA:O	3:C:181:ASN:CB	2.63	0.46
16:P:67:THR:CG2	16:P:68:ASP:N	2.78	0.46
1:A:476:G:H2'	1:A:477:G:H8	1.80	0.46
1:A:775:G:C6	1:A:776:A:N7	2.83	0.46
1:A:1040:G:H2'	1:A:1041:G:O4'	2.16	0.46
1:A:1051:G:H8	1:A:1051:G:OP2	1.99	0.46
2:B:36:ARG:HB2	2:B:41:ILE:HD13	1.96	0.46
2:B:90:MET:HA	2:B:90:MET:CE	2.42	0.46
3:C:50:ALA:HB1	3:C:70:VAL:HG11	1.97	0.46
14:N:36:PHE:CD2	14:N:37:PHE:CE2	3.03	0.46
1:A:892:A:C2'	1:A:893:A:H5'	2.45	0.46
1:A:1488:U:H2'	1:A:1489:G:C8	2.50	0.46
6:F:94:GLN:HB3	18:R:32:ARG:HD2	1.97	0.46
7:G:16:LEU:HD11	9:I:42:ARG:HA	1.97	0.46
16:P:12:LYS:O	16:P:13:HIS:HB2	2.16	0.46
17:Q:59:ILE:HD12	17:Q:59:ILE:HA	1.62	0.46
19:S:6:LYS:HG2	19:S:7:LYS:HE3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:983:A:C8	1:A:1020:C:N3	2.84	0.46
1:A:1355:U:O2'	1:A:1356:G:H5'	2.15	0.46
2:B:140:HIS:CD2	2:B:143:GLU:HG3	2.50	0.46
4:D:121:VAL:O	4:D:134:ASP:HA	2.16	0.46
19:S:6:LYS:C	19:S:7:LYS:HD3	2.41	0.46
20:T:86:ARG:O	20:T:87:LYS:C	2.59	0.46
1:A:148:C:N4	1:A:163:G:H1	2.12	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
6:F:36:ARG:CZ	6:F:36:ARG:HB2	2.46	0.46
7:G:80:VAL:HG12	7:G:81:GLY:N	2.31	0.46
11:K:87:THR:HG22	11:K:91:ARG:NH1	2.31	0.46
18:R:19:LYS:HE2	18:R:19:LYS:HA	1.97	0.46
19:S:29:ARG:O	19:S:31:ILE:N	2.49	0.46
1:A:85:C:H6	1:A:85:C:O5'	1.99	0.45
1:A:86:U:O5'	1:A:86:U:H6	1.99	0.45
1:A:1208:C:H4'	1:A:1209:A:OP1	2.16	0.45
1:A:1387:C:H2'	1:A:1388:G:C8	2.51	0.45
4:D:68:TYR:N	4:D:68:TYR:CD1	2.84	0.45
7:G:15:ASP:O	7:G:19:GLY:HA2	2.16	0.45
9:I:57:GLY:O	9:I:59:PHE:N	2.41	0.45
10:J:3:LYS:HA	10:J:74:ILE:O	2.16	0.45
13:M:108:ARG:HH11	13:M:108:ARG:CG	2.21	0.45
1:A:416:U:O2	1:A:420:G:C2	2.69	0.45
1:A:1073:U:H2'	1:A:1074:U:C6	2.49	0.45
25:A:1614:PAR:O53	25:A:1614:PAR:H21	2.16	0.45
3:C:131:ARG:HH11	5:E:50:GLU:HG2	1.81	0.45
7:G:80:VAL:CG1	7:G:81:GLY:N	2.79	0.45
22:X:4:PSU:H6	22:X:4:PSU:C5'	2.28	0.45
1:A:1327:U:C4	1:A:1360:A:C2	3.05	0.45
1:A:1349:C:C2'	1:A:1350:C:H5'	2.46	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
2:B:187:LEU:HA	2:B:201:ILE:HB	1.98	0.45
6:F:1:MET:HE3	6:F:66:GLU:OE1	2.16	0.45
10:J:22:LYS:C	10:J:24:VAL:H	2.24	0.45
1:A:34:A:N3	12:L:32:PHE:HE2	2.14	0.45
1:A:46:U:H2'	1:A:47:G:C8	2.51	0.45
1:A:81:U:H4'	1:A:82:U:OP1	2.15	0.45
1:A:531:A:H4'	1:A:532:G:O5'	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1258:G:N3	1:A:1264:C:O2'	2.48	0.45
21:U:6:ARG:HH21	21:U:15:ARG:CG	2.24	0.45
1:A:42:G:H2'	1:A:43:G:C8	2.51	0.45
1:A:937:A:C2	1:A:1204:G:O4'	2.69	0.45
1:A:1280:C:H4'	1:A:1281:A:O4'	2.17	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
11:K:87:THR:HG22	11:K:91:ARG:HH12	1.81	0.45
1:A:97:C:P	20:T:17:ARG:HH21	2.39	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
1:A:1472:G:C2'	1:A:1473:U:H5'	2.47	0.45
3:C:132:ARG:HG3	3:C:133:ALA:N	2.32	0.45
4:D:107:ARG:HH21	4:D:194:LEU:HD12	1.82	0.45
6:F:80:ARG:HA	6:F:85:VAL:HG11	1.99	0.45
1:A:961:A:N3	1:A:961:A:C3'	2.76	0.45
1:A:1013:A:N3	1:A:1013:A:OP2	2.50	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
10:J:32:ALA:HB3	10:J:76:ASN:HD21	1.82	0.45
11:K:51:LYS:H	11:K:54:ARG:HH21	1.65	0.45
18:R:32:ARG:HE	18:R:32:ARG:HB2	1.45	0.45
1:A:409:G:N2	1:A:424:G:H1'	2.32	0.45
1:A:604:C:H2'	1:A:605:A:O4'	2.17	0.45
1:A:1046:C:H3'	1:A:1047:G:H2'	1.97	0.45
1:A:1176:U:C2	1:A:1177:C:C5	3.04	0.45
1:A:1280:C:OP2	7:G:114:ARG:NH2	2.46	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
2:B:187:LEU:CD2	2:B:203:GLY:HA3	2.47	0.45
5:E:103:GLY:O	5:E:106:PRO:HD2	2.16	0.45
7:G:58:PRO:O	7:G:59:LEU:C	2.60	0.45
11:K:40:ILE:HD13	11:K:40:ILE:HA	1.78	0.45
14:N:26:ARG:HH11	14:N:47:LEU:CD2	2.30	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
1:A:559:G:C5	1:A:859:G:C2	3.05	0.45
1:A:896:A:H2'	1:A:897:A:O4'	2.16	0.45
1:A:1327:U:C2	1:A:1360:A:N1	2.85	0.45
1:A:1351:G:OP2	9:I:112:LYS:HG3	2.17	0.45
1:A:1401:A:H61	1:A:1460:G:HO2'	1.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:10:LEU:HA	6:F:84:ASN:O	2.17	0.45
17:Q:15:MET:HE3	17:Q:15:MET:HB2	1.75	0.45
19:S:45:VAL:CG2	19:S:46:GLY:N	2.68	0.45
20:T:40:ALA:HB2	20:T:55:ILE:HG22	1.99	0.45
1:A:565:G:O6	1:A:742:G:H3'	2.16	0.45
1:A:722:C:H5''	6:F:69:GLU:HB2	1.98	0.45
1:A:1047:G:H4'	1:A:1048:U:OP1	2.17	0.45
4:D:14:ARG:C	4:D:16:GLY:N	2.73	0.45
10:J:47:PHE:HD1	14:N:34:TYR:CE2	2.35	0.45
12:L:110:VAL:CG2	12:L:120:TYR:HB3	2.47	0.45
15:O:33:THR:HG22	15:O:37:ASN:ND2	2.31	0.45
17:Q:96:GLU:C	17:Q:98:LEU:H	2.25	0.45
1:A:14:U:C5	1:A:894:G:O6	2.70	0.44
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
1:A:999:U:H2'	1:A:1000:G:C8	2.53	0.44
1:A:1270:A:H2	1:A:1334:C:H1'	1.82	0.44
3:C:87:LEU:C	3:C:89:GLU:N	2.75	0.44
3:C:119:ARG:HG2	3:C:140:ARG:NH2	2.32	0.44
4:D:126:ILE:HG22	4:D:127:THR:N	2.32	0.44
9:I:19:LEU:HB3	9:I:59:PHE:CD2	2.52	0.44
13:M:49:THR:CG2	13:M:51:ALA:HB3	2.47	0.44
1:A:378:A:C2	1:A:379:A:C4	3.05	0.44
1:A:380:G:H2'	1:A:381:C:C6	2.52	0.44
1:A:668:A:N6	1:A:669:G:C6	2.86	0.44
1:A:1480:A:C2	1:A:1483:G:N1	2.70	0.44
2:B:67:THR:HG22	2:B:90:MET:CE	2.46	0.44
2:B:132:LYS:HA	2:B:135:GLN:NE2	2.32	0.44
2:B:233:SER:C	2:B:235:SER:H	2.25	0.44
4:D:18:LYS:CG	4:D:31:CYS:HB2	2.47	0.44
4:D:58:LEU:CD2	4:D:62:GLN:HG2	2.42	0.44
6:F:50:TYR:CE1	18:R:77:GLY:HA2	2.53	0.44
6:F:99:ALA:O	18:R:28:GLU:HA	2.17	0.44
9:I:65:VAL:HG21	9:I:77:ILE:HD11	1.99	0.44
10:J:4:ILE:HD13	10:J:99:LYS:O	2.18	0.44
1:A:45:G:N2	1:A:46:U:H1'	2.32	0.44
1:A:521:G:OP1	12:L:113:ARG:NH2	2.50	0.44
1:A:543:A:P	5:E:126:ARG:HH22	2.39	0.44
1:A:700:A:N3	11:K:117:ASN:O	2.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1184:G:O2'	1:A:1185:C:H5'	2.17	0.44
1:A:1375:G:O2'	1:A:1376:U:H5'	2.17	0.44
1:A:1520:U:H3'	1:A:1521:C:C6	2.53	0.44
7:G:32:ARG:O	7:G:34:GLY:N	2.50	0.44
1:A:385:A:N3	1:A:385:A:H2'	2.32	0.44
1:A:409:G:H21	1:A:424:G:H1'	1.82	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
4:D:49:ARG:HA	4:D:49:ARG:NH1	2.32	0.44
19:S:78:ARG:HD2	19:S:81:ARG:NH1	2.32	0.44
1:A:161:G:H2'	1:A:162:G:H8	1.82	0.44
2:B:15:VAL:N	2:B:16:HIS:CE1	2.85	0.44
4:D:36:ARG:HD2	4:D:38:TYR:OH	2.17	0.44
5:E:99:GLY:O	5:E:117:ASP:HA	2.17	0.44
7:G:17:VAL:HG12	7:G:18:TYR:CD1	2.52	0.44
11:K:14:VAL:O	11:K:77:MET:HA	2.17	0.44
13:M:20:THR:C	13:M:22:ILE:N	2.76	0.44
15:O:79:ARG:O	15:O:82:ILE:HD13	2.18	0.44
1:A:43:G:H2'	1:A:44:C:O4'	2.17	0.44
1:A:109:G:H1'	1:A:110:A:N7	2.32	0.44
1:A:453:C:H2'	1:A:454:G:O4'	2.18	0.44
1:A:836:G:C5	1:A:847:G:C8	3.06	0.44
1:A:917:G:H2'	1:A:918:C:C6	2.53	0.44
1:A:927:A:C2	1:A:1215:G:N3	2.86	0.44
1:A:1037:C:H5''	1:A:1037:C:H6	1.82	0.44
1:A:1051:G:N7	1:A:1077:G:O2'	2.35	0.44
1:A:1331:A:C2'	1:A:1332:A:O5'	2.65	0.44
1:A:1410:U:H2'	1:A:1411:A:C8	2.53	0.44
9:I:47:LEU:C	9:I:49:PRO:CD	2.90	0.44
13:M:34:LEU:HD12	13:M:41:PRO:HB3	2.00	0.44
19:S:44:MET:N	19:S:44:MET:SD	2.90	0.44
20:T:73:HIS:O	20:T:74:LYS:CB	2.64	0.44
22:X:3:A:C8	22:X:3:A:C5'	2.99	0.44
1:A:60:A:H1'	1:A:350:G:N2	2.33	0.44
1:A:104:C:H2'	1:A:105:G:O4'	2.18	0.44
1:A:803:A:H8	1:A:803:A:C5'	2.30	0.44
1:A:1350:C:C2'	1:A:1351:G:O5'	2.66	0.44
2:B:102:LEU:N	2:B:102:LEU:CD1	2.80	0.44
10:J:79:ARG:HD3	10:J:82:ILE:HD12	2.00	0.44
15:O:17:ARG:HH11	15:O:17:ARG:CG	2.22	0.44
1:A:380:G:H2'	1:A:381:C:H6	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1172:G:HO2'	3:C:3:ASN:CB	2.28	0.44
2:B:114:ARG:HG3	2:B:114:ARG:NH1	2.27	0.44
6:F:40:VAL:HG22	6:F:41:GLU:N	2.32	0.44
9:I:50:LEU:O	9:I:53:VAL:HG22	2.18	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:956:A:H1'	1:A:1304:C:O2	2.17	0.44
1:A:1188:G:C5	1:A:1189:G:N7	2.85	0.44
1:A:1238:A:N6	1:A:1259:C:H3'	2.33	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:189:ASP:OD2	2:B:205:ASP:OD1	2.36	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
7:G:15:ASP:CB	7:G:20:ASP:H	2.15	0.44
9:I:97:LYS:O	9:I:100:GLY:N	2.46	0.44
1:A:146:A:H2'	1:A:147:A:O4'	2.18	0.43
1:A:715:G:H5'	1:A:750:A:H4'	2.00	0.43
1:A:810:C:H2'	1:A:811:U:C6	2.53	0.43
1:A:812:A:OP1	1:A:812:A:H4'	2.18	0.43
1:A:1162:A:H2'	1:A:1163:G:H5'	1.99	0.43
1:A:1231:C:C5	1:A:1271:A:N6	2.86	0.43
4:D:196:LEU:HA	4:D:196:LEU:HD23	1.55	0.43
11:K:54:ARG:HE	11:K:54:ARG:HB2	1.49	0.43
14:N:57:ARG:HG2	14:N:58:LYS:N	2.32	0.43
18:R:70:ILE:HG22	18:R:71:LYS:N	2.30	0.43
20:T:67:ALA:O	20:T:73:HIS:ND1	2.51	0.43
1:A:720:C:H2'	1:A:721:A:C8	2.53	0.43
1:A:795:C:O2'	1:A:879:A:N1	2.44	0.43
1:A:1117:G:N7	1:A:1118:U:H5	2.16	0.43
25:A:1614:PAR:O43	25:A:1614:PAR:H11	2.19	0.43
2:B:74:LYS:O	2:B:78:GLN:HG2	2.18	0.43
4:D:99:SER:O	4:D:140:VAL:HG23	2.19	0.43
5:E:80:ILE:HD12	5:E:80:ILE:H	1.84	0.43
6:F:22:GLU:HA	6:F:25:ILE:HD12	2.00	0.43
1:A:416:U:H1'	1:A:420:G:N2	2.33	0.43
1:A:979:A:H2'	1:A:980:G:C8	2.53	0.43
1:A:1020:C:O5'	1:A:1020:C:H6	2.01	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
5:E:95:ALA:HA	5:E:96:PRO:HD2	1.75	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:152:ARG:NH2	8:H:107:LEU:O	2.49	0.43
6:F:100:ASN:ND2	18:R:23:LYS:O	2.48	0.43
7:G:111:ARG:HB3	7:G:112:PRO:HD2	1.99	0.43
10:J:38:ILE:HA	10:J:39:PRO:HD3	1.89	0.43
20:T:51:GLU:CD	20:T:51:GLU:H	2.27	0.43
1:A:524:G:H2'	1:A:525:G:O4'	2.19	0.43
1:A:696:A:H2'	1:A:697:G:O4'	2.19	0.43
1:A:836:G:O6	1:A:847:G:C8	2.71	0.43
1:A:1043:C:O2'	1:A:1044:G:H5'	2.18	0.43
1:A:1150:A:H2'	1:A:1151:A:C8	2.54	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
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:N	19:S:49:ILE:HD12	2.33	0.43
1:A:82:U:H6	1:A:82:U:HO2'	1.65	0.43
1:A:331:C:H2'	1:A:332:C:H6	1.83	0.43
1:A:924:A:H2'	1:A:925:G:H8	1.75	0.43
3:C:8:ILE:O	3:C:9:GLY:C	2.61	0.43
3:C:59:ARG:CG	3:C:64:VAL:HG12	2.45	0.43
12:L:78:GLN:O	12:L:80:HIS:N	2.52	0.43
13:M:82:MET:SD	13:M:82:MET:C	3.02	0.43
20:T:26:ASN:OD1	20:T:71:THR:HG23	2.19	0.43
1:A:357:G:C2'	1:A:358:G:H5'	2.48	0.43
1:A:493:A:C8	1:A:493:A:H3'	2.53	0.43
1:A:736:G:H4'	15:O:69:TYR:OH	2.18	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
3:C:91:LEU:CB	3:C:99:VAL:HG11	2.45	0.43
9:I:13:ALA:HB2	9:I:67:GLY:O	2.18	0.43
11:K:41:THR:HG21	11:K:71:LYS:HB3	2.01	0.43
12:L:43:VAL:HG12	12:L:44:THR:O	2.19	0.43
13:M:11:ARG:HG2	13:M:12:ASN:HB2	2.01	0.43
13:M:87:TYR:C	13:M:89:GLY:N	2.76	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
4:D:18:LYS:HG3	4:D:31:CYS:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:70:ASP:OD1	6:F:70:ASP:N	2.47	0.43
15:O:57:LEU:HD23	15:O:57:LEU:HA	1.70	0.43
17:Q:68:ARG:N	17:Q:70:ARG:NH1	2.65	0.43
1:A:804:U:H4'	1:A:805:G:OP2	2.18	0.43
1:A:1017:G:H3'	1:A:1017:G:N3	2.34	0.43
1:A:1173:A:P	3:C:3:ASN:OD1	2.77	0.43
1:A:1218:A:O2'	1:A:1286:G:H4'	2.18	0.43
1:A:1270:A:H1'	1:A:1334:C:O2'	2.18	0.43
1:A:1299:C:H5''	1:A:1300:A:OP2	2.19	0.43
1:A:1335:G:N2	1:A:1336:C:C2	2.87	0.43
2:B:88:ALA:CB	2:B:219:VAL:CG1	2.91	0.43
3:C:32:LEU:HD22	3:C:59:ARG:NH1	2.33	0.43
4:D:106:TYR:CD1	4:D:106:TYR:C	2.95	0.43
7:G:9:VAL:HG13	7:G:94:ARG:HE	1.82	0.43
9:I:97:LYS:HA	9:I:102:LEU:HD12	2.01	0.43
12:L:27:LEU:C	12:L:29:GLY:H	2.26	0.43
12:L:69:TYR:HB2	12:L:90:VAL:HG21	2.01	0.43
14:N:37:PHE:HB3	14:N:39:LEU:HB2	2.00	0.43
16:P:55:ARG:HA	16:P:55:ARG:HD2	1.67	0.43
1:A:1232:A:N3	1:A:1232:A:H5''	2.33	0.43
2:B:52:GLU:HG2	2:B:53:ARG:H	1.82	0.43
2:B:98:LEU:HD23	2:B:98:LEU:N	2.34	0.43
2:B:112:VAL:HG11	2:B:153:ARG:HA	2.01	0.43
5:E:31:LEU:HD23	5:E:31:LEU:HA	1.81	0.43
6:F:43:LEU:HD23	6:F:46:ARG:HH11	1.83	0.43
15:O:44:LYS:HE3	15:O:47:LYS:NZ	2.33	0.43
1:A:60:A:H3'	1:A:327:G:H22	1.84	0.43
1:A:706:A:H3'	1:A:706:A:N3	2.34	0.43
3:C:76:VAL:O	3:C:83:ARG:HB3	2.18	0.43
4:D:61:LYS:O	4:D:62:GLN:C	2.61	0.43
7:G:85:TYR:O	7:G:87:VAL:HG23	2.19	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
20:T:74:LYS:HE3	20:T:74:LYS:HB3	1.62	0.43
1:A:40:G:C4	1:A:482:U:O4	2.72	0.42
1:A:817:U:H2'	1:A:818:C:H6	1.84	0.42
1:A:1049:C:O2'	1:A:1050:A:C5'	2.67	0.42
1:A:1401:A:N6	1:A:1460:G:O2'	2.49	0.42
2:B:75:LYS:HE3	2:B:75:LYS:H	1.84	0.42
3:C:73:PRO:HG3	3:C:105:GLU:HG3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:79:LEU:HD22	9:I:83:ARG:HG3	2.01	0.42
12:L:41:ARG:HH22	12:L:57:LYS:NZ	2.16	0.42
13:M:101:GLN:HE21	13:M:101:GLN:HB3	1.64	0.42
16:P:26:ARG:CG	16:P:27:LYS:N	2.82	0.42
20:T:44:ALA:C	20:T:46:GLU:N	2.77	0.42
1:A:83:U:H1'	1:A:84:A:P	2.59	0.42
1:A:625:U:O4'	8:H:115:SER:HB2	2.19	0.42
1:A:953:A:N6	1:A:1349:C:O2'	2.50	0.42
1:A:985:C:H2'	1:A:986:C:C6	2.54	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
1:A:1404:G:H1	1:A:1457:C:H42	1.67	0.42
2:B:63:MET:HB3	2:B:225:ALA:HB1	1.99	0.42
5:E:41:VAL:HG22	5:E:113:ALA:HB2	2.01	0.42
7:G:58:PRO:C	7:G:60:LYS:N	2.77	0.42
10:J:59:SER:C	10:J:60:ARG:HG3	2.45	0.42
12:L:53:ARG:HG2	12:L:69:TYR:HE1	1.83	0.42
17:Q:17:LYS:H	17:Q:49:GLU:HG2	1.84	0.42
1:A:1292:G:H5'	13:M:77:ASN:HD21	1.83	0.42
3:C:20:SER:O	14:N:54:PRO:HB3	2.19	0.42
3:C:188:LEU:HD13	3:C:189:ALA:H	1.83	0.42
10:J:15:THR:HA	10:J:18:ALA:HB3	2.01	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
1:A:82:U:H6	1:A:82:U:O2'	2.02	0.42
1:A:112:U:H3'	1:A:284:A:H61	1.84	0.42
1:A:775:G:H3'	1:A:775:G:C8	2.54	0.42
1:A:1075:A:H5''	7:G:4:ARG:CZ	2.49	0.42
1:A:1095:C:N3	3:C:178:LEU:HB2	2.35	0.42
1:A:1298:G:O2'	1:A:1300:A:N7	2.47	0.42
1:A:1521:C:O5'	1:A:1521:C:H6	2.02	0.42
2:B:88:ALA:HB2	2:B:219:VAL:HG13	1.93	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
4:D:209:ARG:HH11	4:D:209:ARG:HG3	1.83	0.42
7:G:65:ALA:HB1	7:G:127:ALA:HB3	2.00	0.42
7:G:138:LYS:HD3	7:G:138:LYS:O	2.18	0.42
8:H:75:ARG:HA	8:H:76:PRO:HD3	1.93	0.42
9:I:10:ARG:HD3	9:I:75:ASP:HB2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:9:PHE:CD1	16:P:9:PHE:N	2.88	0.42
19:S:50:ALA:HA	19:S:58:VAL:O	2.19	0.42
1:A:318:C:OP2	1:A:324:C:N4	2.52	0.42
1:A:569:G:N3	1:A:857:C:H4'	2.33	0.42
1:A:1295:U:P	19:S:6:LYS:HG3	2.59	0.42
12:L:68:ALA:HB3	12:L:100:ILE:HD11	2.02	0.42
1:A:211:U:C5'	1:A:211:U:C6	3.02	0.42
1:A:925:G:H2'	1:A:926:C:O4'	2.19	0.42
1:A:1460:G:HO2'	1:A:1461:A:H8	1.59	0.42
1:A:1481:A:C8	1:A:1509:A:H1'	2.55	0.42
2:B:118:LEU:HB2	2:B:142:LEU:CD1	2.48	0.42
3:C:44:GLU:HA	3:C:52:LEU:HD11	2.01	0.42
3:C:126:ARG:O	3:C:127:ARG:C	2.63	0.42
9:I:43:ALA:O	9:I:45:ALA:N	2.51	0.42
16:P:18:ARG:HD3	16:P:35:LYS:CD	2.50	0.42
1:A:17:A:C2'	1:A:18:U:H5'	2.50	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
1:A:445:G:H4'	16:P:41:PRO:HB2	2.00	0.42
1:A:784:G:O5'	1:A:784:G:H8	2.03	0.42
1:A:982:G:H2'	1:A:983:A:C1'	2.49	0.42
1:A:1035:U:O4	1:A:1182:C:C2	2.73	0.42
2:B:81:VAL:HG12	2:B:82:ARG:N	2.34	0.42
2:B:211:ILE:H	2:B:211:ILE:HG13	1.70	0.42
4:D:70:ILE:HD12	4:D:100:ARG:HD2	2.00	0.42
7:G:38:LEU:C	7:G:38:LEU:CD1	2.91	0.42
9:I:9:ARG:HB3	9:I:104:ARG:HH11	1.83	0.42
9:I:114:TYR:CD1	9:I:114:TYR:N	2.87	0.42
10:J:30:SER:HB3	10:J:84:GLN:HE22	1.85	0.42
10:J:47:PHE:HD1	14:N:34:TYR:CD2	2.38	0.42
17:Q:53:LEU:HD11	17:Q:85:VAL:HG11	2.01	0.42
18:R:71:LYS:O	18:R:74:ARG:HB2	2.20	0.42
23:Y:31:A:N3	23:Y:31:A:C2'	2.70	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
1:A:1049:C:O2'	1:A:1050:A:H5'	2.19	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: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
2:B:86:GLU:C	2:B:88:ALA:N	2.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:101:LEU:O	3:C:101:LEU:CD2	2.67	0.42
5:E:131:ILE:HD13	5:E:131:ILE:HA	1.88	0.42
10:J:5:ARG:CG	10:J:73:ASP:OD1	2.58	0.42
10:J:40:LEU:N	10:J:69:ASN:O	2.51	0.42
11:K:11:LYS:HD2	11:K:11:LYS:HA	1.92	0.42
11:K:92:GLU:HB3	11:K:96:ARG:NH1	2.35	0.42
1:A:1049:C:C2'	1:A:1050:A:C5'	2.92	0.42
1:A:1112:C:O5'	1:A:1113:A:O5'	2.37	0.42
1:A:1146:C:C2	1:A:1156:G:N2	2.88	0.42
1:A:1382:C:C2	1:A:1384:G:C5	3.07	0.42
2:B:27:LYS:HG2	2:B:195:ASP:OD2	2.20	0.42
3:C:12:LEU:HD23	3:C:12:LEU:HA	1.73	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
8:H:109:ILE:HG22	8:H:137:VAL:O	2.20	0.42
1:A:94:C:H2'	1:A:95:A:O4'	2.19	0.42
1:A:405:G:H3'	1:A:406:G:H8	1.85	0.42
1:A:475:G:H2'	1:A:476:G:H8	1.85	0.42
1:A:673:C:H2'	1:A:674:G:O4'	2.20	0.42
1:A:1389:U:O2'	1:A:1390:C:H5'	2.20	0.42
1:A:1471:A:C8	22:X:5:G:H1'	2.55	0.42
2:B:42:ILE:O	2:B:42:ILE:HG13	2.19	0.42
4:D:54:TYR:O	4:D:55:ALA:C	2.63	0.42
9:I:85:LEU:HD12	9:I:92:TYR:CD2	2.55	0.42
10:J:8:LEU:HD11	10:J:20:ALA:CB	2.37	0.42
10:J:16:LEU:C	10:J:18:ALA:N	2.76	0.42
11:K:20:TYR:CE1	11:K:83:ILE:HD13	2.55	0.42
13:M:115:LYS:H	13:M:115:LYS:HD3	1.85	0.42
14:N:24:CYS:HB2	14:N:40:CYS:CA	2.50	0.42
20:T:10:LEU:HD12	20:T:12:ALA:H	1.83	0.42
1:A:331:C:O2'	1:A:332:C:H5'	2.20	0.41
1:A:425:U:O2'	4:D:22:LYS:HE2	2.20	0.41
1:A:544:U:H4'	1:A:545:U:H5''	2.02	0.41
1:A:586:A:C2	1:A:621:G:C2	3.08	0.41
1:A:597:C:H3'	1:A:597:C:C6	2.55	0.41
1:A:1040:G:C5	1:A:1186:A:C2	3.08	0.41
1:A:1043:C:C4	3:C:2:GLY:HA3	2.48	0.41
1:A:1269:A:H2'	1:A:1270:A:C8	2.55	0.41
2:B:216:SER:OG	2:B:217:ARG:N	2.53	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:122:LYS:O	11:K:123:LYS:C	2.63	0.41
12:L:126:LYS:CA	12:L:129:ALA:O	2.68	0.41
14:N:26:ARG:HH11	14:N:47:LEU:HD21	1.84	0.41
18:R:37:VAL:HG12	18:R:41:LYS:HE3	2.02	0.41
19:S:18:LYS:HB2	19:S:18:LYS:HE2	1.68	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
1:A:1281:A:C5'	1:A:1282:G:OP2	2.68	0.41
2:B:84:GLU:HA	2:B:87:ARG:HB3	2.01	0.41
4:D:8:VAL:CG1	4:D:21:LEU:CB	2.98	0.41
5:E:7:GLU:O	5:E:8:GLU:HB3	2.19	0.41
8:H:31:PHE:O	8:H:35:ILE:HG13	2.20	0.41
9:I:11:LYS:O	9:I:11:LYS:HG2	2.20	0.41
10:J:57:LYS:HE2	10:J:60:ARG:HH22	1.86	0.41
13:M:49:THR:HG21	13:M:51:ALA:HB3	2.01	0.41
14:N:44:LEU:C	14:N:44:LEU:CD2	2.93	0.41
17:Q:80:GLY:O	17:Q:82:MET:HG2	2.20	0.41
1:A:47:G:O2'	1:A:361:U:H1'	2.19	0.41
1:A:1023:U:O2	1:A:1023:U:H2'	2.20	0.41
1:A:1117:G:C2	1:A:1124:C:C4	3.08	0.41
1:A:1198:G:C2'	1:A:1199:C:H5'	2.50	0.41
1:A:1211:A:C2	1:A:1212:C:C4	3.08	0.41
1:A:1219:C:H4'	1:A:1316:G:N2	2.35	0.41
2:B:21:ARG:CB	2:B:39:ILE:HA	2.47	0.41
2:B:180:LEU:HD23	2:B:180:LEU:HA	1.87	0.41
2:B:208:ILE:HA	2:B:211:ILE:HD12	2.01	0.41
4:D:30:LYS:C	4:D:32:ALA:N	2.78	0.41
8:H:109:ILE:HD12	8:H:109:ILE:HG21	1.90	0.41
9:I:58:ARG:CZ	9:I:58:ARG:HB2	2.49	0.41
10:J:81:THR:O	10:J:83:GLU:N	2.53	0.41
12:L:50:SER:O	12:L:51:ALA:CB	2.68	0.41
16:P:74:LEU:C	16:P:79:VAL:HG23	2.44	0.41
17:Q:69:LYS:O	17:Q:70:ARG:HD2	2.21	0.41
1:A:171:C:H2'	1:A:172:C:C6	2.54	0.41
1:A:344:G:N3	1:A:344:G:C2'	2.83	0.41
1:A:714:G:C5	1:A:715:G:H1'	2.55	0.41
1:A:982:G:C2'	1:A:983:A:H4'	2.50	0.41
1:A:1035:U:O2'	1:A:1038:A:OP2	2.32	0.41
2:B:88:ALA:CB	2:B:219:VAL:HG13	2.50	0.41
2:B:163:PHE:HA	2:B:185:ILE:O	2.20	0.41
3:C:14:ILE:HG22	3:C:15:THR:H	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:203:VAL:O	4:D:204:ILE:C	2.64	0.41
9:I:54:ASP:C	9:I:56:LEU:N	2.78	0.41
10:J:25:GLU:C	10:J:27:ALA:H	2.29	0.41
11:K:62:GLN:O	11:K:63:LEU:C	2.63	0.41
12:L:47:LYS:HG3	12:L:48:PRO:HD3	2.02	0.41
17:Q:48:GLU:O	17:Q:50:LYS:N	2.53	0.41
18:R:74:ARG:HD3	18:R:81:PHE:CD2	2.55	0.41
1:A:83:U:O4'	1:A:83:U:OP1	2.38	0.41
1:A:193:G:C5'	1:A:193:G:C8	3.02	0.41
1:A:554:G:H2'	1:A:555:U:C6	2.55	0.41
1:A:765:A:C5	1:A:786:A:C2	3.09	0.41
1:A:1084:A:OP2	2:B:96:ARG:NH2	2.53	0.41
1:A:1107:G:H4'	10:J:38:ILE:HD13	2.02	0.41
1:A:1108:U:H5'	1:A:1109:U:C4	2.55	0.41
1:A:1168:G:H21	14:N:61:TRP:C	2.28	0.41
1:A:1315:A:H2'	1:A:1316:G:O4'	2.20	0.41
1:A:1351:G:N1	1:A:1352:C:C5	2.88	0.41
3:C:180:ALA:HB1	3:C:182:ILE:HG13	2.03	0.41
7:G:15:ASP:OD1	7:G:44:TYR:OH	2.35	0.41
7:G:56:GLN:H	7:G:56:GLN:HG2	1.64	0.41
7:G:155:ARG:H	7:G:155:ARG:HG3	1.69	0.41
9:I:114:TYR:HD2	10:J:60:ARG:HD2	1.86	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
14:N:24:CYS:SG	14:N:27:CYS:O	2.78	0.41
16:P:28:ARG:HG2	16:P:29:ASP:OD1	2.20	0.41
17:Q:99:SER:O	17:Q:100:LYS:HG3	2.21	0.41
18:R:58:LEU:HD12	18:R:58:LEU:N	2.36	0.41
19:S:29:ARG:C	19:S:31:ILE:N	2.74	0.41
1:A:1001:G:H3'	1:A:1002:G:H8	1.86	0.41
1:A:1022:C:C5	1:A:1023:U:C5	3.09	0.41
1:A:1160:G:N2	1:A:1162:A:H3'	2.35	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
3:C:11:ARG:HD3	3:C:178:LEU:O	2.20	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
1:A:353:G:H2'	1:A:354:U:H6	1.86	0.41
1:A:803:A:C8	1:A:803:A:C5'	3.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1125:G:H5''	1:A:1126:G:OP2	2.21	0.41
7:G:113:GLU:OE1	7:G:122:HIS:HD2	2.04	0.41
8:H:1:MET:O	8:H:2:LEU:CB	2.68	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:9:A:C5	4:D:209:ARG:HB3	2.56	0.41
1:A:389:A:O2'	1:A:390:G:H5'	2.21	0.41
1:A:535:U:H2'	1:A:536:U:C6	2.55	0.41
1:A:1259:C:H2'	1:A:1261:A:C8	2.54	0.41
1:A:1355:U:H2'	1:A:1356:G:C5'	2.50	0.41
1:A:1431:U:H2'	1:A:1433:C:C5	2.56	0.41
4:D:63:LYS:HD2	4:D:198:VAL:HG22	2.03	0.41
18:R:32:ARG:CA	18:R:69:THR:HG21	2.41	0.41
1:A:118:G:C6	1:A:119:U:C4	3.09	0.41
1:A:163:G:C2	1:A:164:C:C5	3.09	0.41
1:A:200:C:H2'	1:A:201:C:C6	2.56	0.41
1:A:258:A:H5'	20:T:74:LYS:HD3	2.01	0.41
1:A:328:G:H2'	1:A:329:G:O5'	2.20	0.41
1:A:394:C:O5'	1:A:394:C:H6	2.04	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
1:A:636:U:C2	1:A:736:G:N2	2.89	0.41
1:A:822:G:H8	1:A:822:G:O5'	2.04	0.41
1:A:900:G:N3	1:A:1381:A:H2	2.19	0.41
1:A:927:A:C2	1:A:1215:G:C4	3.08	0.41
1:A:951:G:O5'	1:A:951:G:H8	2.03	0.41
1:A:1031:G:OP1	14:N:4:LYS:HB2	2.21	0.41
1:A:1164:G:H4'	1:A:1165:A:H5''	2.02	0.41
1:A:1233:A:O2'	1:A:1352:C:O2'	2.39	0.41
1:A:1274:U:P	7:G:41:ARG:NH2	2.94	0.41
1:A:1337:G:O2'	1:A:1338:G:H5'	2.21	0.41
1:A:1349:C:C2	1:A:1350:C:C5	3.09	0.41
1:A:1487:C:H2'	1:A:1488:U:O4'	2.21	0.41
1:A:1518:U:C6	1:A:1518:U:H3'	2.56	0.41
3:C:134:ILE:CD1	3:C:153:VAL:HG23	2.51	0.41
4:D:173:TRP:HB2	4:D:187:ARG:HG3	2.03	0.41
5:E:36:ASP:OD2	5:E:40:ARG:HB2	2.21	0.41
5:E:68:GLU:O	5:E:68:GLU:CG	2.61	0.41
5:E:90:VAL:O	5:E:120:THR:HA	2.21	0.41
7:G:127:ALA:O	7:G:130:GLY:N	2.54	0.41
14:N:53:LEU:HA	14:N:54:PRO:HD3	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:74:LEU:HD23	16:P:74:LEU:HA	1.75	0.41
19:S:67:VAL:C	19:S:69:HIS:H	2.27	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
2:B:69:LEU:HD12	2:B:69:LEU:C	2.45	0.41
4:D:110:PHE:N	4:D:110:PHE:CD1	2.88	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
1:A:53:G:H2'	1:A:54:A:H5'	2.03	0.40
1:A:101:G:C2'	1:A:102:G:H5'	2.50	0.40
1:A:329:G:H4'	20:T:16:HIS:CE1	2.56	0.40
1:A:390:G:H2'	1:A:391:C:C6	2.56	0.40
1:A:1093:A:O5'	1:A:1093:A:H8	2.04	0.40
1:A:1348:G:C6	1:A:1349:C:C4	3.10	0.40
2:B:161:ALA:HB1	2:B:185:ILE:HD11	2.02	0.40
3:C:70:VAL:O	3:C:105:GLU:HA	2.21	0.40
3:C:157:ILE:HG21	3:C:164:ARG:NH2	2.36	0.40
5:E:80:ILE:HA	8:H:104:ARG:NH2	2.36	0.40
10:J:86:MET:HE3	10:J:87:THR:OG1	2.21	0.40
13:M:4:ILE:CD1	13:M:56:LEU:HD13	2.51	0.40
17:Q:58:GLU:C	17:Q:59:ILE:HD13	2.46	0.40
1:A:199:U:C4'	20:T:103:GLY:HA2	2.50	0.40
1:A:536:U:O2'	1:A:537:A:H5'	2.21	0.40
1:A:1263:U:O2	1:A:1263:U:O4'	2.39	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
7:G:17:VAL:O	7:G:17:VAL:HG12	2.21	0.40
9:I:37:PHE:HB3	9:I:43:ALA:HB2	2.02	0.40
1:A:168:U:H5''	1:A:204:A:O4'	2.22	0.40
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:984:A:H5'	1:A:984:A:N3	2.37	0.40
1:A:1077:G:O5'	1:A:1078:U:H5	2.04	0.40
1:A:1252:C:H4'	1:A:1295:U:O2'	2.21	0.40
1:A:1302:C:O2'	1:A:1303:C:H5'	2.21	0.40
1:A:1327:U:N3	1:A:1360:A:C2	2.90	0.40
1:A:1389:U:H2'	1:A:1390:C:H5'	2.04	0.40
4:D:33:MET:O	4:D:33:MET:HG3	2.21	0.40
8:H:112:LEU:C	8:H:112:LEU:CD1	2.87	0.40
11:K:13:GLN:HA	11:K:13:GLN:OE1	2.20	0.40
1:A:416:U:O2	1:A:420:G:N1	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:733:C:OP2	1:A:734:G:OP2	2.39	0.40
1:A:942:A:N3	1:A:947:A:O2'	2.50	0.40
1:A:1057:G:O2'	1:A:1084:A:N1	2.51	0.40
1:A:1107:G:O2'	1:A:1128:C:N4	2.50	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
5:E:36:ASP:OD1	5:E:36:ASP:C	2.65	0.40
11:K:85:ARG:NH1	11:K:111:ASP:OD2	2.55	0.40
19:S:22:LEU:CD1	19:S:26:GLY:HA3	2.48	0.40
1:A:772:U:H2'	1:A:773:U:O4'	2.22	0.40
1:A:1005:G:H1	1:A:1018:A:H61	1.70	0.40
1:A:1092:C:H6	1:A:1092:C:O5'	2.04	0.40
1:A:1314:A:C2	1:A:1315:A:C4	3.09	0.40
2:B:54:THR:HG23	2:B:199:TYR:HB3	2.03	0.40
10:J:99:LYS:HD3	10:J:99:LYS:HA	1.96	0.40
13:M:87:TYR:O	13:M:89:GLY:N	2.55	0.40
20:T:24:LEU:HD22	20:T:24:LEU:HA	1.86	0.40
20:T:53:LEU:HD22	20:T:102:GLY:HA3	2.03	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%)	0	4
3	C	204/206 (99%)	137 (67%)	44 (22%)	23 (11%)	0	2
4	D	206/208 (99%)	163 (79%)	25 (12%)	18 (9%)	0	4
5	E	148/150 (99%)	126 (85%)	17 (12%)	5 (3%)	3	16
6	F	99/101 (98%)	79 (80%)	15 (15%)	5 (5%)	1	10
7	G	153/155 (99%)	122 (80%)	22 (14%)	9 (6%)	1	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	H	136/138 (99%)	120 (88%)	13 (10%)	3 (2%)	5	24
9	I	125/127 (98%)	86 (69%)	25 (20%)	14 (11%)	0	2
10	J	96/98 (98%)	69 (72%)	20 (21%)	7 (7%)	1	5
11	K	117/119 (98%)	101 (86%)	10 (8%)	6 (5%)	1	10
12	L	123/125 (98%)	93 (76%)	21 (17%)	9 (7%)	1	5
13	M	118/120 (98%)	83 (70%)	21 (18%)	14 (12%)	0	1
14	N	58/60 (97%)	37 (64%)	12 (21%)	9 (16%)	0	0
15	O	86/88 (98%)	75 (87%)	9 (10%)	2 (2%)	5	23
16	P	81/83 (98%)	73 (90%)	8 (10%)	0	100	100
17	Q	97/99 (98%)	81 (84%)	14 (14%)	2 (2%)	5	25
18	R	68/70 (97%)	62 (91%)	5 (7%)	1 (2%)	8	32
19	S	76/78 (97%)	54 (71%)	12 (16%)	10 (13%)	0	1
20	T	97/99 (98%)	74 (76%)	15 (16%)	8 (8%)	0	4
21	U	22/24 (92%)	17 (77%)	5 (23%)	0	100	100
All	All	2342/2382 (98%)	1820 (78%)	357 (15%)	165 (7%)	1	5

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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%)	142 (70%)	60 (30%)	0	1
3	C	160/160 (100%)	117 (73%)	43 (27%)	0	2
4	D	180/180 (100%)	142 (79%)	38 (21%)	1	5
5	E	115/115 (100%)	88 (76%)	27 (24%)	1	3
6	F	90/90 (100%)	72 (80%)	18 (20%)	1	6
7	G	126/126 (100%)	101 (80%)	25 (20%)	1	6
8	H	119/119 (100%)	98 (82%)	21 (18%)	2	9
9	I	98/98 (100%)	71 (72%)	27 (28%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	J	88/88 (100%)	60 (68%)	28 (32%)	0	0
11	K	90/90 (100%)	72 (80%)	18 (20%)	1	6
12	L	104/104 (100%)	83 (80%)	21 (20%)	1	5
13	M	96/96 (100%)	59 (62%)	37 (38%)	0	0
14	N	49/49 (100%)	35 (71%)	14 (29%)	0	1
15	O	79/79 (100%)	60 (76%)	19 (24%)	1	3
16	P	72/72 (100%)	53 (74%)	19 (26%)	0	2
17	Q	94/94 (100%)	76 (81%)	18 (19%)	1	7
18	R	61/61 (100%)	48 (79%)	13 (21%)	1	5
19	S	69/69 (100%)	53 (77%)	16 (23%)	1	4
20	T	76/76 (100%)	61 (80%)	15 (20%)	1	6
21	U	19/19 (100%)	13 (68%)	6 (32%)	0	0
All	All	1987/1987 (100%)	1504 (76%)	483 (24%)	1	3

All (483) 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	23	ARG
2	B	27	LYS
2	B	39	ILE
2	B	42	ILE
2	B	48	MET
2	B	60	ASP
2	B	67	THR
2	B	69	LEU
2	B	75	LYS
2	B	76	GLN
2	B	80	ILE
2	B	86	GLU
2	B	90	MET
2	B	96	ARG
2	B	97	TRP

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Mol	Chain	Res	Type
2	B	98	LEU
2	B	102	LEU
2	B	107	THR
2	B	108	ILE
2	B	111	ARG
2	B	112	VAL
2	B	113	HIS
2	B	115	LEU
2	B	119	GLU
2	B	121	LEU
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	165	VAL
2	B	169	LYS
2	B	170	GLU
2	B	172	ILE
2	B	175	ARG
2	B	185	ILE
2	B	187	LEU
2	B	196	LEU
2	B	208	ILE
2	B	209	ARG
2	B	210	SER
2	B	221	LEU
2	B	223	ILE
2	B	229	VAL
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

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Mol	Chain	Res	Type
3	C	16	ARG
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	39	ILE
3	C	40	ARG
3	C	47	LEU
3	C	52	LEU
3	C	54	ARG
3	C	58	GLU
3	C	72	LYS
3	C	82	GLU
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	103	VAL
3	C	107	GLN
3	C	111	LEU
3	C	128	PHE
3	C	144	SER
3	C	156	ARG
3	C	164	ARG
3	C	165	THR
3	C	166	GLU
3	C	172	ARG
3	C	175	LEU
3	C	178	LEU
3	C	188	LEU
3	C	191	THR
3	C	192	THR
3	C	196	LEU
3	C	198	VAL
3	C	202	ILE
3	C	204	LEU
4	D	3	ARG
4	D	9	CYS

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Mol	Chain	Res	Type
4	D	11	LEU
4	D	17	VAL
4	D	19	LEU
4	D	21	LEU
4	D	30	LYS
4	D	33	MET
4	D	34	GLU
4	D	46	LYS
4	D	47	ARG
4	D	49	ARG
4	D	50	ARG
4	D	58	LEU
4	D	59	ARG
4	D	61	LYS
4	D	68	TYR
4	D	70	ILE
4	D	84	LYS
4	D	106	TYR
4	D	108	LEU
4	D	127	THR
4	D	135	LEU
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	198	VAL
4	D	209	ARG
5	E	10	MET
5	E	11	ILE
5	E	12	LEU
5	E	18	ARG
5	E	25	ARG
5	E	27	ARG

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Mol	Chain	Res	Type
5	E	31	LEU
5	E	33	VAL
5	E	41	VAL
5	E	52	PRO
5	E	64	ARG
5	E	68	GLU
5	E	73	ASN
5	E	80	ILE
5	E	82	VAL
5	E	83	GLU
5	E	89	ILE
5	E	90	VAL
5	E	91	LEU
5	E	92	LYS
5	E	101	ILE
5	E	125	SER
5	E	129	ILE
5	E	143	ARG
5	E	145	LYS
5	E	147	ASP
5	E	153	LYS
6	F	17	SER
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	91	VAL
6	F	92	LYS
6	F	98	LEU
7	G	8	GLU
7	G	13	GLN
7	G	27	ILE

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Mol	Chain	Res	Type
7	G	32	ARG
7	G	33	ASP
7	G	38	LEU
7	G	48	LYS
7	G	50	ILE
7	G	61	VAL
7	G	64	GLN
7	G	69	VAL
7	G	77	SER
7	G	79	ARG
7	G	94	ARG
7	G	99	LEU
7	G	104	LEU
7	G	114	ARG
7	G	124	LEU
7	G	131	LYS
7	G	135	VAL
7	G	136	LYS
7	G	141	VAL
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	26	VAL
8	H	38	ILE
8	H	39	LEU
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

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Mol	Chain	Res	Type
8	H	133	LEU
9	I	10	ARG
9	I	14	VAL
9	I	20	ARG
9	I	31	GLN
9	I	34	ASN
9	I	40	LEU
9	I	41	VAL
9	I	47	LEU
9	I	51	ARG
9	I	54	ASP
9	I	58	ARG
9	I	64	THR
9	I	65	VAL
9	I	66	ARG
9	I	70	LYS
9	I	79	LEU
9	I	85	LEU
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	118	LYS
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	23	ILE
10	J	33	GLN
10	J	38	ILE
10	J	45	ARG
10	J	49	VAL
10	J	50	ILE
10	J	55	LYS
10	J	57	LYS
10	J	59	SER
10	J	60	ARG

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Mol	Chain	Res	Type
10	J	70	ARG
10	J	74	ILE
10	J	76	ASN
10	J	79	ARG
10	J	80	LYS
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	48	ILE
11	K	53	SER
11	K	54	ARG
11	K	70	LYS
11	K	77	MET
11	K	80	VAL
11	K	84	VAL
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	7	ILE
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	58	VAL
12	L	60	LEU

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Mol	Chain	Res	Type
12	L	67	THR
12	L	73	GLU
12	L	78	GLN
12	L	79	GLU
12	L	81	SER
12	L	85	ILE
12	L	96	VAL
12	L	100	ILE
12	L	111	LYS
12	L	113	ARG
12	L	114	LYS
13	M	4	ILE
13	M	7	VAL
13	M	8	GLU
13	M	15	VAL
13	M	19	LEU
13	M	20	THR
13	M	25	ILE
13	M	31	LYS
13	M	34	LEU
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
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

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Mol	Chain	Res	Type
13	M	108	ARG
13	M	110	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	29	ARG
14	N	33	VAL
14	N	35	ARG
14	N	42	ILE
14	N	53	LEU
15	O	3	ILE
15	O	4	THR
15	O	5	LYS
15	O	6	GLU
15	O	8	LYS
15	O	13	GLN
15	O	17	ARG
15	O	26	GLU
15	O	28	GLN
15	O	31	LEU
15	O	32	LEU
15	O	39	LEU
15	O	40	SER
15	O	44	LYS
15	O	45	VAL
15	O	65	ARG
15	O	66	LEU
15	O	67	LEU
15	O	82	ILE
16	P	1	MET
16	P	2	VAL
16	P	5	ARG

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Mol	Chain	Res	Type
16	P	8	ARG
16	P	12	LYS
16	P	20	VAL
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	53	VAL
16	P	54	GLU
16	P	65	GLN
16	P	69	THR
16	P	71	ARG
16	P	74	LEU
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	50	LYS
17	Q	52	LYS
17	Q	53	LEU
17	Q	59	ILE
17	Q	65	ILE
17	Q	77	VAL
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	28	GLU
18	R	32	ARG
18	R	46	GLU
18	R	47	THR
18	R	65	ILE
18	R	70	ILE

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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	11	VAL
19	S	22	LEU
19	S	31	ILE
19	S	37	ARG
19	S	41	VAL
19	S	51	VAL
19	S	58	VAL
19	S	62	ILE
19	S	67	VAL
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	100	ILE
20	T	104	LEU
21	U	8	THR
21	U	10	ARG
21	U	12	LYS
21	U	15	ARG
21	U	24	ARG
21	U	25	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	76	GLN
2	B	94	ASN
2	B	95	GLN
2	B	135	GLN
3	C	63	ASN
3	C	110	ASN
4	D	161	ASN
5	E	127	ASN
5	E	130	ASN
6	F	7	ASN
6	F	64	GLN
6	F	73	ASN
6	F	84	ASN
6	F	94	GLN
7	G	84	ASN
7	G	86	GLN
7	G	122	HIS
9	I	31	GLN
9	I	73	GLN
10	J	33	GLN
11	K	62	GLN
11	K	117	ASN
12	L	80	HIS
13	M	62	ASN
15	O	37	ASN
16	P	16	HIS
17	Q	93	GLN
20	T	16	HIS
20	T	90	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1515/1516 (99%)	434 (28%)	87 (5%)
22	X	5/6 (83%)	5 (100%)	0
23	Y	9/10 (90%)	2 (22%)	0
All	All	1529/1532 (99%)	441 (28%)	87 (5%)

All (441) 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
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

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Mol	Chain	Res	Type
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
1	A	222	G
1	A	227	G
1	A	239	A
1	A	240	U
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
1	A	555	U
1	A	556	A
1	A	557	A
1	A	560	G
1	A	566	U
1	A	571	G
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	686	A
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	732	C

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Mol	Chain	Res	Type
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
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	891	A
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
1	A	1033	G
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	1068	U
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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	1268	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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
1	A	1482	G
1	A	1483	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	1509	A
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 ⓘ

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	18,18,22	2.04	8 (44%)	22,26,33	3.31	13 (59%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	PSU	X	4	22,23	18,21,22	1.51	3 (16%)	21,30,33	2.14	4 (19%)

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

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	X	1	PSU	C6-C5	4.54	1.40	1.35
22	X	4	PSU	C6-C5	4.18	1.39	1.35
22	X	1	PSU	C4-C5	2.97	1.52	1.44
22	X	1	PSU	C2-N1	2.94	1.40	1.36
22	X	1	PSU	C2'-C1'	-2.42	1.50	1.53
22	X	4	PSU	C4-N3	-2.33	1.34	1.38
22	X	1	PSU	C4-N3	-2.30	1.34	1.38
22	X	4	PSU	C2'-C1'	-2.13	1.50	1.53
22	X	1	PSU	O2-C2	2.07	1.27	1.23
22	X	1	PSU	C5'-C4'	2.05	1.58	1.51
22	X	1	PSU	O3'-C3'	2.05	1.48	1.43

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	X	4	PSU	N1-C2-N3	6.76	122.30	115.17
22	X	1	PSU	N1-C2-N3	6.11	121.61	115.17
22	X	1	PSU	C4-N3-C2	-5.91	118.22	126.37
22	X	1	PSU	O3'-C3'-C4'	5.77	127.66	111.08
22	X	1	PSU	O5'-C5'-C4'	4.84	127.81	111.33
22	X	1	PSU	O2-C2-N3	-4.65	113.60	121.86
22	X	1	PSU	O4'-C4'-C3'	-3.96	97.29	105.15
22	X	1	PSU	C5-C6-N1	-3.87	116.77	122.14
22	X	1	PSU	C3'-C2'-C1'	3.82	106.19	101.69
22	X	4	PSU	C4-N3-C2	-3.71	121.26	126.37
22	X	4	PSU	O2-C2-N1	-3.51	119.17	122.79
22	X	1	PSU	C4'-O4'-C1'	2.63	115.03	108.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	X	1	PSU	O4-C4-N3	-2.56	115.30	120.11
22	X	4	PSU	C6-N1-C2	-2.49	120.38	122.69
22	X	1	PSU	C5'-C4'-C3'	2.43	120.84	115.10
22	X	1	PSU	C5-C4-N3	2.34	121.69	116.55
22	X	1	PSU	O3'-C3'-C2'	-2.31	104.41	111.82

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	X	1	PSU	C3'-C4'-C5'-O5'
22	X	1	PSU	O4'-C4'-C5'-O5'
22	X	4	PSU	C3'-C4'-C5'-O5'
22	X	4	PSU	O4'-C4'-C5'-O5'

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	-	44,45,45	1.30	6 (13%)	63,67,67	2.00	17 (26%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	PAR	A	1614	-	-	3/18/94/94	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	-4.00	1.48	1.53
25	A	1614	PAR	C13-C23	-3.28	1.48	1.52
25	A	1614	PAR	C33-C43	-2.57	1.46	1.52
25	A	1614	PAR	C31-C21	-2.52	1.50	1.53
25	A	1614	PAR	C62-C12	-2.39	1.48	1.53
25	A	1614	PAR	O41-C41	-2.05	1.37	1.43

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	1614	PAR	O54-C54-C64	-9.02	88.74	106.07
25	A	1614	PAR	C44-C34-C24	-3.66	104.92	110.99
25	A	1614	PAR	O53-C53-C43	-3.30	100.08	111.33
25	A	1614	PAR	C11-O51-C51	-3.27	107.34	113.72
25	A	1614	PAR	C14-O54-C54	3.14	119.86	113.72
25	A	1614	PAR	O44-C44-C34	-2.87	103.61	110.38
25	A	1614	PAR	O41-C41-C31	-2.79	103.81	110.38
25	A	1614	PAR	C14-C24-C34	-2.76	103.38	110.29
25	A	1614	PAR	O23-C23-C13	-2.65	104.36	111.82
25	A	1614	PAR	O41-C41-C51	-2.58	102.98	109.32
25	A	1614	PAR	O43-C13-C23	-2.57	101.72	104.98
25	A	1614	PAR	O51-C51-C61	2.56	112.78	106.44
25	A	1614	PAR	O11-C42-C32	-2.34	103.58	109.18
25	A	1614	PAR	O33-C14-O54	-2.20	104.90	110.69
25	A	1614	PAR	O33-C14-C24	-2.13	104.59	108.08
25	A	1614	PAR	C31-C21-N21	-2.06	106.82	111.05
25	A	1614	PAR	C22-C12-C62	-2.06	107.00	110.08

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	A	1614	PAR	C41-C51-C61-O61

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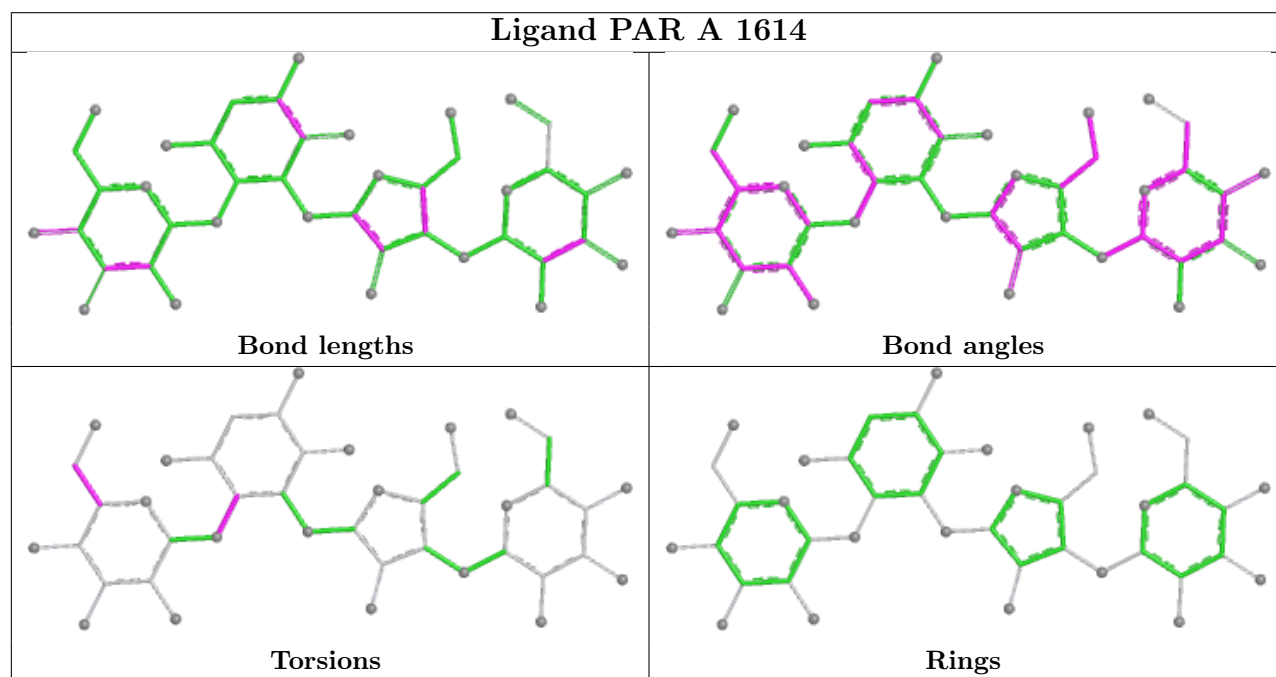
Mol	Chain	Res	Type	Atoms
25	A	1614	PAR	O51-C51-C61-O61
25	A	1614	PAR	C52-C42-O11-C11

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

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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%)	-0.67	16 (1%) 78 59	42, 72, 141, 239	0
2	B	234/234 (100%)	0.20	8 (3%) 48 28	58, 105, 160, 191	0
3	C	206/206 (100%)	-0.03	2 (0%) 79 61	62, 92, 140, 162	0
4	D	208/208 (100%)	-0.13	8 (3%) 44 25	50, 80, 120, 145	0
5	E	150/150 (100%)	-0.52	2 (1%) 75 56	46, 66, 94, 137	0
6	F	101/101 (100%)	-0.30	2 (1%) 65 44	66, 98, 125, 150	0
7	G	155/155 (100%)	-0.17	5 (3%) 50 30	63, 89, 145, 165	0
8	H	138/138 (100%)	-0.57	0 100 100	41, 64, 91, 123	0
9	I	127/127 (100%)	0.24	4 (3%) 51 30	52, 104, 135, 154	0
10	J	98/98 (100%)	0.78	10 (10%) 12 6	57, 126, 180, 221	0
11	K	119/119 (100%)	-0.15	4 (3%) 48 28	44, 76, 113, 168	0
12	L	125/125 (100%)	0.03	8 (6%) 25 14	39, 73, 116, 168	0
13	M	120/120 (100%)	0.11	7 (5%) 29 16	62, 90, 130, 159	0
14	N	60/60 (100%)	0.52	5 (8%) 17 9	69, 91, 114, 127	0
15	O	88/88 (100%)	-0.33	0 100 100	51, 79, 116, 161	0
16	P	83/83 (100%)	-0.36	0 100 100	50, 65, 94, 126	0
17	Q	99/99 (100%)	-0.46	0 100 100	42, 67, 102, 126	0
18	R	70/70 (100%)	-0.38	0 100 100	62, 85, 116, 132	0
19	S	78/78 (100%)	0.22	3 (3%) 44 25	67, 107, 161, 176	0
20	T	99/99 (100%)	-0.02	2 (2%) 65 44	45, 70, 113, 128	0
21	U	24/24 (100%)	0.69	2 (8%) 17 9	59, 79, 106, 136	0
22	X	4/6 (66%)	0.16	0 100 100	66, 67, 83, 93	0
23	Y	10/10 (100%)	0.22	1 (10%) 12 6	76, 96, 145, 188	0
All	All	3912/3914 (99%)	-0.30	89 (2%) 61 39	39, 79, 141, 239	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
21	U	25	LYS	10.7
11	K	128	ALA	8.1
11	K	129	SER	8.0
1	A	1232	A	5.6
12	L	129	ALA	5.6
19	S	81	ARG	5.1
20	T	12	ALA	5.0
7	G	5	ARG	4.2
4	D	26	CYS	3.8
11	K	111	ASP	3.8
1	A	1233	A	3.7
19	S	30	LEU	3.6
2	B	140	HIS	3.6
1	A	707	U	3.6
4	D	9	CYS	3.6
3	C	207	VAL	3.5
2	B	238	LEU	3.3
12	L	28	LYS	3.2
23	Y	40	U	3.2
2	B	96	ARG	3.2
13	M	11	ARG	3.2
10	J	3	LYS	3.1
14	N	2	ALA	3.1
12	L	19	ARG	3.1
20	T	8	ARG	3.0
12	L	128	ALA	3.0
13	M	7	VAL	3.0
19	S	10	PHE	2.9
13	M	8	GLU	2.9
10	J	5	ARG	2.8
10	J	17	ASP	2.8
9	I	39	GLY	2.8
5	E	154	GLY	2.7
1	A	1512	A	2.7
14	N	3	ARG	2.7
13	M	113	PRO	2.7
7	G	81	GLY	2.7
12	L	112	ASP	2.7
4	D	23	GLY	2.6
4	D	31	CYS	2.6
2	B	7	VAL	2.6
1	A	82	U	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	1178	U	2.6
5	E	119	LEU	2.6
7	G	106	GLN	2.5
1	A	81	U	2.5
2	B	230	VAL	2.5
7	G	8	GLU	2.5
2	B	136	VAL	2.5
14	N	33	VAL	2.5
1	A	1234	A	2.4
10	J	77	PRO	2.4
4	D	209	ARG	2.4
1	A	1013	A	2.4
4	D	12	CYS	2.4
13	M	112	GLY	2.3
14	N	28	GLY	2.3
6	F	101	ALA	2.3
9	I	15	ALA	2.3
3	C	167	TRP	2.3
14	N	57	ARG	2.3
13	M	84	ILE	2.3
12	L	111	LYS	2.3
11	K	12	ARG	2.3
10	J	21	GLN	2.2
10	J	59	SER	2.2
2	B	229	VAL	2.2
10	J	6	ILE	2.2
1	A	836	G	2.2
1	A	1230	A	2.2
1	A	1272	G	2.2
10	J	64	GLU	2.2
12	L	47	LYS	2.2
9	I	101	PHE	2.2
1	A	1109	U	2.2
1	A	1012	G	2.2
12	L	26	ALA	2.1
21	U	24	ARG	2.1
2	B	148	TYR	2.1
10	J	37	PRO	2.1
6	F	88	VAL	2.1
13	M	9	ILE	2.1
10	J	100	THR	2.1
4	D	22	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
4	D	5	ILE	2.1
1	A	1231	C	2.1
1	A	1353	G	2.1
9	I	110	GLU	2.1
7	G	156	TRP	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
22	PSU	X	1	17/21	0.87	0.14	29,58,70,82	0
22	PSU	X	4	20/21	0.95	0.07	58,67,81,83	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

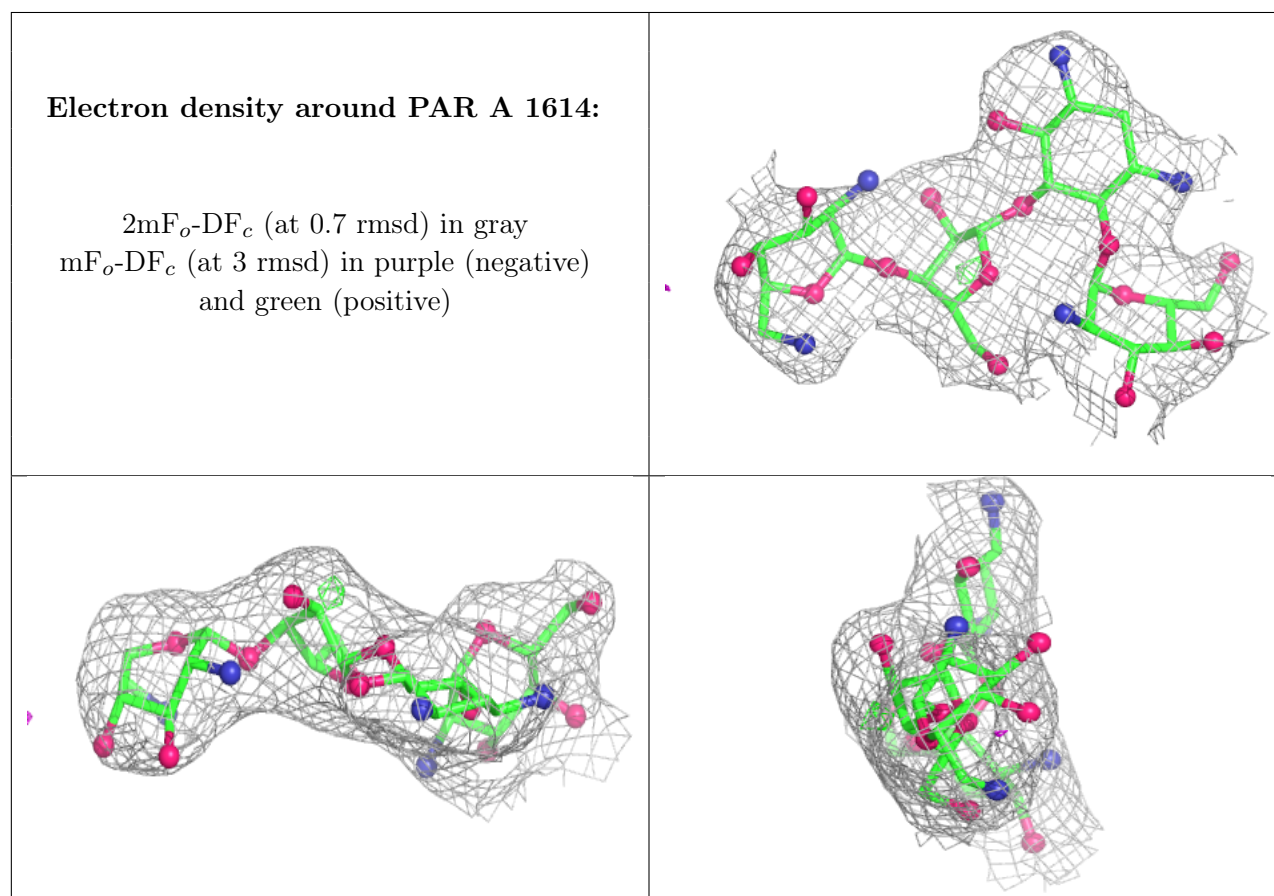
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
24	MG	X	101	1/1	0.85	0.29	55,55,55,55	0
24	MG	A	1603	1/1	0.91	0.25	60,60,60,60	0
24	MG	A	1602	1/1	0.92	0.20	48,48,48,48	0
24	MG	A	1608	1/1	0.94	0.47	52,52,52,52	0
24	MG	A	1604	1/1	0.95	0.26	57,57,57,57	0
24	MG	A	1609	1/1	0.95	0.23	47,47,47,47	0
24	MG	A	1610	1/1	0.95	0.27	43,43,43,43	0
24	MG	A	1612	1/1	0.95	0.28	44,44,44,44	0
24	MG	A	1607	1/1	0.95	0.35	46,46,46,46	0
24	MG	A	1611	1/1	0.96	0.37	51,51,51,51	0
25	PAR	A	1614	42/42	0.96	0.08	49,60,88,106	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	MG	A	1613	1/1	0.97	0.13	41,41,41,41	0
24	MG	A	1605	1/1	0.98	0.14	42,42,42,42	0
24	MG	A	1601	1/1	0.98	0.05	49,49,49,49	0
24	MG	A	1606	1/1	0.99	0.05	52,52,52,52	0

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



6.5 Other polymers ⓘ

There are no such residues in this entry.