



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:04 AM UTC

PDB ID : 3T1H / pdb_00003t1h
Title : Structure of the *Thermus thermophilus* 30S ribosomal subunit complexed with a human anti-codon stem loop (HASL) of transfer RNA lysine 3 (tRNA^{Lys}3) bound to an mRNA with an AAA-codon in the A-site and Paromomycin
Authors : Murphy, F.V.; Vendeix, F.A.P.; Cantara, W.; Leszczynska, G.; Gustilo, E.M.; Sproat, B.; Malkiewicz, A.A.P.; Agris, P.F.
Deposited on : 2011-07-21
Resolution : 3.11 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](#) ①) were used in the production of this report:

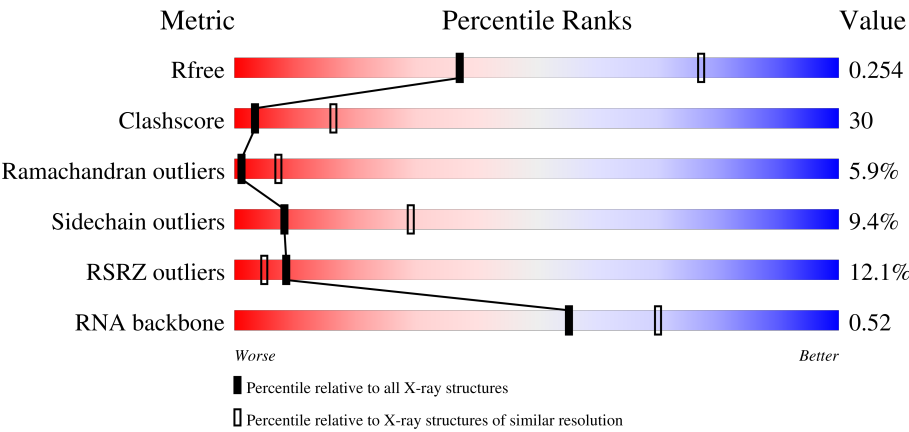
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 3.11 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	1816 (3.14-3.10)
Clashscore	190562	1906 (3.14-3.10)
Ramachandran outliers	187476	1802 (3.14-3.10)
Sidechain outliers	187428	1802 (3.14-3.10)
RSRZ outliers	180081	1816 (3.14-3.10)
RNA backbone	3983	1017 (3.34-2.90)

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	1513	11% 37%38%15%9%
2	B	256	21% 27%52%12%9%
3	C	239	13% 34%39%12%14%
4	D	209	14% 45%47%6%

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Mol	Chain	Length	Quality of chain
5	E	162	
6	F	101	
7	G	156	
8	H	138	
9	I	128	
10	J	105	
11	K	129	
12	L	132	
13	M	126	
14	N	61	
15	O	89	
16	P	88	
17	Q	105	
18	R	88	
19	S	93	
20	T	106	
21	V	27	
22	W	3	
23	X	11	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	12A	X	37	-	-	X	-
23	PSU	X	39	-	-	X	-
24	MG	A	1604	-	-	-	X
24	MG	A	1614	-	-	-	X
24	MG	A	1617	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	MG	A	1621	-	-	-	X
24	MG	A	1625	-	-	-	X
24	MG	A	1635	-	-	-	X
24	MG	A	1638	-	-	-	X
24	MG	A	1644	-	-	-	X
24	MG	A	1646	-	-	-	X
24	MG	A	1652	-	-	-	X
24	MG	A	1666	-	-	-	X
24	MG	A	1678	-	-	-	X
24	MG	A	1683	-	-	-	X
24	MG	A	1693	-	-	-	X
24	MG	A	1694	-	-	-	X
24	MG	A	1695	-	-	-	X
24	MG	A	1699	-	-	-	X
24	MG	A	1700	-	-	-	X
24	MG	A	1701	-	-	-	X
24	MG	A	1703	-	-	-	X
24	MG	A	1704	-	-	-	X
24	MG	A	1706	-	-	-	X
24	MG	A	1707	-	-	-	X
24	MG	A	1713	-	-	-	X
24	MG	A	1718	-	-	-	X
24	MG	A	1721	-	-	-	X
24	MG	A	1722	-	-	-	X
24	MG	A	1725	-	-	-	X
24	MG	A	1729	-	-	-	X
24	MG	A	1739	-	-	-	X
24	MG	A	1743	-	-	-	X
24	MG	A	1754	-	-	-	X
24	MG	A	1756	-	-	-	X
24	MG	A	1766	-	-	-	X
24	MG	A	1774	-	-	-	X
24	MG	L	201	-	-	-	X
24	MG	S	101	-	-	-	X

2 Entry composition

There are 26 unique types of molecules in this entry. The entry contains 52287 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 16s rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1513	Total	C	N	O	P	22	0	0
			32515	14472	6016	10514	1513			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1517	U	-	insertion	GB 55771382
A	1518	U	-	insertion	GB 55771382
A	1519	U	-	insertion	GB 55771382
A	1520	C	-	insertion	GB 55771382
A	1521	U	-	insertion	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			

- 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
			792	498	156	137	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	124	Total	C	N	O	S	0	0	0
			970	611	195	163	1			

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

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

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

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	104	Total	C	N	O	S	0	0	0
			857	547	161	147	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	R	73	Total	C	N	O	0	0	0
			597	380	118	99			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	T	99	Total	C	N	O	S	0	0	0
			762	469	162	129	2			

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

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

- Molecule 22 is a RNA chain called mRNA A-site fragment.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	W	3	Total	C	N	O	P	0	0	0
			67	30	15	19	3			

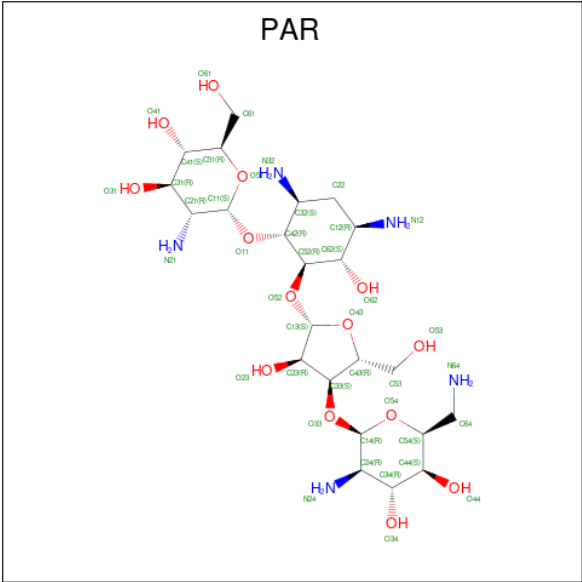
- Molecule 23 is a RNA chain called tRNA ASL human Lys3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
23	X	11	Total	C	N	O	P	S	0	0	0
			247	112	37	85	11	2			

- Molecule 24 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	A	182	Total	Mg	0	0
			182	182		
24	B	1	Total	Mg	0	0
			1	1		
24	L	1	Total	Mg	0	0
			1	1		
24	S	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		

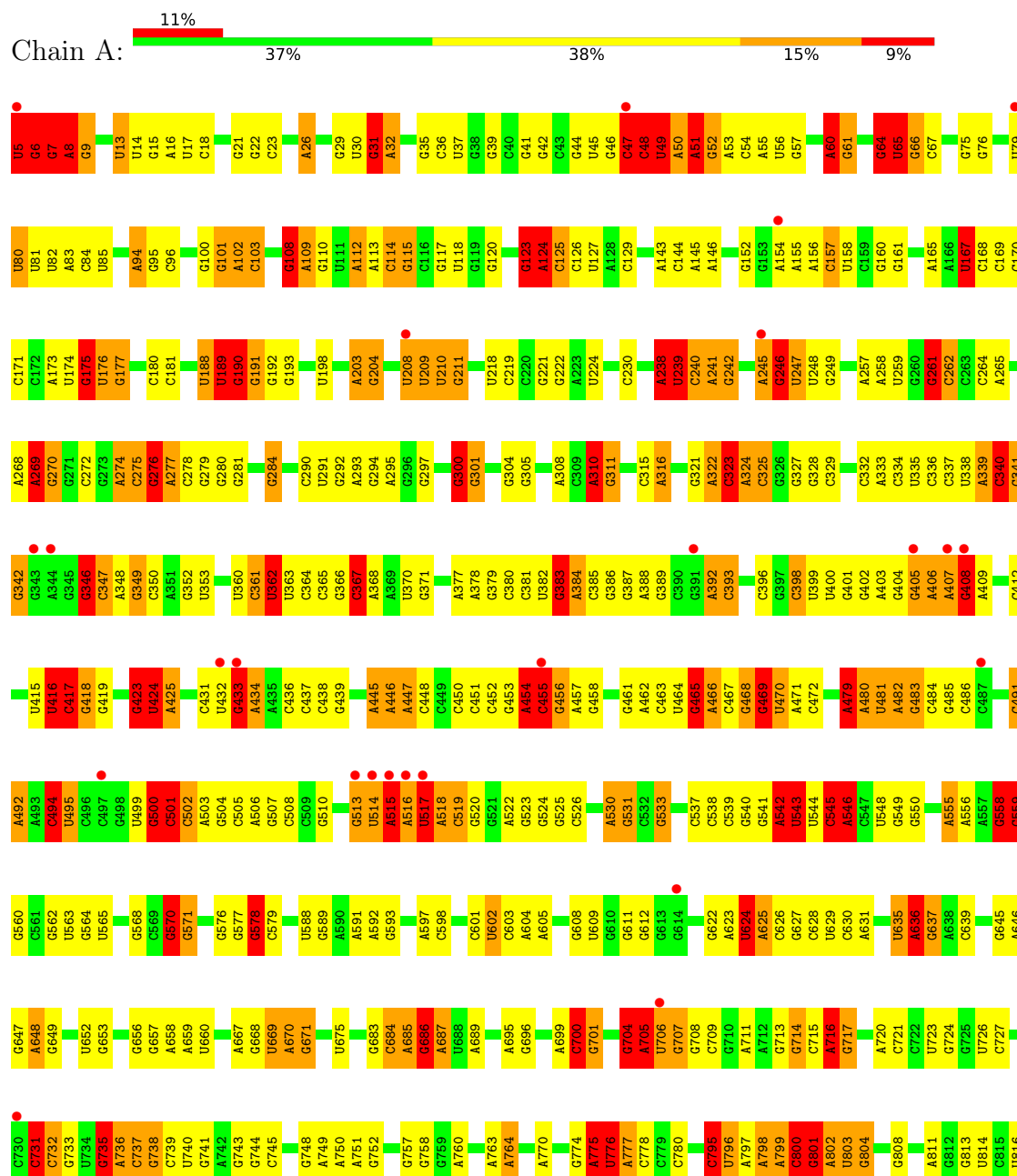
- Molecule 26 is ZINC ION (CCD ID: ZN) (formula: Zn).

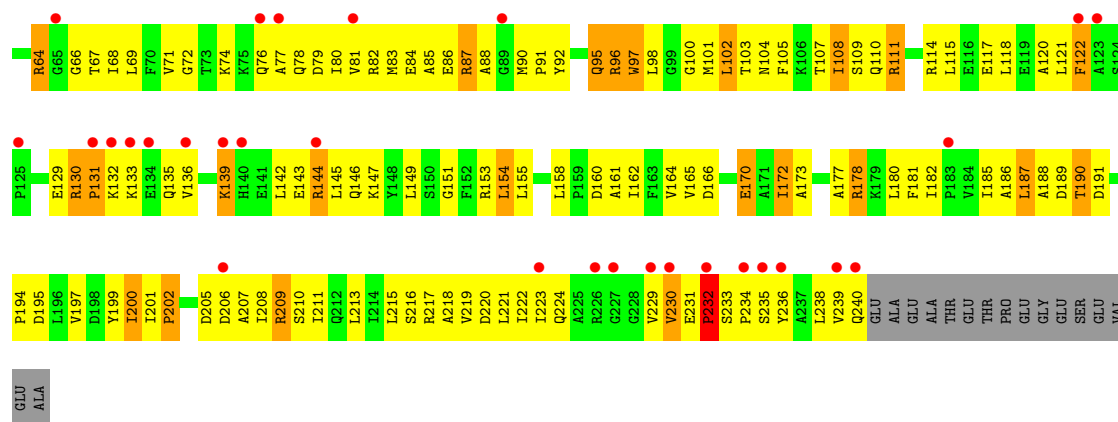
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
26	D	1	Total	Zn	0	0
			1	1		
26	N	1	Total	Zn	0	0
			1	1		

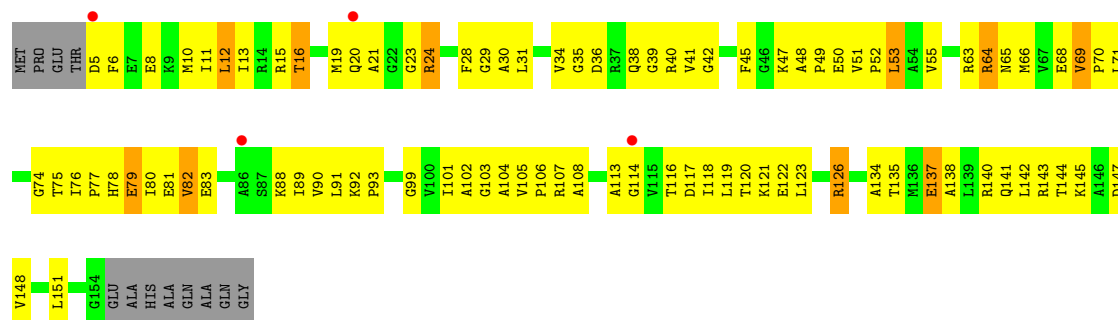
3 Residue-property plots [i](#)

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

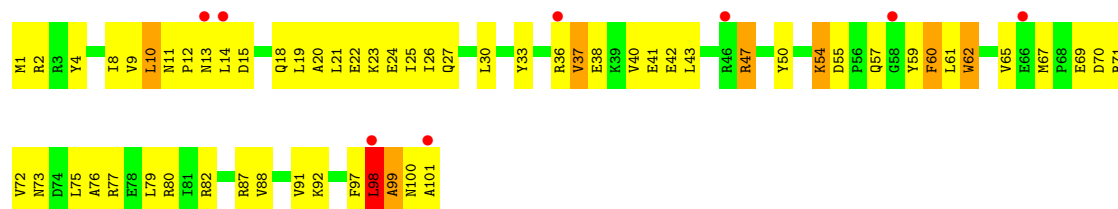
• Molecule 1: 16s rRNA



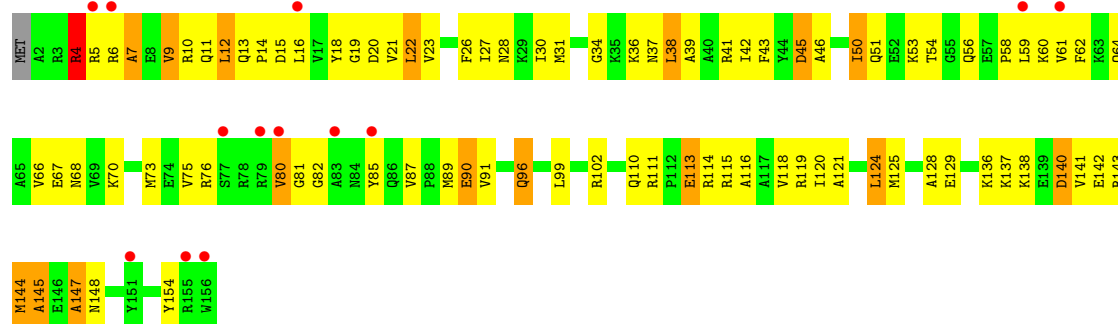




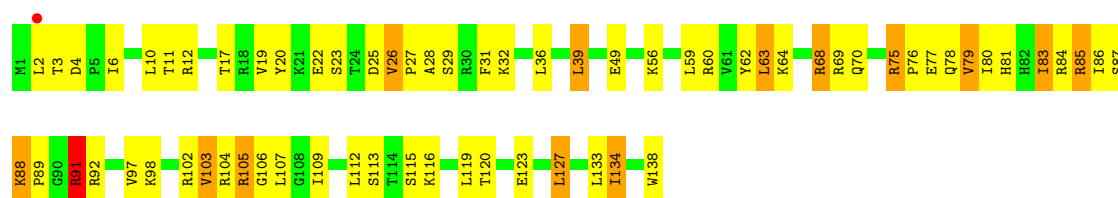
• Molecule 6: 30S ribosomal protein S6



• Molecule 7: 30S ribosomal protein S7

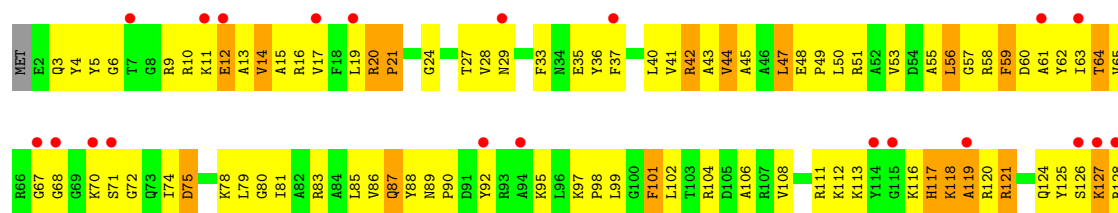


• Molecule 8: 30S ribosomal protein S8

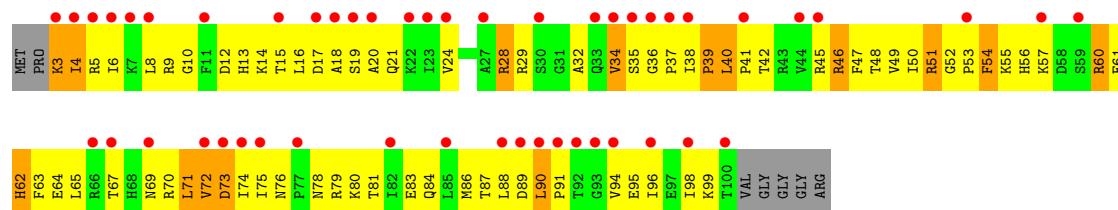


• Molecule 9: 30S ribosomal protein S9

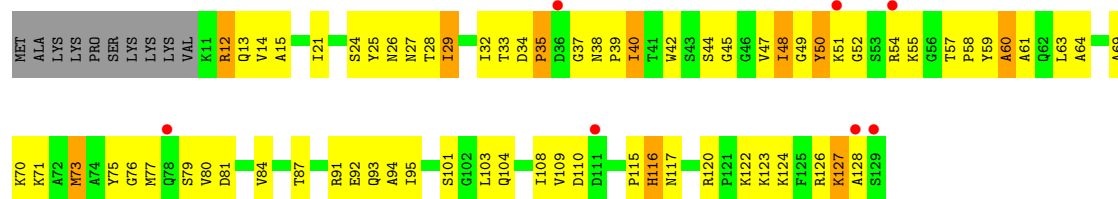




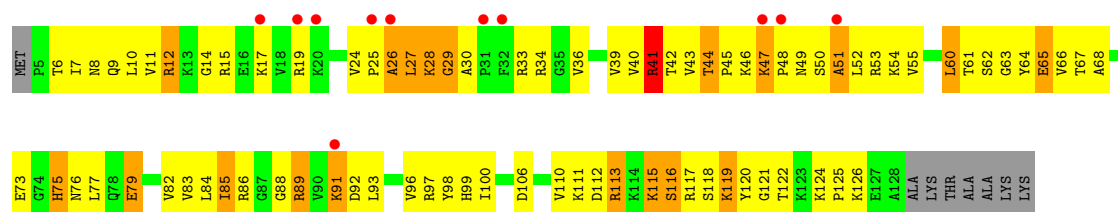
• Molecule 10: 30S ribosomal protein S10



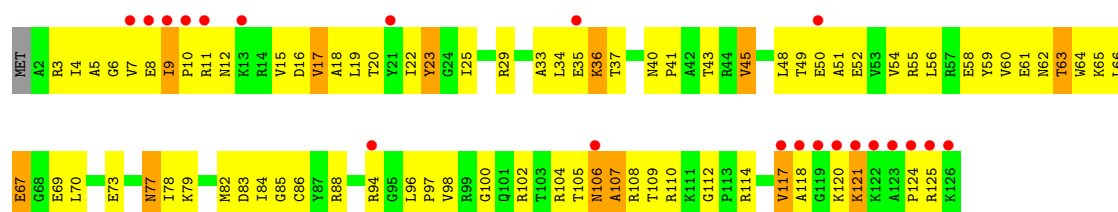
• Molecule 11: 30S ribosomal protein S11



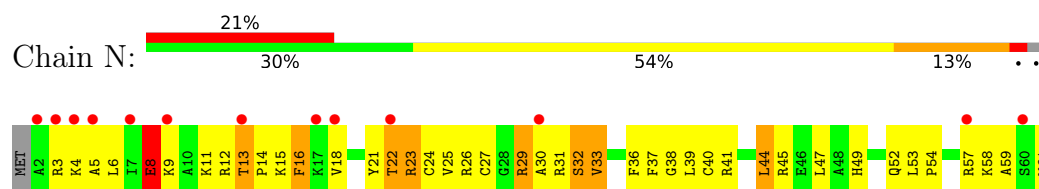
• Molecule 12: 30S ribosomal protein S12



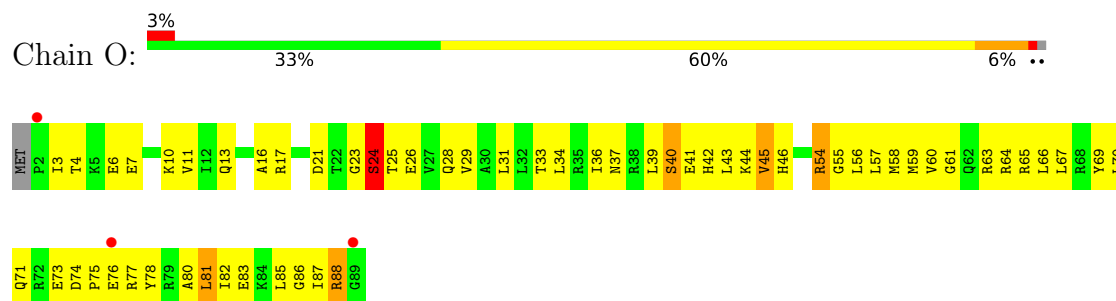
• Molecule 13: 30S ribosomal protein S13



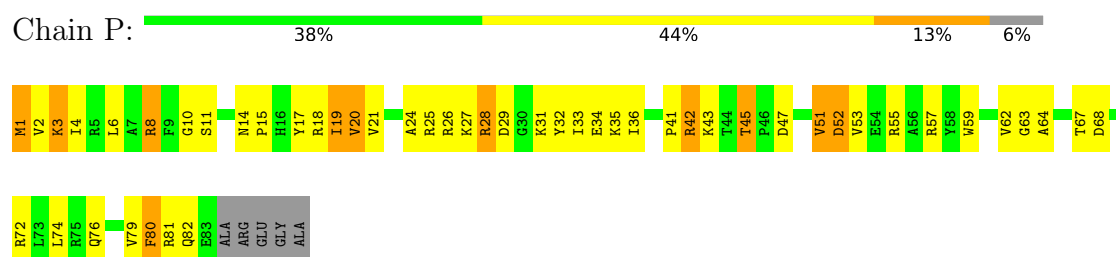
- Molecule 14: 30S ribosomal protein S14 type Z



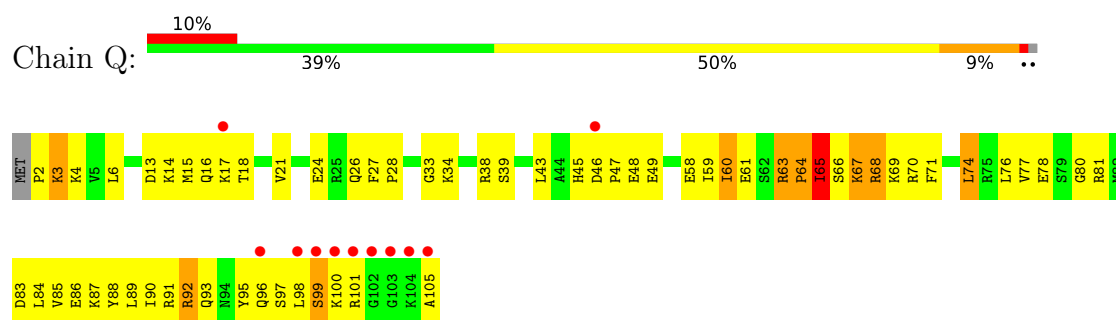
- Molecule 15: 30S ribosomal protein S15



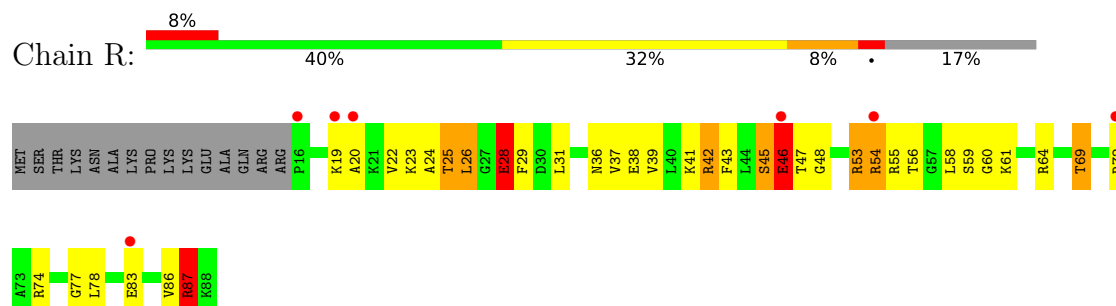
- Molecule 16: 30S ribosomal protein S16



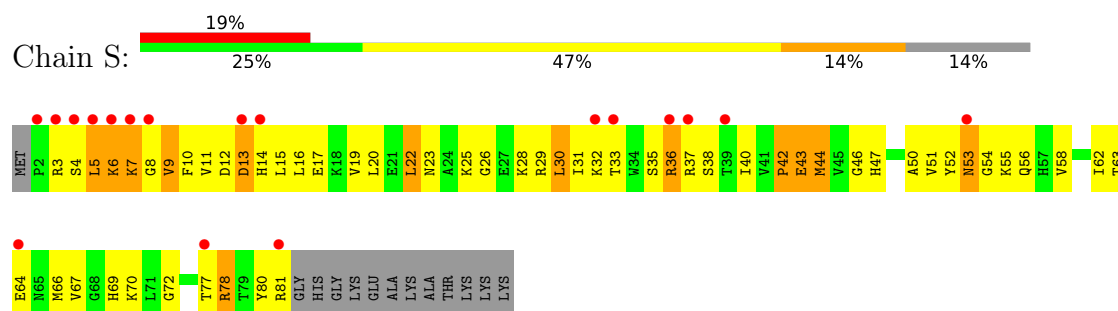
- Molecule 17: 30S ribosomal protein S17



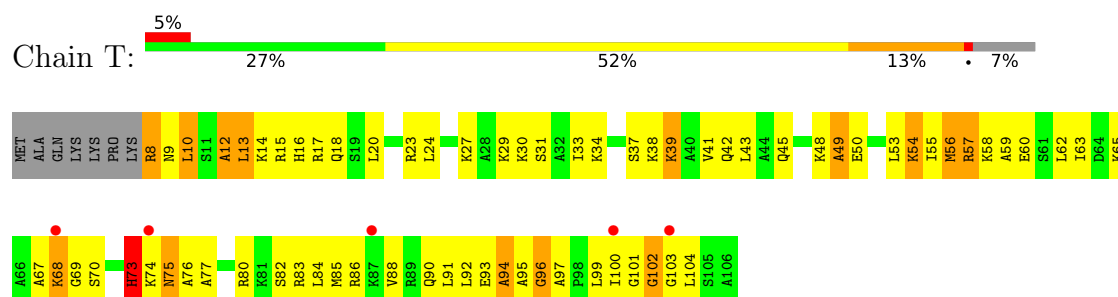
- Molecule 18: 30S ribosomal protein S18



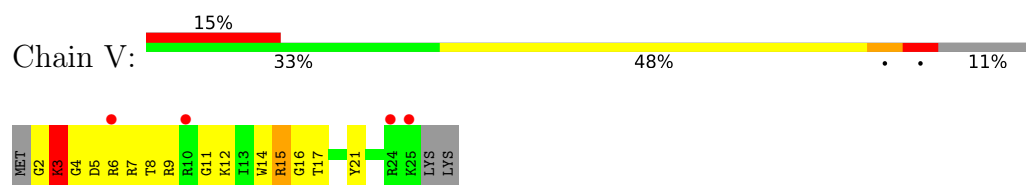
- Molecule 19: 30S ribosomal protein S19



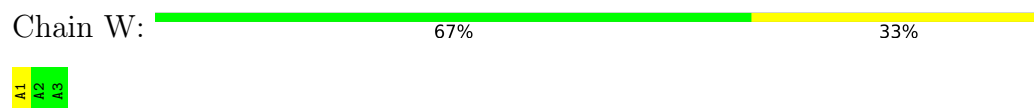
- Molecule 20: 30S ribosomal protein S20



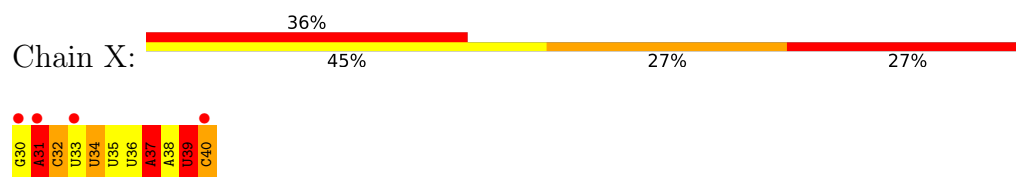
- Molecule 21: 30S ribosomal protein Thx



- Molecule 22: mRNA A-site fragment



- Molecule 23: tRNA ASL human Lys3



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	402.30Å 402.30Å 175.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.72 – 3.11 29.72 – 3.11	Depositor EDS
% Data completeness (in resolution range)	99.0 (29.72-3.11) 98.8 (29.72-3.11)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 2.96Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.247 , 0.276 0.251 , 0.254	Depositor DCC
R_{free} test set	14685 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	61.5	Xtriage
Anisotropy	0.264	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 67.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	52287	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.77% 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: ZN, MG, PSU, 70U, 12A, 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	0.45	2/36395 (0.0%)	0.92	182/56801 (0.3%)
2	B	0.46	0/1935	0.98	7/2609 (0.3%)
3	C	0.48	0/1636	0.96	4/2205 (0.2%)
4	D	0.45	0/1733	0.90	4/2318 (0.2%)
5	E	0.58	0/1162	1.05	4/1564 (0.3%)
6	F	0.44	0/856	0.87	1/1154 (0.1%)
7	G	0.48	0/1276	0.93	6/1709 (0.4%)
8	H	0.58	0/1136	1.16	10/1527 (0.7%)
9	I	0.44	0/1029	0.95	6/1378 (0.4%)
10	J	0.47	0/805	1.01	2/1082 (0.2%)
11	K	0.55	0/900	1.00	4/1213 (0.3%)
12	L	0.56	0/986	1.19	9/1320 (0.7%)
13	M	0.50	0/1008	0.95	1/1347 (0.1%)
14	N	0.51	0/501	1.01	1/664 (0.2%)
15	O	0.48	0/745	0.97	4/992 (0.4%)
16	P	0.55	0/716	1.09	6/963 (0.6%)
17	Q	0.51	0/870	1.15	8/1159 (0.7%)
18	R	0.47	0/603	0.98	1/799 (0.1%)
19	S	0.44	0/661	0.96	1/890 (0.1%)
20	T	0.59	0/764	1.12	7/1006 (0.7%)
21	V	0.51	0/212	0.90	0/277
22	W	0.64	0/75	0.65	0/113
23	X	0.60	0/184	1.45	4/277 (1.4%)
All	All	0.47	2/56188 (0.0%)	0.95	272/83367 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	46

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	517	U	O3'-P	-12.19	1.42	1.61
1	A	980	G	P-OP1	5.41	1.59	1.49

All (272) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	800	C	C2'-C3'-O3'	12.88	128.81	109.50
1	A	367	C	C2'-C3'-O3'	11.81	127.22	109.50
23	X	31	A	C2'-C3'-O3'	11.23	130.54	113.70
1	A	801	G	C2'-C3'-O3'	11.09	126.14	109.50
5	E	64	ARG	N-CA-C	-10.85	96.22	110.53
12	L	26	ALA	N-CA-C	-10.79	100.84	112.93
1	A	1483	U	C2'-C3'-O3'	10.74	125.61	109.50
1	A	491	C	C2'-C3'-O3'	10.72	125.58	109.50
1	A	47	C	C2'-C3'-O3'	10.23	124.85	109.50
1	A	700	C	C2'-C3'-O3'	10.19	124.79	109.50
1	A	108	G	C2'-C3'-O3'	10.13	124.70	109.50
1	A	1025	C	C4'-C3'-O3'	9.93	127.90	113.00
23	X	31	A	C3'-C2'-O2'	9.91	125.57	110.70
1	A	1141	U	C2'-C3'-O3'	9.79	124.19	109.50
1	A	239	U	C2'-C3'-O3'	9.65	123.98	109.50
1	A	1279	C	C2'-C3'-O3'	9.59	123.89	109.50
1	A	31	G	C2'-C3'-O3'	9.49	123.73	109.50
17	Q	67	LYS	N-CA-C	-9.45	98.78	110.41
1	A	1326	U	C2'-C3'-O3'	9.43	123.64	109.50
1	A	65	U	C2'-C3'-O3'	9.31	123.46	109.50
1	A	500	G	C2'-C3'-O3'	9.25	123.38	109.50
1	A	124	A	C2'-C3'-O3'	9.20	123.31	109.50
12	L	28	LYS	N-CA-C	-9.14	102.69	113.38
1	A	861	U	C2'-C3'-O3'	9.07	123.11	109.50
1	A	542	A	C2'-C3'-O3'	9.02	123.03	109.50
1	A	686	G	C2'-C3'-O3'	8.97	122.95	109.50
1	A	238	A	C2'-C3'-O3'	8.92	122.89	109.50
1	A	1345	A	C2'-C3'-O3'	8.84	122.76	109.50
1	A	515	A	P-O3'-C3'	8.73	133.29	120.20
1	A	1362	U	C2'-C3'-O3'	8.66	122.49	109.50
1	A	1206	A	C2'-C3'-O3'	8.60	122.40	109.50
1	A	1505	U	C2'-C3'-O3'	8.53	122.30	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	775	A	C2'-C3'-O3'	8.52	122.28	109.50
1	A	454	A	C2'-C3'-O3'	8.41	122.11	109.50
1	A	800	C	N1-C1'-C2'	8.35	126.53	114.00
1	A	515	A	O3'-P-O5'	8.29	116.44	104.00
1	A	1035	G	C2'-C3'-O3'	-8.28	101.28	113.70
1	A	276	G	C2'-C3'-O3'	8.17	121.75	109.50
15	O	44	LYS	N-CA-C	-8.16	102.35	111.82
20	T	12	ALA	N-CA-C	-8.14	102.91	113.17
11	K	116	HIS	N-CA-C	-8.14	100.40	111.55
1	A	951	A	C2'-C3'-O3'	8.10	121.65	109.50
1	A	445	A	C2'-C3'-O3'	8.08	121.62	109.50
8	H	79	VAL	N-CA-C	-7.99	102.29	111.00
1	A	1432	C	C2'-C3'-O3'	7.98	121.47	109.50
1	A	1282	U	C2'-C3'-O3'	7.94	121.40	109.50
1	A	704	G	C2'-C3'-O3'	7.91	121.37	109.50
11	K	37	GLY	N-CA-C	7.84	125.79	115.36
1	A	323	C	C2'-C3'-O3'	7.84	121.26	109.50
1	A	731	C	C2'-C3'-O3'	7.84	121.26	109.50
1	A	5	U	C2'-C3'-O3'	7.81	121.21	109.50
1	A	1280	A	N9-C1'-C2'	7.75	123.62	112.00
1	A	1283	U	C2'-C3'-O3'	7.70	121.05	109.50
1	A	1205	G	C2'-C3'-O3'	7.69	121.03	109.50
1	A	558	G	C2'-C3'-O3'	7.67	121.00	109.50
1	A	942	A	C2'-C3'-O3'	7.65	120.98	109.50
1	A	362	U	C2'-C3'-O3'	7.59	120.89	109.50
18	R	46	GLU	N-CA-C	-7.56	103.16	112.38
1	A	1516	C	O4'-C4'-C3'	-7.51	96.49	104.00
1	A	735	G	C2'-C3'-O3'	7.49	120.73	109.50
8	H	134	ILE	N-CA-C	7.45	117.98	110.23
1	A	1261	A	C2'-C3'-O3'	7.45	120.67	109.50
1	A	1177	U	C2'-C3'-O3'	7.44	120.66	109.50
1	A	49	U	C2'-C3'-O3'	7.43	120.65	109.50
1	A	1220	A	C2'-C3'-O3'	7.41	120.61	109.50
1	A	1111	C	C2'-C3'-O3'	7.39	120.59	109.50
1	A	705	A	C2'-C3'-O3'	7.37	120.56	109.50
1	A	1278	C	C2'-C3'-O3'	7.30	120.44	109.50
1	A	1346	U	C2'-C3'-O3'	7.28	120.42	109.50
1	A	1316	C	C2'-C3'-O3'	7.27	120.40	109.50
10	J	62	HIS	N-CA-C	7.23	120.45	108.96
1	A	468	G	C2'-C3'-O3'	7.17	120.26	109.50
1	A	1479	A	N9-C1'-C2'	7.16	124.75	114.00
1	A	1381	C	C2'-C3'-O3'	7.16	120.23	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	P	20	VAL	N-CA-C	7.14	118.64	108.42
4	D	33	MET	N-CA-C	-7.13	103.84	112.54
12	L	49	ASN	N-CA-C	7.12	119.94	109.69
1	A	867	G	C2'-C3'-O3'	7.09	120.14	109.50
1	A	175	G	C2'-C3'-O3'	7.01	120.01	109.50
1	A	636	A	C2'-C3'-O3'	6.97	119.95	109.50
8	H	103	VAL	N-CA-C	6.97	118.34	108.93
8	H	116	LYS	N-CA-C	-6.97	103.89	112.88
1	A	1036	C	C4'-C3'-O3'	6.96	123.45	113.00
1	A	211	G	N9-C1'-C2'	6.92	124.38	114.00
1	A	417	C	C2'-C3'-O3'	6.85	119.78	109.50
1	A	1238	U	C2'-C3'-O3'	6.84	119.77	109.50
17	Q	63	ARG	CA-C-N	6.81	128.36	119.84
17	Q	63	ARG	C-N-CA	6.81	128.36	119.84
1	A	570	G	C4'-C3'-O3'	6.79	119.58	109.40
1	A	979	G	C4'-C3'-O3'	-6.78	102.83	113.00
1	A	546	A	C4'-C3'-O3'	-6.77	102.85	113.00
20	T	70	SER	N-CA-C	6.76	120.21	112.57
1	A	340	C	C2'-C3'-O3'	6.75	119.62	109.50
1	A	501	C	C2'-C3'-O3'	6.71	119.57	109.50
8	H	75	ARG	CA-C-N	6.70	126.68	119.78
8	H	75	ARG	C-N-CA	6.70	126.68	119.78
1	A	189	U	C2'-C3'-O3'	6.69	119.54	109.50
1	A	416	U	C2'-C3'-O3'	6.68	119.52	109.50
9	I	72	GLY	N-CA-C	-6.67	104.42	112.49
20	T	92	LEU	N-CA-C	-6.61	105.28	113.15
1	A	239	U	C5'-C4'-C3'	-6.61	105.29	115.20
1	A	545	C	C2'-C3'-O3'	6.61	119.41	109.50
1	A	13	U	C2'-C3'-O3'	6.58	119.37	109.50
1	A	716	A	C4'-C3'-O3'	6.58	119.27	109.40
1	A	624	U	C4'-C3'-O3'	6.55	119.22	109.40
2	B	238	LEU	N-CA-C	-6.53	105.19	113.02
15	O	45	VAL	N-CA-C	-6.52	99.09	109.20
1	A	624	U	C2'-C3'-O3'	-6.52	99.72	109.50
1	A	310	A	C2'-C3'-O3'	6.50	119.26	109.50
1	A	1376	A	C2'-C3'-O3'	6.49	119.24	109.50
1	A	112	A	C2'-C3'-O3'	6.48	119.22	109.50
2	B	133	LYS	N-CA-C	-6.46	104.88	112.89
3	C	21	ARG	N-CA-C	6.45	118.77	110.65
1	A	684	C	C2'-C3'-O3'	6.42	119.14	109.50
1	A	952	A	C2'-C3'-O3'	6.41	119.12	109.50
1	A	937	U	N1-C1'-C2'	6.38	123.57	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	479	A	N9-C1'-C2'	6.38	123.56	114.00
12	L	119	LYS	N-CA-C	-6.35	101.98	110.55
1	A	1207	C	C4'-C3'-O3'	6.34	118.91	109.40
1	A	849	A	C4'-C3'-O3'	6.30	118.86	109.40
1	A	1083	A	C2'-C3'-O3'	6.30	118.95	109.50
1	A	479	A	C2'-C3'-O3'	6.29	118.94	109.50
1	A	64	G	C2'-C3'-O3'	6.28	118.92	109.50
1	A	322	A	C2'-C3'-O3'	6.27	118.90	109.50
1	A	969	U	C2'-C3'-O3'	6.25	118.88	109.50
1	A	1067	U	C2'-C3'-O3'	6.25	118.88	109.50
23	X	31	A	C4'-C3'-O3'	-6.24	103.64	113.00
1	A	60	A	C2'-C3'-O3'	6.23	118.84	109.50
1	A	1031	U	C2'-C3'-O3'	6.21	118.81	109.50
12	L	79	GLU	N-CA-C	6.20	117.72	110.97
1	A	1164	A	C2'-C3'-O3'	6.18	118.77	109.50
8	H	19	VAL	N-CA-C	-6.17	106.31	112.17
1	A	469	G	C2'-C3'-O3'	6.13	118.70	109.50
1	A	1327	A	C2'-C3'-O3'	6.13	118.69	109.50
1	A	238	A	N9-C1'-C2'	6.12	123.18	114.00
1	A	515	A	C2'-C3'-O3'	6.11	122.86	113.70
1	A	1163	G	C2'-C3'-O3'	6.09	118.64	109.50
1	A	300	G	C2'-C3'-O3'	6.09	122.84	113.70
5	E	69	VAL	CA-C-N	6.08	127.45	119.84
5	E	69	VAL	C-N-CA	6.08	127.45	119.84
5	E	23	GLY	N-CA-C	6.08	118.16	110.38
19	S	36	ARG	N-CA-C	-6.05	105.85	113.72
1	A	867	G	N9-C1'-C2'	6.04	123.07	114.00
1	A	433	G	C4'-C3'-O3'	6.04	118.46	109.40
1	A	1221	U	C2'-C3'-O3'	6.02	118.53	109.50
1	A	797	A	C5'-C4'-C3'	-6.01	106.98	116.00
1	A	1516	C	C4'-C3'-O3'	6.01	122.02	113.00
1	A	1262	U	C2'-C3'-O3'	5.99	118.49	109.50
2	B	23	ARG	N-CA-C	-5.99	104.82	113.21
1	A	123	G	C2'-C3'-O3'	5.99	118.49	109.50
7	G	147	ALA	N-CA-C	-5.99	105.97	113.28
14	N	38	GLY	N-CA-C	-5.99	107.40	115.36
1	A	558	G	N9-C1'-C2'	5.97	122.96	114.00
1	A	1475	U	C2'-C3'-O3'	-5.97	100.54	109.50
1	A	1378	A	C2'-C3'-O3'	5.96	118.44	109.50
1	A	48	C	C2'-C3'-O3'	5.95	118.42	109.50
1	A	559	G	C2'-C3'-O3'	5.95	118.42	109.50
20	T	13	LEU	N-CA-C	-5.94	104.93	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1141	U	N1-C1'-C2'	5.92	122.88	114.00
1	A	1139	A	C2'-C3'-O3'	5.91	118.36	109.50
7	G	110	GLN	N-CA-C	-5.89	106.26	113.50
15	O	54	ARG	N-CA-C	-5.88	104.96	111.36
1	A	1076	G	C4'-C3'-O3'	-5.87	104.19	113.00
1	A	383	G	C2'-C3'-O3'	5.86	118.28	109.50
1	A	847	U	C2'-C3'-O3'	5.85	118.28	109.50
1	A	823	C	N1-C1'-C2'	5.85	120.77	112.00
1	A	1483	U	N1-C1'-C2'	5.83	122.74	114.00
1	A	1521	U	C4'-C3'-O3'	-5.82	100.67	109.40
4	D	116	GLN	N-CA-C	-5.80	104.33	111.40
7	G	145	ALA	N-CA-C	-5.79	101.38	110.36
1	A	1510	C	N1-C1'-C2'	5.78	120.67	112.00
16	P	25	ARG	N-CA-C	5.77	119.50	112.23
17	Q	58	GLU	N-CA-C	-5.77	101.15	110.32
9	I	87	GLN	N-CA-C	-5.77	104.91	111.14
1	A	455	C	C2'-C3'-O3'	5.76	118.14	109.50
1	A	423	G	C2'-C3'-O3'	5.76	118.14	109.50
13	M	17	VAL	N-CA-C	-5.75	106.10	111.45
1	A	1047	U	N1-C1'-C2'	5.73	122.60	114.00
1	A	360	U	N1-C1'-C2'	5.73	120.60	112.00
9	I	101	PHE	N-CA-C	-5.72	106.30	113.28
7	G	50	ILE	N-CA-C	-5.71	104.66	113.16
1	A	953	G	C4'-C3'-O3'	5.70	117.96	109.40
3	C	155	GLY	N-CA-C	5.70	121.90	112.89
8	H	17	THR	N-CA-C	5.70	118.26	111.71
12	L	60	LEU	N-CA-C	5.69	118.04	110.53
2	B	36	ARG	N-CA-C	5.67	117.96	107.99
12	L	44	THR	CA-C-N	5.65	126.90	119.84
12	L	44	THR	C-N-CA	5.65	126.90	119.84
6	F	60	PHE	N-CA-C	5.62	119.26	110.32
1	A	1113	G	N9-C1'-C2'	-5.62	103.57	112.00
1	A	776	U	C2'-C3'-O3'	5.61	117.91	109.50
1	A	269	A	C2'-C3'-O3'	5.60	117.90	109.50
1	A	669	U	C2'-C3'-O3'	-5.60	105.30	113.70
1	A	1181	C	C2'-C3'-O3'	5.60	117.90	109.50
1	A	1317	C	C2'-C3'-O3'	5.59	117.88	109.50
1	A	323	C	N1-C1'-C2'	5.57	122.35	114.00
1	A	469	G	C1'-C2'-O2'	-5.55	103.48	111.80
1	A	246	G	N9-C1'-C2'	5.54	122.31	114.00
1	A	937	U	C2'-C3'-O3'	5.53	117.80	109.50
1	A	1312	G	N9-C1'-C2'	5.51	120.26	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	424	U	C2'-C3'-O3'	5.50	117.75	109.50
2	B	110	GLN	N-CA-C	-5.48	106.59	113.28
16	P	3	LYS	N-CA-C	5.48	117.40	109.07
1	A	911	C	C2'-C3'-O3'	-5.47	101.30	109.50
1	A	1111	C	N1-C1'-C2'	5.46	122.19	114.00
17	Q	91	ARG	N-CA-C	-5.45	104.77	111.75
9	I	42	ARG	N-CA-C	5.45	117.02	111.14
16	P	63	GLY	N-CA-C	5.42	119.39	113.58
1	A	795	C	C2'-C3'-O3'	5.42	117.63	109.50
4	D	3	ARG	N-CA-C	-5.42	105.11	112.26
20	T	74	LYS	CB-CA-C	-5.42	108.74	115.89
1	A	558	G	O4'-C1'-C2'	5.41	111.21	105.80
1	A	1036	C	N1-C1'-C2'	-5.40	103.90	112.00
1	A	51	A	C2'-C3'-O3'	5.38	117.58	109.50
4	D	12	CYS	N-CA-C	-5.38	105.49	111.36
1	A	850	A	O4'-C1'-C2'	5.36	111.16	105.80
3	C	147	LYS	N-CA-C	-5.36	106.49	114.64
10	J	21	GLN	N-CA-C	-5.35	106.76	113.28
1	A	848	U	C4'-C3'-O3'	5.35	117.42	109.40
1	A	346	G	O4'-C1'-C2'	5.34	111.14	105.80
1	A	911	C	C4'-C3'-O3'	5.34	117.41	109.40
17	Q	65	ILE	N-CA-C	-5.34	107.18	113.42
9	I	59	PHE	N-CA-C	5.33	117.98	110.14
1	A	1280	A	C4'-C3'-O3'	-5.32	105.02	113.00
20	T	76	ALA	N-CA-C	-5.32	105.15	111.69
1	A	970	G	C2'-C3'-O3'	5.31	117.47	109.50
1	A	47	C	N1-C1'-C2'	5.31	121.97	114.00
16	P	51	VAL	N-CA-C	5.30	120.37	109.34
9	I	60	ASP	N-CA-C	-5.30	99.69	108.75
1	A	8	A	C4'-C3'-O3'	5.28	117.31	109.40
1	A	1480	A	C2'-C3'-O3'	5.27	117.41	109.50
7	G	111	ARG	CA-C-N	5.26	124.95	119.64
7	G	111	ARG	C-N-CA	5.26	124.95	119.64
1	A	555	A	N9-C1'-C2'	5.26	119.89	112.00
1	A	867	G	O4'-C1'-C2'	5.26	111.06	105.80
1	A	1259	U	C2'-C3'-O3'	5.25	117.37	109.50
1	A	800	C	O4'-C1'-C2'	5.23	111.03	105.80
1	A	1345	A	N9-C1'-C2'	5.23	121.84	114.00
11	K	40	ILE	N-CA-C	-5.21	107.08	111.56
1	A	108	G	N9-C1'-C2'	5.21	121.81	114.00
20	T	75	ASN	N-CA-C	-5.18	107.12	112.93
1	A	408	G	N9-C1'-C2'	5.18	119.77	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	494	C	C4'-C3'-O3'	5.17	117.16	109.40
1	A	890	A	O4'-C1'-C2'	5.17	110.97	105.80
12	L	75	HIS	N-CA-C	5.16	117.69	109.65
1	A	261	G	C2'-C3'-O3'	-5.15	105.98	113.70
1	A	7	G	C2'-C3'-O3'	5.14	117.22	109.50
3	C	40	ARG	N-CA-C	-5.14	106.96	113.18
1	A	1278	C	N1-C1'-C2'	5.11	121.66	114.00
1	A	190	G	C2'-C3'-O3'	5.11	117.16	109.50
17	Q	63	ARG	N-CA-C	-5.10	103.22	109.65
11	K	60	ALA	N-CA-C	-5.10	105.16	111.33
23	X	31	A	C5'-C4'-C3'	-5.09	108.36	116.00
1	A	1511	A	O4'-C4'-C3'	5.09	109.09	104.00
1	A	274	A	C2'-C3'-O3'	5.08	117.13	109.50
1	A	47	C	O4'-C1'-C2'	5.08	110.88	105.80
17	Q	80	GLY	N-CA-C	5.07	125.19	113.18
8	H	39	LEU	N-CA-C	-5.07	105.20	111.33
1	A	578	G	C2'-C3'-O3'	-5.06	101.91	109.50
1	A	1133	A	C2'-C3'-O3'	5.05	117.08	109.50
8	H	28	ALA	N-CA-C	5.05	118.30	110.17
1	A	6	G	N9-C1'-C2'	5.05	119.57	112.00
1	A	1376	A	C5'-C4'-C3'	-5.04	107.63	115.20
15	O	10	LYS	N-CA-C	-5.04	105.44	112.45
1	A	1106	G	C4'-C3'-O3'	5.03	116.94	109.40
1	A	953	G	C2'-C3'-O3'	-5.03	101.96	109.50
1	A	948	G	C2'-C3'-O3'	5.03	117.04	109.50
1	A	408	G	C4'-C3'-O3'	-5.02	105.47	113.00
2	B	111	ARG	N-CA-C	-5.01	105.92	112.23
16	P	62	VAL	N-CA-C	5.01	117.00	112.29
2	B	122	PHE	N-CA-C	-5.01	107.34	113.50
1	A	1067	U	O4'-C1'-C2'	5.00	110.80	105.80

There are no chirality outliers.

All (46) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1007	C	Sidechain
1	A	1019	C	Sidechain
1	A	1036	C	Sidechain
1	A	1047	U	Sidechain
1	A	1049	A	Sidechain
1	A	1055	U	Sidechain
1	A	1065	U	Sidechain

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Mol	Chain	Res	Type	Group
1	A	1113	G	Sidechain
1	A	1122	C	Sidechain
1	A	1141	U	Sidechain
1	A	1142	G	Sidechain
1	A	1162	G	Sidechain
1	A	1177	U	Sidechain
1	A	1258	C	Sidechain
1	A	1280	A	Sidechain
1	A	1318	G	Sidechain
1	A	1339	U	Sidechain
1	A	1387	G	Sidechain
1	A	1401	G	Sidechain
1	A	1434	G	Sidechain
1	A	1469	A	Sidechain
1	A	1479	A	Sidechain
1	A	1518	U	Sidechain
1	A	167	U	Sidechain
1	A	190	G	Sidechain
1	A	246	G	Sidechain
1	A	272	C	Sidechain
1	A	362	U	Sidechain
1	A	37	U	Sidechain
1	A	381	C	Sidechain
1	A	382	U	Sidechain
1	A	398	C	Sidechain
1	A	465	G	Sidechain
1	A	47	C	Sidechain
1	A	479	A	Sidechain
1	A	501	C	Sidechain
1	A	543	U	Sidechain
1	A	558	G	Sidechain
1	A	624	U	Sidechain
1	A	800	C	Sidechain
1	A	840	U	Sidechain
1	A	861	U	Sidechain
1	A	875	G	Sidechain
1	A	920	U	Sidechain
1	A	951	A	Sidechain
1	A	959	U	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32515	0	16409	1147	0
2	B	1900	0	1951	188	0
3	C	1612	0	1677	167	0
4	D	1703	0	1764	135	0
5	E	1146	0	1207	100	0
6	F	843	0	857	71	0
7	G	1257	0	1296	86	0
8	H	1116	0	1177	69	0
9	I	1011	0	1043	108	0
10	J	792	0	835	111	0
11	K	885	0	904	66	0
12	L	970	0	1056	99	0
13	M	997	0	1072	97	0
14	N	492	0	530	73	0
15	O	734	0	771	55	0
16	P	700	0	720	55	0
17	Q	857	0	930	72	0
18	R	597	0	668	49	0
19	S	647	0	673	70	0
20	T	762	0	859	71	0
21	V	208	0	221	25	0
22	W	67	0	34	4	0
23	X	247	0	129	33	0
24	A	182	0	0	0	0
24	B	1	0	0	0	0
24	L	1	0	0	0	0
24	S	1	0	0	0	0
25	A	42	0	45	5	0
26	D	1	0	0	0	0
26	N	1	0	0	0	0
All	All	52287	0	36828	2683	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 30.

All (2683) 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:981:G:N2	1:A:982:A:H1'	1.44	1.31
1:A:515:A:H5''	3:C:161:GLU:OE1	1.36	1.21
23:X:39:PSU:C2'	23:X:40:C:H5'	1.74	1.18
1:A:1036:C:H3'	1:A:1036:C:C6	1.80	1.15
1:A:984:C:H2'	1:A:985:C:C6	1.82	1.14
1:A:513:G:H4'	1:A:513:G:OP1	1.35	1.13
2:B:80:ILE:HD11	2:B:208:ILE:HG23	1.28	1.09
23:X:37:12A:H5'	23:X:37:12A:H8	1.32	1.09
9:I:53:VAL:HG21	9:I:85:LEU:HD21	1.36	1.08
1:A:246:G:H4'	1:A:247:U:C5'	1.84	1.07
1:A:980:G:H2'	1:A:981:G:C8	1.87	1.07
20:T:8:ARG:HB2	20:T:8:ARG:HH11	1.14	1.06
1:A:1303:C:H4'	1:A:1304:G:OP1	1.56	1.04
1:A:346:G:H4'	1:A:347:C:OP1	1.57	1.04
1:A:1237:A:C2'	1:A:1238:U:H4'	1.87	1.04
19:S:33:THR:HG22	19:S:35:SER:H	1.18	1.03
1:A:515:A:C5'	3:C:161:GLU:OE1	2.07	1.03
1:A:542:A:H4'	1:A:543:U:H5'	1.36	1.02
1:A:1237:A:H2'	1:A:1238:U:H4'	1.03	1.02
1:A:1237:A:H2'	1:A:1238:U:C4'	1.89	1.02
10:J:8:LEU:HB2	10:J:70:ARG:HB2	1.39	1.01
12:L:41:ARG:NH1	12:L:41:ARG:HB3	1.76	1.00
4:D:189:PRO:HB2	4:D:194:LEU:HD21	1.43	0.99
1:A:241:A:H4'	1:A:242:G:OP1	1.58	0.99
1:A:513:G:C8	23:X:35:U:O2'	2.13	0.99
1:A:515:A:OP2	1:A:515:A:H4'	1.62	0.99
13:M:94:ARG:HH12	19:S:81:ARG:HD3	1.28	0.99
1:A:936:A:H3'	1:A:937:U:H5''	1.43	0.98
1:A:984:C:C5	1:A:985:C:N4	2.30	0.98
1:A:465:G:H4'	1:A:466:A:OP1	1.61	0.97
6:F:2:ARG:HE	6:F:69:GLU:HG2	1.26	0.97
23:X:39:PSU:C3'	23:X:40:C:H5'	1.94	0.97
19:S:7:LYS:HD2	19:S:7:LYS:O	1.65	0.96
10:J:90:LEU:H	10:J:91:PRO:HD2	1.25	0.96
1:A:981:G:N2	1:A:982:A:C1'	2.30	0.95
11:K:54:ARG:O	11:K:57:THR:HG22	1.65	0.95
1:A:1036:C:C6	1:A:1036:C:C3'	2.50	0.95
1:A:1035:G:H5'	1:A:1036:C:H5'	1.49	0.94
15:O:17:ARG:HG3	15:O:17:ARG:HH11	1.32	0.94
4:D:3:ARG:HD3	4:D:118:ARG:NH1	1.82	0.94
1:A:245:A:H4'	1:A:246:G:O5'	1.64	0.94
1:A:981:G:H21	1:A:982:A:H1'	1.29	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:97:SER:O	17:Q:98:LEU:HD23	1.68	0.94
1:A:1286:G:H5''	21:V:4:GLY:HA3	1.49	0.93
4:D:151:LYS:H	4:D:151:LYS:HD2	1.31	0.93
1:A:542:A:H4'	1:A:543:U:C5'	1.99	0.93
10:J:34:VAL:HG12	10:J:36:GLY:H	1.34	0.92
17:Q:67:LYS:HA	17:Q:70:ARG:HH12	1.33	0.92
1:A:1243:C:H2'	1:A:1244:C:H5'	1.51	0.92
1:A:982:A:H3'	1:A:983:A:H4'	1.51	0.92
12:L:75:HIS:HD2	12:L:77:LEU:H	1.17	0.92
8:H:103:VAL:HG21	8:H:109:ILE:O	1.68	0.91
2:B:132:LYS:HA	2:B:135:GLN:HB3	1.52	0.91
6:F:54:LYS:HE2	6:F:54:LYS:N	1.86	0.91
1:A:669:U:H1'	11:K:42:TRP:HE1	1.35	0.91
2:B:7:VAL:HG23	2:B:8:LYS:H	1.36	0.90
1:A:955:A:O2'	1:A:1303:C:N3	2.02	0.90
1:A:647:G:H22	1:A:724:G:H1	1.13	0.90
1:A:1121:G:H4'	1:A:1122:C:OP1	1.71	0.90
14:N:57:ARG:HG2	14:N:58:LYS:H	1.37	0.90
1:A:936:A:H5'	1:A:937:U:OP2	1.73	0.89
1:A:1227:C:H2'	1:A:1228:U:H5'	1.52	0.89
1:A:269:A:HO2'	1:A:270:G:H8	1.18	0.89
4:D:104:VAL:HG11	4:D:146:ILE:HD12	1.53	0.89
1:A:1243:C:H42	1:A:1254:G:H1	1.17	0.89
2:B:91:PRO:HG3	2:B:154:LEU:HB3	1.54	0.88
1:A:1286:G:HO2'	1:A:1287:A:H8	0.90	0.88
2:B:197:VAL:HB	2:B:200:ILE:HG12	1.55	0.88
1:A:501:C:C5	1:A:513:G:H5''	2.09	0.88
1:A:1124:G:H2'	1:A:1125:G:H5'	1.56	0.88
6:F:11:ASN:HD22	6:F:13:ASN:H	1.21	0.88
1:A:985:C:H2'	1:A:986:C:C6	2.09	0.88
1:A:1083:A:H4'	1:A:1084:A:O5'	1.72	0.87
4:D:19:LEU:CD2	4:D:67:ILE:HG12	2.04	0.87
1:A:1262:U:H5'	1:A:1263:C:C5	2.08	0.87
19:S:29:ARG:H	19:S:29:ARG:HD2	1.37	0.87
8:H:68:ARG:HB3	8:H:68:ARG:HH11	1.40	0.87
9:I:125:TYR:HE1	9:I:128:ARG:HB3	1.39	0.87
3:C:195:VAL:C	3:C:196:LEU:HD23	1.99	0.86
20:T:39:LYS:HD2	20:T:55:ILE:CD1	2.05	0.86
6:F:54:LYS:HE2	6:F:54:LYS:H	1.38	0.86
1:A:736:A:H4'	1:A:737:C:O5'	1.74	0.86
1:A:984:C:H2'	1:A:985:C:C5	2.09	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:39:PRO:O	10:J:40:LEU:HB2	1.76	0.86
5:E:148:VAL:HG21	8:H:107:LEU:HD22	1.57	0.86
1:A:1479:A:H2	1:A:1482:G:H1	1.24	0.85
23:X:36:U:H2'	23:X:37:12A:H5''	1.59	0.85
1:A:102:A:H2'	1:A:321:G:N2	1.91	0.85
12:L:41:ARG:HG2	12:L:42:THR:H	1.41	0.85
1:A:984:C:C4	1:A:985:C:N4	2.45	0.85
1:A:1301:C:H5'	19:S:70:LYS:HD2	1.56	0.85
13:M:49:THR:HG22	13:M:51:ALA:H	1.42	0.85
1:A:983:A:OP2	1:A:984:C:C4	2.30	0.84
1:A:1286:G:O2'	1:A:1287:A:H8	1.60	0.84
11:K:84:VAL:HG23	11:K:110:ASP:HA	1.59	0.84
3:C:88:ARG:HG3	3:C:101:LEU:HD12	1.60	0.84
1:A:716:A:H4'	1:A:717:G:OP1	1.76	0.84
20:T:8:ARG:HB2	20:T:8:ARG:NH1	1.92	0.84
1:A:1004:G:H1	1:A:1018:G:H1	1.25	0.84
1:A:1098:C:H2'	1:A:1099:G:H5''	1.58	0.84
1:A:1231:A:H4'	9:I:68:GLY:H	1.41	0.84
1:A:1119:C:OP2	1:A:1120:G:H5''	1.78	0.83
1:A:1409:U:H2'	1:A:1410:A:C8	2.13	0.83
2:B:60:ASP:HB3	2:B:64:ARG:NH2	1.92	0.83
3:C:75:VAL:O	3:C:83:ARG:HG2	1.77	0.83
1:A:1417:G:H2'	1:A:1418:U:C6	2.14	0.83
1:A:980:G:C6	1:A:981:G:O6	2.32	0.82
12:L:41:ARG:HB3	12:L:41:ARG:HH11	1.41	0.82
1:A:1036:C:H3'	1:A:1036:C:H6	1.38	0.82
1:A:246:G:H4'	1:A:247:U:H5''	1.62	0.82
3:C:16:ARG:HH11	3:C:16:ARG:HG3	1.44	0.82
4:D:19:LEU:HD21	4:D:67:ILE:HG12	1.59	0.82
5:E:88:LYS:HB3	5:E:123:LEU:HB2	1.62	0.82
9:I:112:LYS:HE2	9:I:117:HIS:O	1.80	0.82
1:A:1206:A:H3'	1:A:1207:C:C6	2.14	0.82
1:A:689:A:H1'	11:K:29:ILE:HD11	1.59	0.81
5:E:81:GLU:HG3	5:E:90:VAL:HG22	1.62	0.81
1:A:341:G:H2'	1:A:342:G:H5'	1.62	0.81
2:B:80:ILE:HD11	2:B:208:ILE:CG2	2.09	0.81
1:A:980:G:H2'	1:A:981:G:H8	1.42	0.81
5:E:13:ILE:HD12	5:E:13:ILE:O	1.80	0.81
1:A:180:C:O2	20:T:85:MET:HE1	1.79	0.81
11:K:84:VAL:HG11	11:K:95:ILE:HD11	1.61	0.81
13:M:49:THR:HB	13:M:52:GLU:HG3	1.63	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:48:GLU:HA	9:I:51:ARG:HH11	1.44	0.81
1:A:501:C:H5	1:A:513:G:H5''	1.43	0.81
1:A:505:C:H41	12:L:53:ARG:NH2	1.79	0.80
16:P:74:LEU:HG	16:P:79:VAL:HG21	1.62	0.80
13:M:40:ASN:HD22	13:M:41:PRO:CD	1.94	0.80
1:A:530:A:H4'	1:A:531:G:O5'	1.81	0.80
1:A:1170:C:H5'	1:A:1171:G:OP2	1.81	0.80
1:A:1207:C:H4'	1:A:1208:A:OP1	1.81	0.80
20:T:68:LYS:HE3	20:T:68:LYS:HA	1.64	0.80
3:C:15:THR:O	3:C:16:ARG:HB2	1.80	0.80
7:G:147:ALA:C	7:G:148:ASN:HD22	1.90	0.80
2:B:83:MET:HG3	2:B:235:SER:OG	1.81	0.80
2:B:84:GLU:HB3	2:B:219:VAL:HG21	1.62	0.80
13:M:117:VAL:HG12	13:M:118:ALA:H	1.46	0.80
1:A:955:A:H1'	1:A:1303:C:O2	1.81	0.79
1:A:1006:C:H42	1:A:1016:G:N2	1.79	0.79
8:H:113:SER:HB2	8:H:134:ILE:HD11	1.64	0.79
16:P:28:ARG:HG2	16:P:28:ARG:HH11	1.47	0.79
2:B:14:GLY:O	2:B:15:VAL:HG13	1.82	0.79
2:B:178:ARG:HH11	2:B:178:ARG:HG3	1.46	0.79
14:N:3:ARG:NH2	14:N:6:LEU:HD11	1.98	0.79
1:A:499:U:O2	1:A:516:A:N6	2.16	0.79
1:A:849:A:H4'	1:A:850:A:OP1	1.82	0.79
13:M:40:ASN:HD22	13:M:41:PRO:HD2	1.47	0.79
1:A:562:G:H5'	1:A:711:A:H1'	1.63	0.79
1:A:1049:A:H4'	1:A:1050:G:O5'	1.82	0.79
2:B:105:PHE:O	2:B:109:SER:HB2	1.82	0.79
23:X:39:PSU:H6	23:X:39:PSU:H5'	1.48	0.79
8:H:64:LYS:HG2	8:H:79:VAL:HG21	1.63	0.79
8:H:120:THR:OG1	8:H:123:GLU:HG3	1.82	0.79
1:A:1228:U:H6	1:A:1228:U:H3'	1.47	0.79
23:X:39:PSU:H2'	23:X:40:C:H5'	1.62	0.79
1:A:1106:G:H2'	1:A:1127:C:C5	2.17	0.79
1:A:35:G:H2'	1:A:36:C:C6	2.17	0.79
1:A:516:A:H4'	1:A:517:U:OP1	1.81	0.79
1:A:1267:A:H8	1:A:1268:A:H4'	1.48	0.79
1:A:246:G:H4'	1:A:247:U:H5'	1.62	0.78
2:B:60:ASP:HB3	2:B:64:ARG:HH22	1.47	0.78
2:B:21:ARG:HG3	2:B:22:LYS:H	1.46	0.78
1:A:347:C:H4'	1:A:349:G:OP1	1.82	0.78
1:A:1123:C:H2'	1:A:1124:G:H5'	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1098:C:H2'	1:A:1099:G:C5'	2.12	0.78
3:C:14:ILE:HG22	3:C:15:THR:H	1.49	0.78
5:E:105:VAL:HB	5:E:106:PRO:HD3	1.65	0.78
10:J:64:GLU:HG2	14:N:59:ALA:HB2	1.65	0.78
25:A:1783:PAR:H11	25:A:1783:PAR:O52	1.81	0.78
15:O:36:ILE:O	15:O:40:SER:HB2	1.83	0.78
1:A:1509:U:H2'	1:A:1510:C:C5'	2.14	0.78
1:A:923:A:H2'	1:A:924:G:C8	2.19	0.78
3:C:70:VAL:O	3:C:106:VAL:HG23	1.84	0.77
3:C:59:ARG:HG3	3:C:63:ASN:O	1.85	0.77
12:L:27:LEU:C	12:L:29:GLY:H	1.91	0.77
19:S:33:THR:HG22	19:S:35:SER:N	1.99	0.77
23:X:36:U:C2'	23:X:37:12A:H5''	2.13	0.77
1:A:461:G:O2'	1:A:462:A:H5'	1.84	0.77
1:A:980:G:N1	1:A:981:G:C6	2.53	0.77
1:A:1266:A:H4'	1:A:1267:A:O5'	1.83	0.77
1:A:515:A:OP2	1:A:515:A:C4'	2.33	0.77
1:A:982:A:C2'	1:A:983:A:OP1	2.31	0.77
1:A:1105:A:H2	10:J:39:PRO:HG3	1.48	0.77
2:B:101:MET:HA	2:B:108:ILE:HG21	1.65	0.77
1:A:181:C:O4'	20:T:85:MET:HE2	1.85	0.77
18:R:37:VAL:O	18:R:41:LYS:HG3	1.84	0.77
18:R:55:ARG:NH1	18:R:55:ARG:HB3	2.00	0.77
1:A:936:A:H3'	1:A:937:U:C5'	2.15	0.77
1:A:1286:G:N2	1:A:1312:G:O2'	2.18	0.77
10:J:78:ASN:HB2	10:J:81:THR:OG1	1.85	0.77
9:I:97:LYS:HB3	9:I:98:PRO:HD3	1.67	0.76
7:G:41:ARG:O	7:G:45:ASP:HB2	1.85	0.76
1:A:1042:C:C5	3:C:2:GLY:HA2	2.20	0.76
16:P:28:ARG:HG2	16:P:29:ASP:OD2	1.85	0.76
9:I:48:GLU:N	9:I:49:PRO:HD2	2.01	0.76
13:M:15:VAL:HG23	13:M:43:THR:O	1.85	0.76
20:T:58:LYS:O	20:T:62:LEU:HD12	1.85	0.76
1:A:513:G:H5''	1:A:513:G:N3	2.00	0.76
12:L:26:ALA:O	12:L:27:LEU:O	2.03	0.76
13:M:121:LYS:HA	13:M:125:ARG:HD3	1.67	0.76
1:A:102:A:H2'	1:A:321:G:H21	1.47	0.76
1:A:899:G:H5'	5:E:20:GLN:NE2	2.01	0.76
19:S:30:LEU:O	19:S:31:ILE:HD13	1.86	0.76
20:T:39:LYS:HD2	20:T:55:ILE:HD13	1.66	0.76
7:G:12:LEU:H	7:G:12:LEU:HD12	1.51	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:X:34:70U:H2'	23:X:35:U:C6	2.21	0.76
1:A:501:C:H4'	1:A:502:C:H5''	1.66	0.75
10:J:86:MET:HA	10:J:86:MET:HE3	1.68	0.75
12:L:91:LYS:HA	12:L:91:LYS:HE3	1.66	0.75
5:E:51:VAL:HB	5:E:52:PRO:HD3	1.67	0.75
1:A:1351:C:H2'	1:A:1352:G:C8	2.22	0.75
1:A:433:G:H4'	1:A:434:A:OP1	1.87	0.75
1:A:1302:C:H5''	1:A:1303:C:H2'	1.69	0.75
7:G:15:ASP:HB3	7:G:19:GLY:N	2.00	0.75
1:A:392:A:N7	1:A:530:A:O2'	2.19	0.75
1:A:1134:A:H5''	10:J:13:HIS:CD2	2.21	0.75
3:C:32:LEU:HD22	3:C:59:ARG:HH11	1.51	0.75
4:D:35:ARG:HD2	4:D:35:ARG:N	2.01	0.75
15:O:16:ALA:HB1	15:O:21:ASP:HB3	1.69	0.75
1:A:366:G:O2'	1:A:367:C:H5'	1.87	0.75
1:A:513:G:C2'	1:A:514:U:OP2	2.33	0.75
3:C:191:THR:HG21	3:C:193:TYR:CZ	2.21	0.74
1:A:102:A:H4'	1:A:103:C:OP2	1.86	0.74
1:A:982:A:H2'	1:A:983:A:OP1	1.87	0.74
2:B:230:VAL:HG12	2:B:231:GLU:H	1.51	0.74
1:A:15:G:H4'	5:E:24:ARG:HH12	1.52	0.74
1:A:689:A:C1'	11:K:29:ILE:HD11	2.16	0.74
1:A:1022:U:H2'	1:A:1023:A:H8	1.53	0.74
1:A:198:U:H1'	20:T:103:GLY:HA2	1.69	0.74
1:A:203:A:H4'	1:A:204:G:O5'	1.84	0.74
1:A:1042:C:H2'	1:A:1043:G:H8	1.52	0.74
1:A:297:G:H5''	12:L:17:LYS:HE2	1.69	0.74
8:H:91:ARG:HG3	12:L:7:ILE:HG13	1.69	0.74
12:L:41:ARG:HG2	12:L:42:THR:N	2.02	0.74
13:M:10:PRO:HB2	13:M:18:ALA:HB1	1.70	0.74
1:A:952:A:H4'	1:A:953:G:H5'	1.68	0.74
1:A:1147:C:H2'	1:A:1148:G:H5'	1.68	0.74
4:D:34:GLU:O	4:D:35:ARG:HB2	1.87	0.74
1:A:238:A:H4'	1:A:239:U:H5'	1.67	0.74
5:E:78:HIS:ND1	8:H:104:ARG:HD2	2.03	0.74
1:A:980:G:H1	1:A:1020:C:H42	1.36	0.74
2:B:107:THR:C	2:B:109:SER:H	1.95	0.74
1:A:123:G:N3	1:A:189:U:H5'	2.01	0.74
6:F:2:ARG:NE	6:F:69:GLU:HG2	2.01	0.74
23:X:36:U:H2'	23:X:37:12A:C5'	2.18	0.74
9:I:4:TYR:CE2	9:I:88:TYR:HA	2.22	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1098:C:C2'	1:A:1099:G:H5''	2.18	0.73
2:B:162:ILE:HD12	2:B:177:ALA:HB2	1.70	0.73
4:D:70:ILE:HD11	4:D:100:ARG:CD	2.18	0.73
9:I:19:LEU:HD23	9:I:61:ALA:HB2	1.69	0.73
1:A:1036:C:C4	23:X:34:70U:H4'	2.23	0.73
1:A:1136:G:H2'	1:A:1137:G:H8	1.52	0.73
1:A:1267:A:C8	1:A:1268:A:H4'	2.23	0.73
3:C:52:LEU:HD12	3:C:52:LEU:O	1.88	0.73
4:D:62:GLN:HE22	4:D:65:ARG:NH1	1.86	0.73
12:L:36:VAL:HG22	12:L:82:VAL:HG12	1.71	0.73
1:A:923:A:H2'	1:A:924:G:H8	1.52	0.73
4:D:199:ASN:HD21	4:D:201:GLN:HB3	1.53	0.73
1:A:264:C:H2'	1:A:265:A:C8	2.23	0.73
1:A:514:U:O2'	1:A:515:A:P	2.46	0.73
1:A:714:G:OP1	1:A:749:A:H1'	1.88	0.73
1:A:1479:A:H5''	1:A:1480:A:OP2	1.88	0.73
19:S:64:GLU:O	19:S:67:VAL:HG23	1.88	0.73
20:T:103:GLY:O	20:T:104:LEU:HD23	1.89	0.73
1:A:1227:C:C2'	1:A:1228:U:H5'	2.17	0.73
12:L:28:LYS:O	12:L:30:ALA:N	2.22	0.73
1:A:31:G:O2'	1:A:32:A:OP1	2.07	0.73
1:A:916:G:H5''	7:G:102:ARG:NH2	2.04	0.73
16:P:74:LEU:O	16:P:79:VAL:HG23	1.88	0.73
1:A:803:U:H4'	1:A:804:G:OP2	1.87	0.73
1:A:949:C:O5'	10:J:57:LYS:HD3	1.89	0.73
1:A:1197:G:O2'	1:A:1198:C:H5'	1.88	0.73
1:A:1261:A:O2'	1:A:1262:U:OP1	2.05	0.73
1:A:733:G:N3	15:O:23:GLY:HA3	2.03	0.72
1:A:821:G:H2'	1:A:822:U:H5''	1.71	0.72
4:D:140:VAL:HG11	4:D:146:ILE:HD11	1.70	0.72
1:A:35:G:H2'	1:A:36:C:H6	1.54	0.72
1:A:513:G:H2'	1:A:514:U:OP2	1.89	0.72
17:Q:59:ILE:HG22	17:Q:71:PHE:CD1	2.25	0.72
1:A:1082:C:C6	1:A:1082:C:H3'	2.24	0.72
1:A:1349:C:H5'	10:J:60:ARG:HH12	1.54	0.72
4:D:3:ARG:HD3	4:D:118:ARG:HH11	1.55	0.72
16:P:51:VAL:O	16:P:52:ASP:HB3	1.89	0.72
1:A:982:A:C3'	1:A:983:A:H4'	2.19	0.72
23:X:31:A:H2'	23:X:31:A:N3	2.04	0.72
23:X:37:12A:H5'	23:X:37:12A:C8	2.17	0.72
4:D:127:THR:HG22	4:D:147:ALA:HB3	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:79:LYS:HG2	13:M:83:ASP:OD2	1.89	0.72
19:S:47:HIS:O	19:S:62:ILE:HG22	1.89	0.72
1:A:1004:G:H2'	1:A:1005:C:H5'	1.71	0.72
8:H:85:ARG:NE	8:H:87:SER:O	2.22	0.72
18:R:25:THR:HG22	18:R:42:ARG:HH11	1.54	0.72
2:B:86:GLU:C	2:B:88:ALA:H	1.97	0.72
10:J:47:PHE:CE2	14:N:37:PHE:HE1	2.07	0.72
16:P:34:GLU:OE2	16:P:55:ARG:HD3	1.89	0.71
1:A:994:A:H2'	1:A:995:G:O4'	1.90	0.71
3:C:157:ILE:HD13	3:C:166:GLU:HB2	1.72	0.71
4:D:151:LYS:HD2	4:D:151:LYS:N	2.04	0.71
20:T:57:ARG:HH21	20:T:100:ILE:HG22	1.54	0.71
1:A:269:A:O2'	1:A:270:G:H8	1.72	0.71
1:A:366:G:C2'	1:A:367:C:H5'	2.20	0.71
1:A:170:C:H2'	1:A:171:C:H6	1.54	0.71
10:J:39:PRO:HA	10:J:70:ARG:HH21	1.55	0.71
12:L:25:PRO:C	12:L:27:LEU:H	1.98	0.71
12:L:27:LEU:C	12:L:29:GLY:N	2.44	0.71
1:A:337:C:H2'	1:A:338:U:H5'	1.73	0.71
1:A:763:A:O2'	1:A:764:A:H5''	1.90	0.71
1:A:1449:U:H2'	1:A:1450:A:H8	1.54	0.71
10:J:50:ILE:HA	10:J:60:ARG:HD2	1.71	0.71
16:P:20:VAL:HG21	16:P:32:TYR:CG	2.26	0.71
3:C:91:LEU:HB3	3:C:99:VAL:HG21	1.72	0.71
1:A:513:G:H8	23:X:35:U:O2'	1.68	0.71
1:A:774:G:H2'	1:A:775:A:H5'	1.72	0.71
1:A:1254:G:H2'	1:A:1255:G:O4'	1.89	0.71
9:I:16:ARG:HE	9:I:64:THR:CG2	2.02	0.71
1:A:984:C:C6	1:A:985:C:C5	2.79	0.71
9:I:70:LYS:O	9:I:74:ILE:HG13	1.91	0.71
1:A:1124:G:C2'	1:A:1125:G:H5'	2.21	0.71
2:B:69:LEU:HD12	2:B:155:LEU:HD11	1.72	0.71
5:E:137:GLU:O	5:E:141:GLN:HG3	1.91	0.71
10:J:10:GLY:N	10:J:16:LEU:HD11	2.06	0.71
1:A:1035:G:C5'	1:A:1036:C:H5'	2.20	0.70
21:V:6:ARG:HD2	21:V:15:ARG:HH12	1.55	0.70
1:A:1348:C:H2'	1:A:1349:C:C6	2.25	0.70
4:D:104:VAL:HG11	4:D:146:ILE:CD1	2.20	0.70
5:E:42:GLY:HA3	5:E:66:MET:HE2	1.73	0.70
23:X:39:PSU:O2'	23:X:40:C:H5'	1.90	0.70
14:N:37:PHE:CE2	14:N:53:LEU:HD13	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:76:ARG:HG2	4:D:76:ARG:HH11	1.55	0.70
10:J:90:LEU:N	10:J:91:PRO:HD2	2.04	0.70
5:E:12:LEU:CD1	5:E:31:LEU:HB2	2.20	0.70
7:G:145:ALA:C	7:G:147:ALA:H	1.98	0.70
1:A:1279:C:C5	7:G:114:ARG:HD3	2.26	0.70
2:B:47:THR:HA	2:B:202:PRO:HG2	1.74	0.70
3:C:108:ASN:HD21	3:C:110:ASN:ND2	1.90	0.70
4:D:62:GLN:O	4:D:66:ARG:HB2	1.91	0.70
17:Q:21:VAL:HG21	17:Q:59:ILE:HD11	1.73	0.70
9:I:16:ARG:HG2	9:I:16:ARG:HH11	1.57	0.70
12:L:28:LYS:C	12:L:30:ALA:H	2.00	0.70
6:F:14:LEU:HA	6:F:18:GLN:NE2	2.07	0.69
13:M:49:THR:HG22	13:M:51:ALA:N	2.07	0.69
15:O:26:GLU:HG3	15:O:81:LEU:HG	1.72	0.69
1:A:238:A:C5'	1:A:239:U:H5'	2.22	0.69
1:A:1281:G:O2'	1:A:1282:U:H6	1.75	0.69
3:C:108:ASN:HD21	3:C:110:ASN:HD22	1.39	0.69
6:F:14:LEU:HB3	6:F:18:GLN:HB3	1.74	0.69
16:P:67:THR:HG22	16:P:68:ASP:N	2.06	0.69
8:H:86:ILE:O	8:H:88:LYS:HG2	1.93	0.69
11:K:80:VAL:HG13	11:K:103:LEU:HD22	1.73	0.69
12:L:6:THR:OG1	12:L:9:GLN:HG3	1.92	0.69
14:N:9:LYS:HG3	14:N:21:TYR:O	1.92	0.69
1:A:238:A:H5''	1:A:239:U:H5'	1.74	0.69
2:B:102:LEU:HD21	2:B:162:ILE:HD11	1.74	0.69
3:C:119:ARG:NE	3:C:140:ARG:HH12	1.90	0.69
4:D:35:ARG:O	4:D:36:ARG:HG3	1.92	0.69
1:A:242:G:N7	17:Q:96:GLN:NE2	2.40	0.69
1:A:1449:U:H2'	1:A:1450:A:C8	2.27	0.69
4:D:189:PRO:HB2	4:D:194:LEU:CD2	2.20	0.69
18:R:54:ARG:HD3	18:R:55:ARG:HG2	1.73	0.69
19:S:29:ARG:HD2	19:S:29:ARG:N	2.08	0.69
1:A:238:A:H4'	1:A:239:U:C5'	2.22	0.69
1:A:516:A:H8	1:A:516:A:O5'	1.75	0.69
1:A:780:C:OP1	11:K:124:LYS:HE2	1.93	0.69
18:R:31:LEU:O	18:R:69:THR:HG21	1.92	0.69
2:B:136:VAL:HA	2:B:139:LYS:NZ	2.09	0.69
2:B:213:LEU:O	2:B:217:ARG:HG2	1.93	0.69
10:J:12:ASP:HB3	10:J:15:THR:CG2	2.22	0.69
1:A:1228:U:H3'	1:A:1228:U:C6	2.29	0.68
5:E:12:LEU:HD12	5:E:31:LEU:HB2	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:930:G:H5'	1:A:942:A:H61	1.56	0.68
1:A:1328:G:N2	1:A:1355:G:H2'	2.06	0.68
13:M:17:VAL:O	13:M:20:THR:HB	1.93	0.68
17:Q:3:LYS:HB2	17:Q:60:ILE:HD11	1.75	0.68
1:A:1082:C:H3'	1:A:1082:C:H6	1.56	0.68
1:A:1475:U:H2'	1:A:1520:C:OP1	1.94	0.68
9:I:78:LYS:HE2	9:I:101:PHE:CD2	2.29	0.68
1:A:635:U:H2'	1:A:735:G:H1	1.58	0.68
1:A:748:G:H1	1:A:795:C:H2'	1.59	0.68
1:A:458:G:H5''	16:P:81:ARG:NH1	2.09	0.68
1:A:980:G:C2	1:A:981:G:C6	2.82	0.68
10:J:3:LYS:N	10:J:75:ILE:HG22	2.09	0.68
13:M:22:ILE:HD12	13:M:25:ILE:HD12	1.76	0.68
17:Q:67:LYS:HA	17:Q:70:ARG:NH1	2.08	0.68
1:A:341:G:H2'	1:A:342:G:C5'	2.23	0.68
1:A:1006:C:H3'	1:A:1006:C:C6	2.28	0.68
2:B:7:VAL:HG23	2:B:8:LYS:N	2.07	0.68
1:A:670:A:H4'	1:A:671:G:O5'	1.94	0.67
14:N:22:THR:HB	14:N:33:VAL:HG21	1.76	0.67
17:Q:63:ARG:HG2	17:Q:64:PRO:HD2	1.76	0.67
3:C:111:LEU:HD21	3:C:144:SER:O	1.93	0.67
21:V:3:LYS:H	21:V:3:LYS:HD2	1.60	0.67
1:A:1221:U:OP1	7:G:116:ALA:HB2	1.94	0.67
6:F:101:ALA:HB2	18:R:28:GLU:HG3	1.76	0.67
3:C:23:TYR:CD2	3:C:24:ALA:N	2.63	0.67
1:A:60:A:H4'	1:A:61:G:O5'	1.94	0.67
1:A:1026:A:H8	1:A:1026:A:OP1	1.77	0.67
1:A:1355:G:H5''	7:G:36:LYS:HB2	1.76	0.67
1:A:525:G:P	4:D:10:ARG:HH22	2.18	0.67
12:L:60:LEU:HD11	12:L:85:ILE:HD12	1.77	0.67
15:O:87:ILE:HG22	15:O:88:ARG:HG3	1.75	0.67
1:A:525:G:H2'	1:A:526:C:H6	1.59	0.67
2:B:51:LEU:HD22	2:B:55:PHE:CE2	2.29	0.67
10:J:53:PRO:HA	14:N:41:ARG:HH21	1.59	0.67
20:T:23:ARG:HH12	20:T:27:LYS:HZ1	1.42	0.67
11:K:57:THR:HG23	11:K:60:ALA:H	1.59	0.67
14:N:16:PHE:HB2	14:N:18:VAL:HG22	1.77	0.67
1:A:361:C:O2'	1:A:389:G:N2	2.28	0.67
1:A:1260:A:H5''	1:A:1261:A:OP1	1.94	0.66
2:B:21:ARG:HG3	2:B:22:LYS:N	2.10	0.66
9:I:78:LYS:HE2	9:I:101:PHE:HD2	1.59	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1379:C:H4'	1:A:1380:A:OP2	1.96	0.66
1:A:1521:U:O3'	22:W:1:A:P	2.53	0.66
13:M:11:ARG:HG2	13:M:12:ASN:N	2.10	0.66
1:A:774:G:C2'	1:A:775:A:H5'	2.25	0.66
1:A:960:A:H5'	1:A:961:C:OP2	1.96	0.66
2:B:211:ILE:HG22	2:B:215:LEU:HD12	1.76	0.66
3:C:129:ALA:HB3	3:C:132:ARG:HE	1.60	0.66
7:G:54:THR:HG22	7:G:56:GLN:H	1.60	0.66
1:A:1231:A:H4'	9:I:68:GLY:N	2.10	0.66
12:L:40:VAL:O	12:L:40:VAL:HG12	1.96	0.66
12:L:75:HIS:CD2	12:L:77:LEU:H	2.07	0.66
2:B:104:ASN:ND2	2:B:107:THR:HB	2.10	0.66
1:A:1130:U:H2'	1:A:1131:C:O4'	1.96	0.66
3:C:20:SER:O	14:N:54:PRO:HB3	1.96	0.66
7:G:75:VAL:HG21	7:G:144:MET:HE3	1.77	0.66
11:K:32:ILE:CG2	11:K:77:MET:HE2	2.24	0.66
1:A:670:A:N6	1:A:686:G:H1'	2.11	0.66
3:C:188:LEU:HD13	3:C:189:ALA:H	1.60	0.66
8:H:23:SER:HA	8:H:63:LEU:HD22	1.76	0.66
1:A:208:U:H5''	1:A:209:U:OP2	1.95	0.66
1:A:469:G:O2'	1:A:470:U:OP2	2.13	0.66
16:P:18:ARG:HG3	16:P:35:LYS:HE3	1.76	0.65
1:A:392:A:H5'	1:A:393:C:OP1	1.95	0.65
1:A:899:G:H4'	5:E:20:GLN:HA	1.77	0.65
1:A:1337:G:H2'	1:A:1338:A:C8	2.31	0.65
4:D:31:CYS:C	4:D:33:MET:H	2.03	0.65
6:F:2:ARG:HE	6:F:69:GLU:CG	2.06	0.65
1:A:424:U:H1'	1:A:425:A:H5''	1.78	0.65
1:A:738:G:OP2	15:O:65:ARG:HD2	1.96	0.65
2:B:211:ILE:O	2:B:215:LEU:HB2	1.96	0.65
3:C:188:LEU:O	3:C:189:ALA:HB2	1.94	0.65
4:D:3:ARG:HE	4:D:3:ARG:CA	2.09	0.65
1:A:930:G:C5'	1:A:942:A:H61	2.10	0.65
3:C:22:TRP:HB3	3:C:59:ARG:HB3	1.79	0.65
3:C:131:ARG:O	3:C:135:LYS:HG3	1.97	0.65
8:H:112:LEU:HD12	8:H:112:LEU:N	2.11	0.65
1:A:578:G:H2'	1:A:624:U:O4	1.96	0.65
9:I:48:GLU:OE2	9:I:51:ARG:HD2	1.96	0.65
23:X:39:PSU:C3'	23:X:40:C:C5'	2.73	0.65
1:A:1509:U:H2'	1:A:1510:C:H5'	1.78	0.65
11:K:87:THR:HG23	11:K:91:ARG:NH2	2.12	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:67:LYS:CA	17:Q:70:ARG:HH12	2.07	0.65
1:A:371:G:OP2	16:P:67:THR:HG21	1.96	0.65
1:A:1046:G:O2'	1:A:1171:G:N2	2.30	0.65
1:A:1506:G:H5''	1:A:1507:G:OP2	1.97	0.65
3:C:139:GLN:HA	3:C:139:GLN:HE21	1.62	0.65
1:A:513:G:N3	1:A:513:G:C5'	2.60	0.65
1:A:1205:G:O2'	1:A:1206:A:OP1	2.13	0.65
11:K:58:PRO:HB2	11:K:93:GLN:HG3	1.79	0.65
12:L:68:ALA:HB1	12:L:100:ILE:HG13	1.79	0.65
15:O:4:THR:OG1	15:O:7:GLU:HG3	1.97	0.65
1:A:465:G:H2'	1:A:467:C:N4	2.12	0.65
1:A:704:G:H4'	1:A:705:A:O5'	1.96	0.65
15:O:56:LEU:HA	15:O:59:MET:HE2	1.79	0.65
21:V:5:ASP:O	21:V:11:GLY:HA3	1.97	0.65
1:A:230:C:H5'	17:Q:70:ARG:HG2	1.78	0.65
1:A:931:G:H21	1:A:1208:A:H62	1.43	0.65
3:C:64:VAL:HG12	3:C:66:VAL:HG23	1.78	0.65
13:M:84:ILE:O	13:M:86:CYS:N	2.30	0.65
1:A:981:G:N2	1:A:1020:C:C2	2.64	0.64
1:A:1461:C:H2'	1:A:1462:U:H5'	1.79	0.64
2:B:88:ALA:C	2:B:90:MET:H	2.04	0.64
2:B:98:LEU:O	2:B:101:MET:HG3	1.96	0.64
1:A:400:U:H3'	1:A:401:G:H5'	1.78	0.64
1:A:432:U:H5''	4:D:155:LEU:HD22	1.79	0.64
1:A:1227:C:H2'	1:A:1228:U:C5'	2.27	0.64
1:A:1345:A:H1'	1:A:1347:G:N7	2.12	0.64
1:A:515:A:H5''	3:C:161:GLU:CD	2.20	0.64
1:A:545:C:O2'	12:L:15:ARG:HB3	1.97	0.64
1:A:824:U:C6	1:A:825:C:H1'	2.32	0.64
1:A:986:C:H42	1:A:1000:G:N2	1.96	0.64
19:S:53:ASN:HD22	19:S:53:ASN:N	1.94	0.64
1:A:1243:C:H2'	1:A:1244:C:C5'	2.26	0.64
1:A:323:C:O2	1:A:323:C:H2'	1.96	0.64
5:E:120:THR:HG22	5:E:121:LYS:N	2.11	0.64
21:V:6:ARG:HG2	21:V:15:ARG:NH1	2.12	0.64
1:A:238:A:C4'	1:A:239:U:H5'	2.27	0.64
2:B:117:GLU:O	2:B:120:ALA:HB3	1.97	0.64
3:C:139:GLN:HA	3:C:139:GLN:NE2	2.12	0.64
12:L:24:VAL:HG23	12:L:24:VAL:O	1.97	0.64
1:A:825:C:C6	1:A:825:C:H3'	2.32	0.64
1:A:1121:G:N2	1:A:1125:G:H21	1.95	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:96:ARG:N	2:B:96:ARG:HD2	2.12	0.64
2:B:118:LEU:HB2	2:B:142:LEU:HD12	1.78	0.64
3:C:58:GLU:H	3:C:65:ALA:HB3	1.62	0.64
9:I:29:ASN:HD21	9:I:65:VAL:HG12	1.63	0.64
12:L:55:VAL:CG1	12:L:67:THR:HG23	2.28	0.64
1:A:866:A:H4'	1:A:867:G:O5'	1.97	0.64
1:A:1139:A:H5'	1:A:1140:C:C6	2.32	0.64
1:A:1297:G:N2	1:A:1299:A:H3'	2.13	0.64
1:A:1333:C:H2'	1:A:1334:G:C8	2.33	0.64
1:A:1433:G:H2'	1:A:1434:G:O4'	1.98	0.64
1:A:387:G:H2'	1:A:388:A:H8	1.63	0.64
1:A:516:A:O2'	1:A:518:A:OP2	2.09	0.64
1:A:934:U:H3	1:A:937:U:C5'	2.10	0.64
1:A:1482:G:H4'	1:A:1483:U:O5'	1.97	0.64
1:A:1258:C:H3'	1:A:1258:C:C6	2.33	0.64
3:C:148:GLY:HA3	3:C:172:ARG:O	1.98	0.64
3:C:156:ARG:H	3:C:163:ALA:HA	1.63	0.64
6:F:4:TYR:CZ	6:F:72:VAL:HG21	2.33	0.64
20:T:82:SER:O	20:T:86:ARG:HB2	1.97	0.63
1:A:1036:C:N3	23:X:34:70U:H4'	2.13	0.63
1:A:1349:C:H5'	10:J:60:ARG:NH1	2.13	0.63
5:E:63:ARG:HA	5:E:66:MET:HE3	1.80	0.63
5:E:81:GLU:CD	5:E:88:LYS:HE2	2.24	0.63
13:M:106:ASN:O	13:M:107:ALA:HB2	1.99	0.63
2:B:132:LYS:HG2	2:B:135:GLN:OE1	1.98	0.63
4:D:117:ALA:O	4:D:121:VAL:HG23	1.98	0.63
1:A:1258:C:H3'	1:A:1258:C:H6	1.64	0.63
2:B:189:ASP:O	2:B:191:ASP:N	2.30	0.63
6:F:26:ILE:O	6:F:30:LEU:HG	1.99	0.63
19:S:6:LYS:HG2	19:S:7:LYS:H	1.62	0.63
1:A:1022:U:H2'	1:A:1023:A:C8	2.33	0.63
1:A:1163:G:O2'	1:A:1164:A:OP2	2.16	0.63
1:A:1301:C:N4	19:S:36:ARG:HG3	2.13	0.63
15:O:17:ARG:HG3	15:O:17:ARG:NH1	2.07	0.63
17:Q:65:ILE:HD12	17:Q:65:ILE:N	2.13	0.63
13:M:5:ALA:HB3	13:M:8:GLU:HB2	1.79	0.63
1:A:173:A:H2'	1:A:174:U:C6	2.34	0.63
3:C:204:LEU:N	3:C:204:LEU:HD23	2.14	0.63
13:M:50:GLU:O	13:M:54:VAL:HG23	1.99	0.63
8:H:56:LYS:HD2	8:H:56:LYS:N	2.14	0.63
19:S:53:ASN:N	19:S:53:ASN:ND2	2.46	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:8:LEU:HD12	10:J:20:ALA:HB2	1.81	0.63
1:A:669:U:O4	1:A:686:G:O2'	2.11	0.62
1:A:981:G:H22	1:A:982:A:H1'	1.58	0.62
4:D:22:LYS:HB3	4:D:26:CYS:SG	2.38	0.62
4:D:24:GLU:O	4:D:25:ARG:HB3	1.98	0.62
4:D:70:ILE:HD11	4:D:100:ARG:NE	2.13	0.62
8:H:4:ASP:OD2	8:H:85:ARG:NH1	2.32	0.62
8:H:64:LYS:CG	8:H:79:VAL:HG21	2.29	0.62
9:I:5:TYR:O	9:I:87:GLN:HG3	1.99	0.62
19:S:16:LEU:O	19:S:19:VAL:HG12	1.98	0.62
6:F:11:ASN:O	6:F:14:LEU:HD11	1.99	0.62
1:A:275:C:H4'	1:A:276:G:OP2	1.97	0.62
1:A:986:C:O5'	1:A:986:C:H6	1.81	0.62
1:A:1035:G:N7	1:A:1181:C:H5''	2.15	0.62
4:D:100:ARG:NH1	4:D:137:SER:HA	2.14	0.62
5:E:99:GLY:O	5:E:117:ASP:HA	1.99	0.62
17:Q:67:LYS:O	17:Q:69:LYS:N	2.29	0.62
1:A:446:A:O2'	1:A:447:A:O5'	2.15	0.62
1:A:900:A:OP1	5:E:21:ALA:HB2	1.99	0.62
2:B:178:ARG:HG3	2:B:178:ARG:NH1	2.13	0.62
5:E:145:LYS:HA	8:H:107:LEU:HD21	1.81	0.62
1:A:1121:G:H21	1:A:1125:G:H21	1.47	0.62
1:A:1197:G:H5''	14:N:5:ALA:HB2	1.80	0.62
1:A:1425:G:H5''	1:A:1426:A:H4'	1.82	0.62
1:A:1425:G:H5''	1:A:1426:A:H5'	1.82	0.62
1:A:1328:G:O2'	1:A:1329:U:OP2	2.18	0.62
10:J:49:VAL:O	10:J:60:ARG:HA	2.00	0.62
1:A:8:A:H4'	1:A:9:G:OP1	1.97	0.62
1:A:276:G:O2'	1:A:277:A:OP2	2.18	0.62
5:E:29:GLY:HA2	5:E:47:LYS:HG3	1.82	0.62
5:E:79:GLU:HG3	5:E:93:PRO:HD2	1.81	0.62
7:G:115:ARG:HB2	7:G:118:VAL:HG23	1.82	0.62
9:I:125:TYR:CE1	9:I:128:ARG:HB3	2.29	0.62
20:T:37:SER:O	20:T:41:VAL:HG23	1.99	0.62
1:A:423:G:H4'	1:A:424:U:O5'	1.99	0.62
2:B:9:GLU:HA	2:B:12:GLU:OE2	1.99	0.62
3:C:14:ILE:HG22	3:C:15:THR:N	2.15	0.62
6:F:19:LEU:HD23	6:F:20:ALA:N	2.15	0.62
9:I:16:ARG:HE	9:I:64:THR:HG21	1.65	0.62
1:A:937:U:O2'	1:A:1204:C:H4'	1.99	0.61
25:A:1783:PAR:H13	25:A:1783:PAR:O62	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:199:ASN:ND2	4:D:201:GLN:HB3	2.13	0.61
20:T:10:LEU:O	20:T:13:LEU:HG	2.00	0.61
1:A:501:C:N4	1:A:513:G:N2	2.48	0.61
1:A:570:G:H4'	1:A:571:G:OP1	1.98	0.61
1:A:775:A:H4'	1:A:776:U:C5'	2.30	0.61
2:B:51:LEU:HD22	2:B:55:PHE:HE2	1.64	0.61
4:D:11:LEU:O	4:D:15:GLU:HB2	2.00	0.61
9:I:9:ARG:HA	9:I:13:ALA:O	1.99	0.61
19:S:51:VAL:O	19:S:58:VAL:HG22	1.99	0.61
1:A:1521:U:O2'	22:W:1:A:OP1	2.07	0.61
16:P:36:ILE:O	16:P:51:VAL:O	2.18	0.61
2:B:230:VAL:HG12	2:B:231:GLU:N	2.15	0.61
7:G:15:ASP:HB3	7:G:20:ASP:H	1.65	0.61
12:L:28:LYS:C	12:L:30:ALA:N	2.54	0.61
13:M:25:ILE:HD11	13:M:60:VAL:CG1	2.30	0.61
1:A:407:A:N1	4:D:35:ARG:HG3	2.15	0.61
7:G:26:PHE:CE2	7:G:30:ILE:HD11	2.35	0.61
9:I:86:VAL:HG13	9:I:90:PRO:HA	1.83	0.61
10:J:32:ALA:CB	10:J:75:ILE:HG13	2.30	0.61
11:K:126:ARG:O	11:K:127:LYS:HB2	1.99	0.61
12:L:39:VAL:HG12	12:L:41:ARG:H	1.64	0.61
14:N:12:ARG:C	14:N:14:PRO:HD3	2.26	0.61
1:A:1031:U:H2'	14:N:3:ARG:HH11	1.66	0.61
1:A:1222:G:H2'	1:A:1223:C:C6	2.36	0.61
11:K:48:ILE:HD11	11:K:64:ALA:HA	1.82	0.61
12:L:115:LYS:O	12:L:117:ARG:N	2.30	0.61
13:M:25:ILE:HD11	13:M:60:VAL:HG11	1.81	0.61
20:T:57:ARG:NH2	20:T:100:ILE:HG22	2.16	0.61
2:B:76:GLN:HG3	2:B:206:ASP:OD1	2.00	0.61
3:C:58:GLU:HB2	3:C:65:ALA:CB	2.31	0.61
3:C:132:ARG:O	3:C:136:GLN:HG3	1.99	0.61
3:C:155:GLY:HA3	3:C:163:ALA:HB1	1.83	0.61
4:D:3:ARG:NH2	4:D:71:SER:HB3	2.15	0.61
6:F:8:ILE:HD11	6:F:79:LEU:HD13	1.81	0.61
7:G:15:ASP:CB	7:G:20:ASP:H	2.12	0.61
15:O:61:GLY:O	15:O:64:ARG:HG2	2.01	0.61
1:A:830:G:O2'	1:A:831:G:H5'	2.01	0.61
1:A:1082:C:C6	1:A:1082:C:C3'	2.83	0.61
3:C:40:ARG:O	3:C:44:GLU:HB3	2.01	0.61
10:J:8:LEU:HB3	10:J:16:LEU:HD22	1.82	0.61
17:Q:24:GLU:HG2	17:Q:39:SER:HB3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:91:LYS:HA	12:L:91:LYS:CE	2.31	0.61
1:A:1373:U:H2'	1:A:1374:G:C8	2.36	0.61
1:A:1387:G:P	25:A:1783:PAR:HO34	2.24	0.61
2:B:161:ALA:HB1	2:B:185:ILE:HD11	1.83	0.61
11:K:14:VAL:HG21	11:K:40:ILE:HD11	1.83	0.61
21:V:14:TRP:C	21:V:16:GLY:H	2.08	0.61
1:A:341:G:C2'	1:A:342:G:H5'	2.31	0.60
1:A:944:C:O2'	9:I:128:ARG:HD3	2.00	0.60
1:A:966:C:H42	1:A:1197:G:H1	1.48	0.60
1:A:1003:U:H3'	1:A:1003:U:H6	1.65	0.60
1:A:1008:C:N4	1:A:1014:G:N1	2.49	0.60
2:B:36:ARG:HD2	2:B:41:ILE:HD13	1.82	0.60
2:B:47:THR:HG23	2:B:202:PRO:O	2.00	0.60
4:D:15:GLU:HG3	4:D:63:LYS:HG3	1.83	0.60
4:D:36:ARG:N	4:D:37:PRO:HD3	2.16	0.60
17:Q:76:LEU:HD23	17:Q:77:VAL:N	2.16	0.60
19:S:29:ARG:H	19:S:29:ARG:CD	2.12	0.60
1:A:952:A:H5'	1:A:952:A:H8	1.65	0.60
1:A:983:A:OP2	1:A:984:C:C5	2.54	0.60
7:G:38:LEU:HA	7:G:41:ARG:HD3	1.83	0.60
14:N:14:PRO:C	14:N:16:PHE:H	2.08	0.60
15:O:25:THR:HG21	15:O:70:LEU:HB2	1.83	0.60
1:A:1120:G:H3'	1:A:1120:G:N3	2.16	0.60
3:C:14:ILE:HG22	3:C:15:THR:HG23	1.83	0.60
3:C:82:GLU:HG3	3:C:83:ARG:H	1.67	0.60
1:A:472:C:O5'	1:A:472:C:H6	1.83	0.60
10:J:4:ILE:N	10:J:4:ILE:HD12	2.16	0.60
18:R:25:THR:HG21	18:R:42:ARG:HD3	1.83	0.60
1:A:635:U:H2'	1:A:735:G:N1	2.16	0.60
2:B:33:TYR:HB3	2:B:41:ILE:HG13	1.82	0.60
2:B:80:ILE:CD1	2:B:208:ILE:HG23	2.19	0.60
9:I:48:GLU:HA	9:I:51:ARG:NH1	2.14	0.60
9:I:55:ALA:C	9:I:57:GLY:H	2.09	0.60
10:J:61:GLU:OE1	14:N:45:ARG:NH1	2.34	0.60
23:X:33:U:H5'	23:X:34:70U:OP2	2.02	0.60
1:A:448:C:H41	1:A:462:A:H2	1.50	0.60
1:A:1080:C:H2'	1:A:1081:G:C8	2.36	0.60
1:A:1109:G:H21	1:A:1128:A:H62	1.50	0.60
1:A:1131:C:H2'	1:A:1132:U:C6	2.36	0.60
6:F:33:TYR:CD1	6:F:75:LEU:HD23	2.37	0.60
9:I:47:LEU:C	9:I:49:PRO:HD2	2.26	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:41:ARG:HB3	12:L:41:ARG:CZ	2.31	0.60
14:N:13:THR:O	14:N:13:THR:HG22	2.01	0.60
2:B:142:LEU:HD21	2:B:146:GLN:OE1	2.01	0.60
5:E:116:THR:HG23	5:E:117:ASP:OD2	2.02	0.60
15:O:55:GLY:HA2	15:O:58:MET:HE2	1.81	0.60
23:X:39:PSU:H5'	23:X:39:PSU:C6	2.35	0.60
1:A:171:C:OP1	20:T:65:LYS:NZ	2.28	0.60
8:H:83:ILE:HG23	8:H:83:ILE:O	2.01	0.60
10:J:12:ASP:HB3	10:J:15:THR:HG22	1.82	0.60
1:A:84:C:H6	1:A:84:C:O5'	1.85	0.60
1:A:916:G:H5''	7:G:102:ARG:HH22	1.67	0.60
1:A:959:U:OP1	1:A:959:U:H6	1.84	0.60
1:A:1509:U:C2'	1:A:1510:C:H5'	2.31	0.60
2:B:132:LYS:O	2:B:136:VAL:HG23	2.00	0.60
4:D:189:PRO:CB	4:D:194:LEU:HD21	2.27	0.60
9:I:13:ALA:HA	9:I:67:GLY:O	2.02	0.60
18:R:38:GLU:HA	18:R:41:LYS:HE2	1.82	0.60
1:A:795:C:H4'	1:A:796:U:H5'	1.82	0.59
1:A:1193:U:O2'	1:A:1194:A:C8	2.49	0.59
1:A:1406:C:O2'	1:A:1407:U:H5'	2.01	0.59
4:D:127:THR:CG2	4:D:147:ALA:HB3	2.31	0.59
6:F:1:MET:HA	6:F:1:MET:HE2	1.83	0.59
9:I:19:LEU:CD2	9:I:61:ALA:HB2	2.32	0.59
16:P:26:ARG:HD2	16:P:31:LYS:O	2.02	0.59
17:Q:13:ASP:C	17:Q:15:MET:H	2.10	0.59
1:A:17:U:H2'	1:A:18:C:C6	2.37	0.59
2:B:28:PHE:CD2	2:B:190:THR:HA	2.37	0.59
3:C:58:GLU:HB2	3:C:65:ALA:HB2	1.83	0.59
10:J:8:LEU:CD1	10:J:20:ALA:HB2	2.31	0.59
14:N:8:GLU:HB2	14:N:11:LYS:HB2	1.83	0.59
17:Q:27:PHE:HB2	17:Q:28:PRO:HD2	1.84	0.59
1:A:954:A:H2'	1:A:955:A:H5''	1.84	0.59
2:B:21:ARG:O	2:B:22:LYS:HD2	2.01	0.59
3:C:139:GLN:HE21	3:C:139:GLN:CA	2.14	0.59
6:F:11:ASN:ND2	6:F:13:ASN:H	1.96	0.59
13:M:40:ASN:ND2	13:M:41:PRO:HD2	2.17	0.59
14:N:32:SER:HB3	14:N:41:ARG:HB3	1.84	0.59
1:A:1035:G:H5'	1:A:1036:C:C5'	2.29	0.59
3:C:175:LEU:HD21	3:C:201:TYR:HE2	1.66	0.59
5:E:76:ILE:HG23	5:E:142:LEU:HD13	1.84	0.59
20:T:59:ALA:O	20:T:63:ILE:HG13	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:969:U:O2'	1:A:970:G:OP2	2.20	0.59
1:A:1006:C:H2'	1:A:1007:C:O4'	2.02	0.59
5:E:120:THR:CG2	5:E:121:LYS:N	2.64	0.59
8:H:89:PRO:HA	8:H:92:ARG:NH1	2.17	0.59
18:R:46:GLU:H	18:R:46:GLU:CD	2.11	0.59
18:R:55:ARG:HB3	18:R:55:ARG:CZ	2.33	0.59
1:A:625:A:C8	8:H:115:SER:HA	2.38	0.59
1:A:984:C:C6	1:A:985:C:H5	2.21	0.59
1:A:1394:C:H2'	1:A:1395:A:C8	2.37	0.59
12:L:124:LYS:HD2	12:L:125:PRO:HD2	1.85	0.59
1:A:1005:C:H2'	1:A:1006:C:C5	2.37	0.59
6:F:67:MET:HE1	6:F:75:LEU:HB2	1.84	0.59
23:X:39:PSU:H2'	23:X:40:C:O4'	2.03	0.59
9:I:111:ARG:HD2	14:N:61:TRP:OXT	2.03	0.59
14:N:8:GLU:O	14:N:11:LYS:HB2	2.02	0.59
1:A:1082:C:N4	1:A:1085:C:OP1	2.35	0.59
1:A:1461:C:C2'	1:A:1462:U:H5'	2.32	0.59
9:I:16:ARG:HG2	9:I:16:ARG:NH1	2.18	0.59
10:J:71:LEU:CD1	10:J:73:ASP:HB2	2.33	0.59
12:L:65:GLU:CD	12:L:65:GLU:N	2.61	0.59
15:O:21:ASP:OD1	15:O:24:SER:HB3	2.02	0.59
16:P:8:ARG:HB2	16:P:28:ARG:NH1	2.17	0.59
18:R:86:VAL:O	18:R:87:ARG:HB2	2.02	0.59
1:A:328:G:H4'	20:T:16:HIS:CE1	2.38	0.59
1:A:396:C:H1'	1:A:605:A:H1'	1.84	0.59
1:A:408:G:H22	1:A:424:U:H5''	1.68	0.59
1:A:417:C:O2'	1:A:418:G:OP2	2.17	0.59
1:A:981:G:H21	1:A:982:A:C1'	2.08	0.59
14:N:3:ARG:HH21	14:N:6:LEU:HD11	1.65	0.59
1:A:999:G:O2'	1:A:1000:G:H5'	2.03	0.58
6:F:101:ALA:HB2	18:R:28:GLU:CG	2.33	0.58
8:H:68:ARG:HB3	8:H:68:ARG:NH1	2.14	0.58
9:I:16:ARG:NE	9:I:64:THR:CG2	2.66	0.58
10:J:4:ILE:HD13	10:J:74:ILE:O	2.03	0.58
11:K:69:ALA:O	11:K:73:MET:HG2	2.03	0.58
13:M:94:ARG:NH1	19:S:81:ARG:HD3	2.09	0.58
16:P:52:ASP:O	16:P:52:ASP:OD1	2.21	0.58
18:R:26:LEU:N	18:R:26:LEU:HD23	2.18	0.58
1:A:1231:A:C4'	9:I:68:GLY:H	2.14	0.58
1:A:1253:G:O2'	1:A:1254:G:H5'	2.03	0.58
1:A:1324:G:H2'	1:A:1325:C:C6	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1387:G:P	25:A:1783:PAR:O34	2.61	0.58
2:B:12:GLU:OE1	2:B:12:GLU:N	2.35	0.58
13:M:37:THR:CG2	13:M:55:ARG:HD2	2.33	0.58
19:S:44:MET:O	19:S:47:HIS:HB2	2.03	0.58
1:A:929:U:O4	13:M:104:ARG:HD3	2.03	0.58
1:A:1288:U:H5'	13:M:109:THR:HG21	1.85	0.58
3:C:22:TRP:CH2	3:C:32:LEU:HB2	2.37	0.58
3:C:155:GLY:O	3:C:196:LEU:HD22	2.03	0.58
4:D:64:LEU:HD21	4:D:97:LEU:CD1	2.33	0.58
4:D:196:LEU:HB3	4:D:198:VAL:HG22	1.84	0.58
6:F:37:VAL:HA	6:F:65:VAL:HG12	1.84	0.58
21:V:2:GLY:C	21:V:4:GLY:H	2.11	0.58
1:A:446:A:HO2'	1:A:447:A:C5'	2.16	0.58
1:A:685:A:H4'	1:A:686:G:OP2	2.04	0.58
2:B:61:LEU:HD21	2:B:160:ASP:CB	2.32	0.58
2:B:208:ILE:C	2:B:210:SER:H	2.11	0.58
4:D:151:LYS:H	4:D:151:LYS:CD	2.10	0.58
5:E:76:ILE:HG22	5:E:78:HIS:H	1.69	0.58
7:G:9:VAL:O	7:G:10:ARG:C	2.45	0.58
10:J:61:GLU:OE2	14:N:58:LYS:NZ	2.36	0.58
11:K:57:THR:OG1	11:K:58:PRO:HD2	2.04	0.58
12:L:47:LYS:HB2	12:L:47:LYS:NZ	2.17	0.58
13:M:40:ASN:HD22	13:M:41:PRO:N	2.00	0.58
15:O:17:ARG:HH11	15:O:17:ARG:CG	2.12	0.58
1:A:980:G:C2	1:A:981:G:C5	2.91	0.58
2:B:118:LEU:CB	2:B:142:LEU:HD12	2.33	0.58
1:A:1006:C:O5'	1:A:1006:C:H6	1.87	0.58
1:A:1062:A:O3'	5:E:16:THR:OG1	2.21	0.58
1:A:1295:C:C5	19:S:6:LYS:HE2	2.39	0.58
7:G:66:VAL:O	7:G:70:LYS:HG3	2.03	0.58
1:A:1286:G:N2	1:A:1312:G:HO2'	2.02	0.58
3:C:175:LEU:HD21	3:C:201:TYR:CE2	2.39	0.58
4:D:64:LEU:HD21	4:D:97:LEU:HD13	1.84	0.58
10:J:49:VAL:HG13	14:N:41:ARG:HB2	1.85	0.58
18:R:22:VAL:HB	18:R:56:THR:HA	1.85	0.58
1:A:1354:U:O2'	1:A:1355:G:H5'	2.04	0.58
2:B:95:GLN:C	2:B:96:ARG:HD2	2.29	0.58
4:D:15:GLU:CG	4:D:63:LYS:HG3	2.34	0.58
1:A:713:G:N2	1:A:748:G:H5''	2.19	0.58
1:A:824:U:C5	1:A:825:C:H1'	2.39	0.58
1:A:1301:C:C2'	1:A:1302:C:O5'	2.51	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1301:C:H2'	1:A:1302:C:O5'	2.03	0.58
1:A:1505:U:O2'	1:A:1506:G:H3'	2.04	0.58
4:D:62:GLN:HE22	4:D:65:ARG:HH12	1.51	0.58
5:E:82:VAL:HG21	5:E:138:ALA:HA	1.85	0.58
9:I:9:ARG:HD3	9:I:14:VAL:CG1	2.34	0.58
10:J:29:ARG:NH1	10:J:29:ARG:HG2	2.17	0.58
16:P:20:VAL:HG23	16:P:34:GLU:O	2.03	0.58
1:A:406:A:C4	1:A:408:G:H1'	2.39	0.58
1:A:603:C:H2'	1:A:604:A:O4'	2.03	0.58
1:A:629:U:H2'	1:A:630:C:C6	2.39	0.58
1:A:705:A:H4'	1:A:706:U:OP1	2.04	0.58
1:A:726:U:H2'	1:A:727:C:C6	2.39	0.58
1:A:1157:A:H2'	1:A:1158:G:C8	2.39	0.58
1:A:1206:A:H3'	1:A:1207:C:C5	2.39	0.58
1:A:1299:A:H8	1:A:1299:A:OP2	1.87	0.58
3:C:11:ARG:O	3:C:14:ILE:O	2.20	0.58
8:H:49:GLU:HG2	8:H:62:TYR:HE2	1.68	0.58
23:X:34:70U:H2'	23:X:35:U:H6	1.69	0.58
1:A:670:A:H62	1:A:686:G:H1'	1.69	0.57
1:A:823:C:H4'	1:A:824:U:OP1	2.04	0.57
4:D:157:LEU:HD23	4:D:157:LEU:O	2.04	0.57
7:G:23:VAL:O	7:G:27:ILE:HG13	2.03	0.57
7:G:38:LEU:HD12	7:G:38:LEU:O	2.04	0.57
1:A:656:G:H2'	1:A:657:G:C8	2.40	0.57
1:A:1458:U:H2'	1:A:1459:G:H5'	1.86	0.57
2:B:7:VAL:HB	2:B:8:LYS:NZ	2.18	0.57
3:C:193:TYR:HE1	3:C:196:LEU:HD21	1.69	0.57
4:D:3:ARG:HE	4:D:3:ARG:HA	1.68	0.57
4:D:196:LEU:CD2	4:D:197:PRO:HD2	2.34	0.57
9:I:121:ARG:HG2	9:I:121:ARG:HH11	1.69	0.57
1:A:52:G:O2'	1:A:53:A:H5'	2.04	0.57
1:A:1287:A:C2	1:A:1288:U:H1'	2.39	0.57
10:J:60:ARG:HG2	10:J:60:ARG:HH11	1.69	0.57
13:M:35:GLU:C	13:M:37:THR:H	2.12	0.57
1:A:120:G:HO2'	17:Q:2:PRO:N	2.03	0.57
1:A:500:G:O2'	1:A:501:C:OP2	2.21	0.57
2:B:7:VAL:CG2	2:B:8:LYS:HZ3	2.16	0.57
3:C:126:ARG:HH11	3:C:126:ARG:HG3	1.69	0.57
3:C:129:ALA:CB	3:C:132:ARG:HE	2.17	0.57
5:E:24:ARG:HG2	5:E:24:ARG:HH11	1.70	0.57
9:I:79:LEU:HD22	9:I:83:ARG:HG3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:3:LYS:N	10:J:75:ILE:HA	2.19	0.57
13:M:3:ARG:HA	13:M:8:GLU:O	2.04	0.57
15:O:71:GLN:HB2	15:O:78:TYR:CD1	2.40	0.57
1:A:984:C:C2'	1:A:985:C:C5	2.86	0.57
2:B:101:MET:HG2	2:B:108:ILE:HD13	1.85	0.57
7:G:18:TYR:CD1	7:G:59:LEU:HB2	2.40	0.57
7:G:38:LEU:O	7:G:42:ILE:HG13	2.04	0.57
7:G:121:ALA:O	7:G:125:MET:HG3	2.04	0.57
16:P:28:ARG:HG2	16:P:28:ARG:NH1	2.16	0.57
1:A:109:A:H2'	1:A:110:G:O4'	2.04	0.57
1:A:1131:C:O2'	1:A:1261:A:N1	2.37	0.57
1:A:1183:G:H2'	1:A:1184:C:C5'	2.34	0.57
4:D:8:VAL:HG11	4:D:115:ARG:NH1	2.19	0.57
8:H:2:LEU:H	8:H:2:LEU:HD12	1.70	0.57
1:A:432:U:O2'	4:D:123:HIS:HD2	1.87	0.57
1:A:520:G:OP1	12:L:113:ARG:NH2	2.37	0.57
5:E:13:ILE:HD12	5:E:13:ILE:C	2.29	0.57
6:F:99:ALA:O	6:F:100:ASN:HB2	2.04	0.57
10:J:29:ARG:HG2	10:J:29:ARG:HH11	1.68	0.57
12:L:60:LEU:HB2	12:L:64:TYR:O	2.05	0.57
17:Q:68:ARG:HH11	17:Q:68:ARG:HG3	1.69	0.57
20:T:23:ARG:HH12	20:T:27:LYS:NZ	2.03	0.57
1:A:170:C:H2'	1:A:171:C:C6	2.37	0.57
1:A:909:C:H5'	7:G:4:ARG:HG2	1.87	0.57
2:B:14:GLY:C	2:B:15:VAL:HG22	2.30	0.57
3:C:10:PHE:CE2	3:C:178:LEU:HD13	2.40	0.57
20:T:23:ARG:HG2	20:T:23:ARG:HH11	1.69	0.57
1:A:241:A:C4'	1:A:242:G:OP1	2.44	0.57
1:A:796:U:OP1	1:A:881:C:H5'	2.05	0.57
1:A:980:G:N1	1:A:981:G:O6	2.37	0.57
6:F:47:ARG:N	6:F:47:ARG:HD3	2.20	0.57
9:I:97:LYS:HG2	9:I:102:LEU:HD12	1.87	0.57
10:J:80:LYS:O	10:J:83:GLU:HB3	2.04	0.57
14:N:44:LEU:HD12	14:N:44:LEU:O	2.05	0.57
1:A:1031:U:H1'	1:A:1182:A:C8	2.40	0.57
10:J:24:VAL:O	10:J:28:ARG:HG2	2.05	0.57
13:M:33:ALA:HA	13:M:59:TYR:HE2	1.70	0.57
14:N:57:ARG:HG2	14:N:58:LYS:N	2.14	0.57
1:A:242:G:OP1	1:A:242:G:H4'	2.05	0.56
2:B:87:ARG:NE	2:B:233:SER:HB3	2.20	0.56
10:J:75:ILE:O	10:J:76:ASN:HB2	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:16:LEU:HA	19:S:19:VAL:HG12	1.87	0.56
1:A:181:C:C1'	20:T:85:MET:HE2	2.35	0.56
1:A:500:G:H5'	1:A:502:C:C2	2.40	0.56
1:A:953:G:O2'	1:A:954:A:H5'	2.03	0.56
1:A:1126:G:H8	1:A:1126:G:H3'	1.71	0.56
1:A:1220:A:H4'	1:A:1221:U:O5'	2.05	0.56
1:A:1303:C:C4'	1:A:1304:G:OP1	2.40	0.56
5:E:144:THR:O	5:E:148:VAL:HG23	2.04	0.56
8:H:68:ARG:HH11	8:H:68:ARG:CB	2.17	0.56
21:V:6:ARG:CD	21:V:15:ARG:HH12	2.17	0.56
1:A:501:C:H5	1:A:513:G:C5'	2.18	0.56
1:A:996:C:O5'	1:A:996:C:H6	1.87	0.56
1:A:1311:U:H2'	1:A:1312:G:H5'	1.87	0.56
2:B:136:VAL:HA	2:B:139:LYS:HZ3	1.71	0.56
10:J:90:LEU:H	10:J:91:PRO:CD	2.09	0.56
13:M:5:ALA:HB3	13:M:8:GLU:HG3	1.87	0.56
13:M:65:LYS:O	13:M:66:LEU:HD23	2.05	0.56
1:A:66:G:H8	1:A:66:G:OP1	1.88	0.56
1:A:818:U:OP1	18:R:64:ARG:NH2	2.35	0.56
1:A:1042:C:H5	3:C:2:GLY:HA2	1.69	0.56
3:C:155:GLY:HA2	3:C:164:ARG:O	2.06	0.56
3:C:191:THR:HG21	3:C:193:TYR:CE2	2.40	0.56
4:D:194:LEU:HD22	4:D:194:LEU:N	2.20	0.56
6:F:8:ILE:HG22	6:F:10:LEU:HD23	1.88	0.56
23:X:37:12A:H8	23:X:37:12A:C5'	2.22	0.56
1:A:1006:C:N4	1:A:1016:G:N2	2.52	0.56
1:A:1301:C:N3	19:S:36:ARG:NE	2.52	0.56
2:B:79:ASP:O	2:B:82:ARG:HB3	2.06	0.56
2:B:98:LEU:HB2	2:B:108:ILE:HD11	1.87	0.56
2:B:218:ALA:O	2:B:222:ILE:HG13	2.05	0.56
4:D:175:SER:HB3	4:D:184:LYS:HB2	1.87	0.56
4:D:209:ARG:HG2	4:D:209:ARG:HH11	1.71	0.56
5:E:48:ALA:HB1	5:E:49:PRO:HD2	1.87	0.56
6:F:19:LEU:HD23	6:F:19:LEU:C	2.31	0.56
16:P:3:LYS:O	16:P:21:VAL:HA	2.06	0.56
17:Q:90:ILE:HA	17:Q:93:GLN:HB2	1.87	0.56
1:A:79:U:H3'	1:A:79:U:C6	2.41	0.56
1:A:713:G:H21	1:A:748:G:H5''	1.71	0.56
1:A:1006:C:C6	1:A:1006:C:C3'	2.87	0.56
1:A:1286:G:H22	1:A:1312:G:C2'	2.18	0.56
5:E:11:ILE:HB	5:E:31:LEU:HB3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:5:ARG:HD2	10:J:99:LYS:HB2	1.87	0.56
10:J:49:VAL:HG11	14:N:41:ARG:O	2.06	0.56
21:V:6:ARG:CG	21:V:15:ARG:NH1	2.69	0.56
1:A:66:G:OP1	1:A:66:G:C8	2.59	0.56
1:A:401:G:H5''	4:D:5:ILE:HG23	1.87	0.56
1:A:1123:C:H2'	1:A:1124:G:C5'	2.35	0.56
1:A:1136:G:H2'	1:A:1137:G:C8	2.39	0.56
1:A:1262:U:H4'	1:A:1263:C:OP2	2.06	0.56
3:C:79:ARG:HG2	3:C:82:GLU:OE1	2.06	0.56
20:T:23:ARG:HG2	20:T:23:ARG:NH1	2.20	0.56
1:A:686:G:O2'	1:A:687:A:OP2	2.23	0.56
14:N:29:ARG:HH22	14:N:41:ARG:HH12	1.52	0.56
1:A:224:U:H5''	16:P:33:ILE:HD13	1.88	0.56
1:A:916:G:H2'	1:A:917:C:C6	2.41	0.56
1:A:1039:G:H5''	3:C:154:SER:HB2	1.88	0.56
3:C:107:GLN:O	3:C:108:ASN:HB3	2.06	0.56
10:J:48:THR:OG1	10:J:62:HIS:CD2	2.58	0.56
12:L:53:ARG:HG2	12:L:53:ARG:HH11	1.71	0.56
15:O:64:ARG:HH11	15:O:64:ARG:HG3	1.71	0.56
17:Q:60:ILE:HD13	17:Q:61:GLU:N	2.21	0.56
1:A:985:C:C2	1:A:986:C:C4	2.94	0.56
2:B:46:LYS:HA	2:B:49:GLU:HB2	1.88	0.56
10:J:94:VAL:HG12	10:J:95:GLU:N	2.21	0.56
13:M:9:ILE:HD12	13:M:9:ILE:N	2.21	0.56
15:O:39:LEU:HD23	15:O:39:LEU:C	2.31	0.56
1:A:123:G:O2'	1:A:189:U:H5''	2.06	0.55
1:A:387:G:H2'	1:A:388:A:C8	2.41	0.55
1:A:949:C:P	10:J:57:LYS:HD3	2.47	0.55
8:H:80:ILE:O	8:H:80:ILE:HG22	2.05	0.55
10:J:24:VAL:HG21	10:J:37:PRO:HD3	1.87	0.55
12:L:110:VAL:O	12:L:122:THR:HG21	2.06	0.55
13:M:59:TYR:O	13:M:63:THR:HG22	2.06	0.55
19:S:52:TYR:HA	19:S:56:GLN:O	2.06	0.55
21:V:7:ARG:HB2	21:V:21:TYR:CE1	2.40	0.55
1:A:79:U:H2'	1:A:81:U:OP2	2.06	0.55
1:A:1105:A:C2	10:J:39:PRO:HG3	2.37	0.55
1:A:1125:G:H2'	1:A:1126:G:C4	2.41	0.55
1:A:1516:C:N4	7:G:82:GLY:HA2	2.22	0.55
2:B:162:ILE:HG22	2:B:164:VAL:HG23	1.88	0.55
4:D:3:ARG:HH21	4:D:71:SER:HB3	1.69	0.55
1:A:379:G:H2'	1:A:380:C:C6	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:816:U:H2'	1:A:817:C:C6	2.42	0.55
1:A:1006:C:H3'	1:A:1006:C:H6	1.71	0.55
1:A:1382:C:H4'	1:A:1383:G:OP2	2.06	0.55
2:B:88:ALA:HB1	2:B:90:MET:HG2	1.87	0.55
4:D:107:ARG:C	4:D:109:GLY:H	2.14	0.55
8:H:10:LEU:CD2	8:H:83:ILE:HD11	2.37	0.55
9:I:48:GLU:N	9:I:49:PRO:CD	2.69	0.55
20:T:54:LYS:HB2	20:T:100:ILE:CD1	2.36	0.55
1:A:188:U:H4'	1:A:189:U:OP1	2.06	0.55
1:A:482:A:O2'	1:A:483:G:C8	2.60	0.55
3:C:65:ALA:O	3:C:66:VAL:HB	2.05	0.55
12:L:42:THR:HG21	12:L:52:LEU:HB3	1.89	0.55
5:E:78:HIS:HD1	8:H:104:ARG:HD2	1.71	0.55
19:S:78:ARG:HG2	19:S:78:ARG:HH11	1.71	0.55
1:A:1320:A:H2'	1:A:1321:A:O4'	2.06	0.55
3:C:73:PRO:C	3:C:75:VAL:H	2.15	0.55
3:C:134:ILE:HG23	3:C:151:VAL:HB	1.89	0.55
4:D:34:GLU:C	4:D:35:ARG:HD2	2.32	0.55
4:D:196:LEU:HD22	4:D:197:PRO:HD2	1.89	0.55
13:M:84:ILE:C	13:M:86:CYS:H	2.15	0.55
19:S:9:VAL:HG12	19:S:10:PHE:N	2.20	0.55
1:A:247:U:H5'	1:A:247:U:H6	1.72	0.55
1:A:652:U:H2'	1:A:653:G:C8	2.42	0.55
2:B:71:VAL:CG2	2:B:164:VAL:HG22	2.37	0.55
3:C:46:GLU:C	3:C:47:LEU:HD12	2.31	0.55
6:F:80:ARG:NH1	6:F:88:VAL:HB	2.22	0.55
1:A:300:G:O2'	1:A:301:G:OP2	2.13	0.55
1:A:963:A:H1'	19:S:54:GLY:O	2.06	0.55
1:A:1039:G:H2'	1:A:1040:G:O4'	2.06	0.55
1:A:1243:C:N4	1:A:1254:G:H1	1.96	0.55
1:A:1479:A:H2	1:A:1482:G:N1	1.99	0.55
2:B:139:LYS:NZ	2:B:139:LYS:HB3	2.22	0.55
5:E:12:LEU:O	5:E:12:LEU:HD13	2.07	0.55
5:E:51:VAL:O	5:E:55:VAL:HG23	2.07	0.55
16:P:26:ARG:CD	16:P:31:LYS:O	2.55	0.55
19:S:50:ALA:HA	19:S:58:VAL:O	2.06	0.55
20:T:49:ALA:HB1	20:T:99:LEU:HG	1.88	0.55
1:A:123:G:HO2'	1:A:189:U:H3'	1.72	0.55
1:A:1181:C:O2'	1:A:1182:A:OP2	2.18	0.55
2:B:115:LEU:HD23	2:B:153:ARG:HD3	1.88	0.55
2:B:215:LEU:O	2:B:219:VAL:HG23	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:15:GLU:C	4:D:17:VAL:H	2.14	0.55
7:G:50:ILE:HG23	7:G:125:MET:SD	2.46	0.55
10:J:16:LEU:HB3	10:J:70:ARG:HG3	1.89	0.55
1:A:636:A:O2'	1:A:637:G:OP1	2.24	0.55
1:A:838:G:O2'	1:A:839:C:H5'	2.07	0.55
3:C:22:TRP:CB	3:C:59:ARG:HB3	2.37	0.55
4:D:52:SER:O	4:D:53:ASP:C	2.50	0.55
13:M:22:ILE:CD1	13:M:25:ILE:HD12	2.36	0.55
16:P:20:VAL:HG21	16:P:32:TYR:CB	2.38	0.55
17:Q:92:ARG:O	17:Q:95:TYR:HB2	2.06	0.55
1:A:75:G:O2'	1:A:76:G:H5'	2.07	0.54
1:A:1118:U:O5'	1:A:1118:U:H6	1.89	0.54
1:A:1247:G:N2	1:A:1250:A:OP2	2.40	0.54
1:A:1316:C:O2'	1:A:1317:C:OP2	2.15	0.54
2:B:7:VAL:HG13	2:B:221:LEU:HD11	1.89	0.54
2:B:97:TRP:HZ2	2:B:102:LEU:HD13	1.73	0.54
9:I:28:VAL:HA	9:I:63:ILE:O	2.08	0.54
9:I:95:LYS:O	9:I:99:LEU:HD23	2.07	0.54
13:M:88:ARG:NH1	19:S:3:ARG:HH21	2.05	0.54
16:P:11:SER:OG	16:P:14:ASN:HB3	2.07	0.54
1:A:209:U:H4'	1:A:210:U:OP1	2.07	0.54
1:A:484:C:H2'	1:A:485:G:H8	1.70	0.54
1:A:601:C:H3'	1:A:602:U:C5'	2.37	0.54
1:A:1129:C:HO2'	9:I:5:TYR:HH	1.54	0.54
19:S:40:ILE:HG21	19:S:62:ILE:HD11	1.89	0.54
1:A:332:C:H2'	1:A:333:A:C8	2.42	0.54
1:A:525:G:H2'	1:A:526:C:C6	2.42	0.54
1:A:825:C:C6	1:A:825:C:C3'	2.89	0.54
1:A:969:U:H4'	1:A:970:G:O5'	2.08	0.54
1:A:1193:U:O2	1:A:1193:U:H2'	2.07	0.54
1:A:1225:C:OP2	21:V:9:ARG:HB2	2.07	0.54
4:D:170:VAL:HG12	4:D:171:GLY:N	2.22	0.54
1:A:51:A:OP2	1:A:52:G:H8	1.91	0.54
1:A:453:G:H3'	1:A:454:A:C5'	2.38	0.54
1:A:985:C:O2	1:A:986:C:C4	2.60	0.54
1:A:997:C:H2'	1:A:998:U:O4'	2.07	0.54
1:A:1111:C:N4	1:A:1117:U:H3	2.04	0.54
1:A:1286:G:C5'	21:V:4:GLY:HA3	2.30	0.54
13:M:65:LYS:HE2	13:M:69:GLU:OE2	2.07	0.54
15:O:7:GLU:O	15:O:11:VAL:HG23	2.08	0.54
4:D:190:ASP:HB2	4:D:193:ASP:OD2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:143:ARG:NH1	8:H:77:GLU:OE2	2.40	0.54
12:L:113:ARG:HH12	12:L:116:SER:HB2	1.72	0.54
14:N:11:LYS:O	14:N:11:LYS:HG2	2.06	0.54
1:A:647:G:N2	1:A:724:G:H1	1.96	0.54
1:A:1035:G:C4'	1:A:1036:C:H5'	2.38	0.54
1:A:1143:C:O2'	1:A:1144:C:H5'	2.07	0.54
1:A:1329:U:H4'	9:I:120:ARG:HD2	1.89	0.54
2:B:81:VAL:O	2:B:81:VAL:HG12	2.06	0.54
7:G:13:GLN:HE21	7:G:14:PRO:HD2	1.73	0.54
1:A:601:C:H3'	1:A:602:U:H5'	1.89	0.54
1:A:622:G:O2'	1:A:623:A:H5'	2.08	0.54
1:A:903:G:H3'	1:A:1482:G:H21	1.73	0.54
1:A:1194:A:H4'	1:A:1195:C:OP1	2.08	0.54
6:F:98:LEU:H	6:F:98:LEU:HD12	1.72	0.54
9:I:16:ARG:NE	9:I:64:THR:HG21	2.23	0.54
10:J:42:THR:HG23	10:J:67:THR:C	2.32	0.54
17:Q:83:ASP:O	17:Q:86:GLU:HB2	2.08	0.54
22:W:1:A:H62	23:X:37:12A:HG22	1.73	0.54
1:A:264:C:H2'	1:A:265:A:H8	1.67	0.54
1:A:578:G:N1	1:A:624:U:H2'	2.23	0.54
1:A:1004:G:N2	1:A:1018:G:H22	2.06	0.54
3:C:16:ARG:HH11	3:C:16:ARG:CG	2.18	0.54
5:E:80:ILE:HG22	8:H:104:ARG:NH2	2.23	0.54
7:G:73:MET:HA	7:G:91:VAL:HG23	1.88	0.54
1:A:145:A:H2'	1:A:146:A:O4'	2.08	0.54
1:A:424:U:H4'	1:A:425:A:O5'	2.08	0.54
1:A:1164:A:O2'	1:A:1165:G:OP1	2.19	0.54
1:A:1350:G:O2'	1:A:1351:C:H5'	2.08	0.54
1:A:1447:G:O2'	1:A:1448:G:H5'	2.08	0.54
3:C:51:GLY:O	3:C:70:VAL:HG12	2.08	0.54
8:H:10:LEU:HD23	8:H:83:ILE:HD11	1.90	0.54
9:I:125:TYR:CE1	9:I:128:ARG:NE	2.76	0.54
12:L:91:LYS:HE3	12:L:91:LYS:CA	2.37	0.54
18:R:25:THR:HG22	18:R:42:ARG:NH1	2.20	0.54
1:A:123:G:O2'	1:A:189:U:H3'	2.07	0.54
1:A:1289:U:C5'	13:M:110:ARG:HH21	2.20	0.54
6:F:10:LEU:HD11	6:F:59:TYR:HD2	1.71	0.54
10:J:38:ILE:HD12	10:J:71:LEU:HD12	1.89	0.54
21:V:2:GLY:O	21:V:4:GLY:N	2.41	0.54
1:A:188:U:O2'	1:A:189:U:O5'	2.20	0.53
1:A:455:C:O2'	1:A:456:G:OP1	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:635:U:H4'	1:A:636:A:OP1	2.08	0.53
1:A:980:G:C6	1:A:981:G:C6	2.95	0.53
1:A:986:C:H42	1:A:1000:G:H22	1.56	0.53
1:A:1348:C:H2'	1:A:1349:C:H6	1.72	0.53
1:A:1469:A:OP1	12:L:47:LYS:N	2.41	0.53
3:C:23:TYR:O	3:C:24:ALA:HB2	2.08	0.53
4:D:31:CYS:O	4:D:31:CYS:SG	2.65	0.53
7:G:138:LYS:HD3	7:G:138:LYS:C	2.33	0.53
9:I:106:ALA:O	9:I:108:VAL:HG23	2.07	0.53
20:T:53:LEU:HD21	20:T:104:LEU:HD12	1.90	0.53
1:A:108:G:H1'	1:A:109:A:N7	2.23	0.53
1:A:383:G:O2'	1:A:384:A:P	2.67	0.53
1:A:385:C:H2'	1:A:386:G:C8	2.43	0.53
1:A:824:U:H3'	1:A:825:C:O4'	2.09	0.53
1:A:1170:C:OP1	10:J:51:ARG:NH2	2.40	0.53
1:A:1272:G:OP1	7:G:37:ASN:ND2	2.41	0.53
11:K:109:VAL:HG22	18:R:86:VAL:HG13	1.89	0.53
20:T:96:GLY:O	20:T:97:ALA:HB3	2.06	0.53
1:A:125:C:OP1	1:A:190:G:N2	2.42	0.53
1:A:515:A:H5'	3:C:161:GLU:OE1	2.02	0.53
1:A:578:G:C6	1:A:624:U:H2'	2.43	0.53
1:A:1215:C:H5'	1:A:1347:G:OP1	2.08	0.53
1:A:1241:C:OP1	1:A:1265:C:H4'	2.08	0.53
1:A:1431:A:H4'	1:A:1432:C:OP2	2.05	0.53
5:E:36:ASP:CG	5:E:40:ARG:HB2	2.33	0.53
5:E:126:ARG:NH1	5:E:126:ARG:HG3	2.22	0.53
7:G:18:TYR:CD1	7:G:59:LEU:HD22	2.44	0.53
7:G:50:ILE:HG21	7:G:61:VAL:HG21	1.90	0.53
7:G:87:VAL:HG11	7:G:154:TYR:O	2.09	0.53
10:J:14:LYS:O	10:J:18:ALA:HB3	2.07	0.53
10:J:46:ARG:HG3	10:J:46:ARG:NH1	2.24	0.53
10:J:60:ARG:NH1	10:J:60:ARG:HG2	2.23	0.53
11:K:79:SER:CB	11:K:104:GLN:HB3	2.38	0.53
12:L:119:LYS:O	12:L:120:TYR:HB2	2.08	0.53
16:P:28:ARG:NH1	16:P:29:ASP:OD2	2.41	0.53
1:A:494:C:HO2'	1:A:495:U:H6	1.57	0.53
1:A:648:A:N3	1:A:715:C:H2'	2.24	0.53
1:A:886:A:H2'	1:A:887:C:O4'	2.08	0.53
9:I:16:ARG:HE	9:I:64:THR:HG23	1.71	0.53
11:K:24:SER:C	11:K:26:ASN:H	2.16	0.53
14:N:8:GLU:O	14:N:11:LYS:CB	2.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:14:PRO:O	14:N:15:LYS:HB2	2.07	0.53
1:A:49:U:O2'	1:A:50:A:OP1	2.25	0.53
1:A:268:A:H1'	17:Q:16:GLN:NE2	2.23	0.53
1:A:1126:G:H3'	1:A:1126:G:C8	2.44	0.53
1:A:1150:A:H2'	1:A:1151:A:C8	2.43	0.53
1:A:1206:A:H3'	1:A:1207:C:H6	1.71	0.53
1:A:1381:C:H4'	1:A:1382:C:O5'	2.09	0.53
2:B:71:VAL:HG21	2:B:164:VAL:HG22	1.89	0.53
3:C:29:TYR:CZ	14:N:54:PRO:HG2	2.44	0.53
6:F:14:LEU:N	6:F:14:LEU:HD12	2.24	0.53
7:G:6:ARG:O	7:G:7:ALA:O	2.25	0.53
15:O:39:LEU:HD23	15:O:39:LEU:O	2.09	0.53
20:T:53:LEU:O	20:T:54:LYS:C	2.52	0.53
21:V:3:LYS:HB3	21:V:14:TRP:CG	2.43	0.53
1:A:22:G:H2'	1:A:23:C:C6	2.44	0.53
1:A:821:G:C2'	1:A:822:U:H5''	2.39	0.53
1:A:1036:C:C3'	1:A:1036:C:H6	2.09	0.53
1:A:1184:C:H6	1:A:1184:C:O5'	1.91	0.53
1:A:160:G:O2'	1:A:161:G:H5'	2.08	0.53
1:A:603:C:C2	4:D:135:LEU:HD13	2.42	0.53
1:A:1024:G:H2'	1:A:1025:C:H6	1.73	0.53
1:A:1098:C:H2'	1:A:1099:G:H5'	1.90	0.53
1:A:1460:A:H2'	1:A:1461:C:O5'	2.09	0.53
3:C:130:VAL:HG11	3:C:157:ILE:HG23	1.90	0.53
4:D:19:LEU:HD21	4:D:67:ILE:CG1	2.33	0.53
5:E:143:ARG:HH12	8:H:77:GLU:CD	2.16	0.53
6:F:50:TYR:CE1	18:R:77:GLY:HA2	2.44	0.53
10:J:24:VAL:HG13	10:J:28:ARG:NH1	2.23	0.53
11:K:14:VAL:O	11:K:15:ALA:HB3	2.09	0.53
11:K:93:GLN:OE1	11:K:93:GLN:HA	2.08	0.53
1:A:1077:U:H2'	1:A:1078:C:O4'	2.09	0.53
2:B:97:TRP:CZ2	2:B:102:LEU:HD13	2.43	0.53
3:C:14:ILE:O	3:C:15:THR:C	2.52	0.53
8:H:92:ARG:HG2	8:H:92:ARG:HH11	1.74	0.53
9:I:36:TYR:CD2	9:I:37:PHE:CE2	2.97	0.53
1:A:338:U:H2'	1:A:340:C:C4	2.43	0.53
1:A:453:G:H3'	1:A:454:A:H5''	1.91	0.53
1:A:465:G:H2'	1:A:467:C:H41	1.72	0.53
2:B:86:GLU:C	2:B:88:ALA:N	2.67	0.53
2:B:87:ARG:HD2	2:B:234:PRO:HD2	1.91	0.53
7:G:145:ALA:C	7:G:147:ALA:N	2.64	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:12:GLU:HG2	9:I:12:GLU:O	2.09	0.53
1:A:980:G:C4	1:A:981:G:N7	2.76	0.53
1:A:1300:A:H4'	19:S:37:ARG:NH1	2.24	0.53
9:I:111:ARG:HG2	9:I:112:LYS:N	2.24	0.53
15:O:3:ILE:HD12	15:O:3:ILE:N	2.23	0.53
16:P:1:MET:O	16:P:24:ALA:HB2	2.09	0.53
1:A:516:A:C4'	1:A:517:U:OP1	2.53	0.52
1:A:927:U:H5	13:M:102:ARG:NE	2.07	0.52
1:A:953:G:N7	1:A:1339:U:C2	2.77	0.52
1:A:1113:G:C8	1:A:1113:G:H3'	2.44	0.52
1:A:1286:G:O2'	1:A:1287:A:C8	2.45	0.52
1:A:1287:A:N6	1:A:1312:G:H1'	2.25	0.52
5:E:71:LEU:HD11	5:E:114:GLY:HA3	1.90	0.52
7:G:137:LYS:O	7:G:141:VAL:HG23	2.09	0.52
10:J:49:VAL:CG1	14:N:41:ARG:HD2	2.39	0.52
12:L:43:VAL:HG12	12:L:44:THR:N	2.24	0.52
1:A:501:C:O2'	1:A:502:C:OP2	2.23	0.52
1:A:1134:A:H2'	1:A:1135:C:C6	2.44	0.52
1:A:1362:U:O2'	1:A:1363:U:OP2	2.24	0.52
1:A:1521:U:O3'	22:W:1:A:OP1	2.28	0.52
5:E:39:GLY:O	5:E:68:GLU:HA	2.09	0.52
5:E:147:ASP:O	5:E:151:LEU:HD13	2.09	0.52
19:S:19:VAL:HG13	19:S:20:LEU:N	2.24	0.52
1:A:952:A:H5'	1:A:952:A:C8	2.44	0.52
5:E:45:PHE:CE2	5:E:47:LYS:HD2	2.44	0.52
10:J:39:PRO:HA	10:J:70:ARG:NH2	2.24	0.52
16:P:18:ARG:CG	16:P:35:LYS:HE3	2.40	0.52
18:R:22:VAL:HG23	18:R:55:ARG:O	2.09	0.52
1:A:611:G:O2'	1:A:612:G:H5'	2.09	0.52
1:A:1031:U:O2'	1:A:1032:G:OP2	2.25	0.52
2:B:19:HIS:O	2:B:20:GLU:C	2.52	0.52
2:B:74:LYS:HG2	2:B:76:GLN:H	1.74	0.52
3:C:188:LEU:O	3:C:189:ALA:CB	2.57	0.52
3:C:188:LEU:CD1	3:C:189:ALA:H	2.21	0.52
6:F:30:LEU:HA	6:F:75:LEU:HD21	1.91	0.52
10:J:84:GLN:C	10:J:86:MET:H	2.17	0.52
13:M:45:VAL:HA	13:M:48:LEU:HG	1.90	0.52
1:A:335:U:H2'	1:A:336:C:C6	2.44	0.52
1:A:1172:A:OP2	3:C:3:ASN:ND2	2.42	0.52
2:B:107:THR:C	2:B:109:SER:N	2.62	0.52
2:B:166:ASP:O	2:B:170:GLU:HB2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:18:TYR:CE1	7:G:59:LEU:HB2	2.45	0.52
10:J:64:GLU:CG	14:N:59:ALA:HB2	2.38	0.52
11:K:33:THR:HG22	11:K:39:PRO:HA	1.91	0.52
17:Q:64:PRO:C	17:Q:65:ILE:HD12	2.34	0.52
1:A:102:A:C4'	1:A:103:C:OP2	2.57	0.52
2:B:7:VAL:CG2	2:B:8:LYS:H	2.16	0.52
2:B:189:ASP:OD2	2:B:205:ASP:OD2	2.27	0.52
3:C:23:TYR:OH	10:J:9:ARG:HD3	2.10	0.52
4:D:104:VAL:HG21	4:D:140:VAL:HG21	1.90	0.52
6:F:43:LEU:HD22	6:F:43:LEU:N	2.25	0.52
6:F:100:ASN:ND2	18:R:23:LYS:NZ	2.57	0.52
16:P:67:THR:CG2	16:P:68:ASP:N	2.72	0.52
1:A:94:A:O2'	1:A:95:G:H5'	2.09	0.52
1:A:114:C:H4'	1:A:115:G:OP1	2.10	0.52
1:A:795:C:O2'	1:A:796:U:P	2.68	0.52
2:B:77:ALA:HB2	2:B:211:ILE:HG21	1.91	0.52
3:C:55:VAL:O	3:C:55:VAL:HG12	2.10	0.52
10:J:15:THR:O	10:J:94:VAL:HG21	2.10	0.52
11:K:15:ALA:HA	11:K:76:GLY:O	2.10	0.52
12:L:60:LEU:HD23	12:L:66:VAL:HG22	1.92	0.52
17:Q:69:LYS:C	17:Q:70:ARG:HD2	2.35	0.52
17:Q:89:LEU:O	17:Q:92:ARG:HB2	2.10	0.52
18:R:53:ARG:HD3	18:R:58:LEU:O	2.10	0.52
6:F:20:ALA:O	6:F:24:GLU:HB2	2.09	0.52
7:G:115:ARG:HB2	7:G:118:VAL:CG2	2.39	0.52
19:S:80:TYR:CG	19:S:81:ARG:N	2.78	0.52
1:A:1171:G:OP1	3:C:4:LYS:HA	2.10	0.52
3:C:87:LEU:O	3:C:91:LEU:HB2	2.10	0.52
10:J:46:ARG:HG3	10:J:46:ARG:HH11	1.75	0.52
11:K:52:GLY:H	11:K:55:LYS:HE2	1.75	0.52
15:O:17:ARG:NH1	15:O:17:ARG:CG	2.73	0.52
1:A:21:G:H2'	1:A:22:G:C8	2.45	0.52
1:A:522:A:H2'	1:A:523:G:C8	2.45	0.52
1:A:1094:C:O2	3:C:179:ARG:HB3	2.10	0.52
2:B:120:ALA:C	2:B:122:PHE:H	2.18	0.52
3:C:43:LEU:O	3:C:47:LEU:HD13	2.10	0.52
3:C:196:LEU:HD23	3:C:196:LEU:N	2.24	0.52
7:G:85:TYR:O	7:G:87:VAL:HG23	2.10	0.52
9:I:118:LYS:NZ	9:I:118:LYS:CB	2.72	0.52
12:L:89:ARG:H	12:L:89:ARG:CD	2.22	0.52
14:N:57:ARG:CG	14:N:58:LYS:H	2.17	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:59:SER:C	18:R:61:LYS:N	2.63	0.52
1:A:1008:C:N4	1:A:1014:G:H1	2.09	0.51
2:B:187:LEU:HD23	2:B:201:ILE:O	2.10	0.51
2:B:208:ILE:HA	2:B:211:ILE:HD12	1.91	0.51
3:C:91:LEU:HD23	3:C:99:VAL:HG21	1.92	0.51
10:J:16:LEU:HD21	10:J:94:VAL:HG13	1.90	0.51
1:A:364:C:H2'	1:A:365:C:C6	2.45	0.51
1:A:1100:C:H1'	1:A:1160:A:C4	2.46	0.51
2:B:58:ILE:HG23	2:B:68:ILE:CD1	2.41	0.51
2:B:95:GLN:OE1	2:B:95:GLN:HA	2.10	0.51
7:G:58:PRO:O	7:G:61:VAL:HG22	2.10	0.51
11:K:12:ARG:HG2	11:K:12:ARG:O	2.09	0.51
19:S:55:LYS:HG2	19:S:56:GLN:HG3	1.90	0.51
20:T:91:LEU:C	20:T:93:GLU:H	2.17	0.51
1:A:124:A:O2'	1:A:125:C:O5'	2.25	0.51
1:A:506:A:H61	12:L:92:ASP:HB2	1.74	0.51
1:A:854:C:OP1	8:H:88:LYS:HE2	2.10	0.51
1:A:1186:U:O2'	3:C:195:VAL:HG23	2.10	0.51
1:A:1286:G:O2'	1:A:1287:A:P	2.68	0.51
3:C:33:LEU:HD21	14:N:53:LEU:CD2	2.40	0.51
5:E:79:GLU:CG	5:E:93:PRO:HD2	2.41	0.51
12:L:27:LEU:O	12:L:29:GLY:N	2.43	0.51
13:M:4:ILE:CD1	13:M:56:LEU:HD13	2.40	0.51
13:M:5:ALA:HB3	13:M:8:GLU:CB	2.40	0.51
1:A:701:G:H4'	11:K:117:ASN:ND2	2.26	0.51
1:A:1286:G:N2	1:A:1312:G:C2'	2.72	0.51
1:A:1461:C:C6	1:A:1461:C:H3'	2.45	0.51
6:F:15:ASP:CG	6:F:18:GLN:HB2	2.35	0.51
10:J:79:ARG:O	10:J:83:GLU:HB2	2.09	0.51
13:M:3:ARG:HG2	13:M:9:ILE:HG23	1.93	0.51
13:M:88:ARG:HH11	19:S:3:ARG:HH21	1.57	0.51
14:N:29:ARG:HG2	14:N:29:ARG:HH11	1.75	0.51
15:O:74:ASP:C	15:O:76:GLU:H	2.17	0.51
20:T:24:LEU:HD12	20:T:27:LYS:CE	2.41	0.51
1:A:798:A:O2'	1:A:799:A:P	2.68	0.51
1:A:801:G:O2'	1:A:803:U:C5	2.63	0.51
1:A:1153:C:H2'	1:A:1154:G:C8	2.45	0.51
1:A:1213:U:H5''	9:I:124:GLN:O	2.10	0.51
1:A:1259:U:O2'	1:A:1260:A:OP2	2.26	0.51
1:A:1300:A:C4'	19:S:37:ARG:HH12	2.22	0.51
2:B:80:ILE:C	2:B:82:ARG:H	2.17	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:107:THR:O	2:B:109:SER:N	2.43	0.51
3:C:191:THR:HG22	3:C:193:TYR:H	1.76	0.51
4:D:98:GLU:HG2	4:D:189:PRO:HG3	1.92	0.51
5:E:148:VAL:CG2	8:H:107:LEU:HD22	2.34	0.51
7:G:125:MET:O	7:G:129:GLU:HG2	2.10	0.51
15:O:78:TYR:CZ	15:O:82:ILE:HD11	2.46	0.51
16:P:51:VAL:O	16:P:52:ASP:CB	2.56	0.51
1:A:377:A:H2'	1:A:378:A:C8	2.45	0.51
1:A:1328:G:H22	1:A:1355:G:H2'	1.76	0.51
1:A:245:A:C4'	1:A:246:G:O5'	2.49	0.51
1:A:983:A:OP1	1:A:984:C:P	2.69	0.51
1:A:1172:A:OP1	3:C:4:LYS:NZ	2.42	0.51
1:A:1302:C:H5''	1:A:1303:C:C2'	2.39	0.51
4:D:126:ILE:HG22	4:D:127:THR:N	2.26	0.51
7:G:15:ASP:HB3	7:G:19:GLY:CA	2.41	0.51
9:I:17:VAL:HG11	9:I:81:ILE:HG12	1.93	0.51
9:I:33:PHE:CE2	9:I:47:LEU:HD11	2.45	0.51
13:M:11:ARG:HG2	13:M:12:ASN:H	1.74	0.51
1:A:41:G:H2'	1:A:42:G:C8	2.46	0.51
1:A:364:C:H2'	1:A:365:C:H6	1.75	0.51
1:A:911:C:H5'	1:A:912:A:OP1	2.10	0.51
1:A:934:U:H3	1:A:937:U:H5'	1.76	0.51
1:A:1054:G:H2'	1:A:1055:U:C6	2.45	0.51
1:A:1133:A:O2'	1:A:1134:A:O5'	2.29	0.51
1:A:1261:A:O4'	10:J:41:PRO:HG3	2.10	0.51
2:B:104:ASN:HD21	2:B:107:THR:HB	1.75	0.51
2:B:206:ASP:O	2:B:207:ALA:HB3	2.09	0.51
11:K:14:VAL:HG21	11:K:40:ILE:CD1	2.41	0.51
12:L:8:ASN:O	12:L:12:ARG:HB2	2.11	0.51
12:L:34:ARG:O	12:L:61:THR:HG23	2.10	0.51
15:O:37:ASN:O	15:O:41:GLU:HB2	2.11	0.51
20:T:34:LYS:O	20:T:38:LYS:HG3	2.10	0.51
1:A:402:G:O2'	4:D:116:GLN:HG3	2.11	0.51
1:A:735:G:O2'	1:A:736:A:P	2.69	0.51
1:A:1057:C:H5'	2:B:103:THR:HG21	1.93	0.51
1:A:1210:A:C2	1:A:1211:C:C4	2.99	0.51
1:A:1408:C:O2'	1:A:1409:U:H5'	2.10	0.51
2:B:143:GLU:O	2:B:147:LYS:HG3	2.11	0.51
10:J:16:LEU:O	10:J:19:SER:N	2.44	0.51
12:L:111:LYS:HG2	12:L:112:ASP:N	2.26	0.51
1:A:82:U:C6	1:A:82:U:H3'	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:700:C:O2'	1:A:701:G:OP2	2.22	0.51
1:A:1051:C:O2'	1:A:1173:C:H1'	2.11	0.51
1:A:1187:G:H1'	3:C:193:TYR:O	2.11	0.51
1:A:1228:U:C6	1:A:1228:U:C3'	2.92	0.51
4:D:58:LEU:O	4:D:58:LEU:HD22	2.11	0.51
11:K:27:ASN:OD1	11:K:28:THR:N	2.42	0.51
1:A:352:G:O2'	1:A:353:U:H5'	2.10	0.50
1:A:402:G:H2'	1:A:403:A:C8	2.46	0.50
1:A:981:G:N2	1:A:1020:C:N3	2.59	0.50
1:A:1434:G:O2'	1:A:1435:G:H5'	2.10	0.50
7:G:28:ASN:HD21	7:G:36:LYS:CE	2.23	0.50
1:A:823:C:H5''	1:A:824:U:OP2	2.11	0.50
1:A:1269:A:H2'	1:A:1270:A:C8	2.46	0.50
1:A:1307:C:OP1	21:V:12:LYS:NZ	2.44	0.50
2:B:42:ILE:HG22	2:B:43:ASP:N	2.25	0.50
2:B:80:ILE:C	2:B:82:ARG:N	2.70	0.50
12:L:60:LEU:N	12:L:64:TYR:O	2.41	0.50
12:L:86:ARG:HH11	12:L:86:ARG:HG3	1.77	0.50
13:M:54:VAL:HG12	13:M:58:GLU:HG2	1.92	0.50
1:A:245:A:H5'	1:A:247:U:O4'	2.11	0.50
1:A:332:C:H2'	1:A:333:A:H8	1.76	0.50
1:A:1029:G:O2'	1:A:1030:G:H5'	2.12	0.50
1:A:1202:G:OP1	1:A:1301:C:N4	2.44	0.50
1:A:1286:G:H22	1:A:1312:G:H2'	1.76	0.50
1:A:1388:U:O2'	1:A:1389:C:H5'	2.11	0.50
4:D:150:GLU:C	4:D:152:SER:H	2.19	0.50
6:F:54:LYS:HE2	6:F:54:LYS:CA	2.41	0.50
6:F:97:PHE:O	6:F:98:LEU:O	2.30	0.50
8:H:26:VAL:HG23	8:H:27:PRO:O	2.11	0.50
8:H:36:LEU:HD12	8:H:59:LEU:HD13	1.93	0.50
8:H:77:GLU:HG2	8:H:78:GLN:N	2.26	0.50
9:I:126:SER:O	9:I:127:LYS:C	2.54	0.50
11:K:45:GLY:HA3	11:K:55:LYS:HG2	1.94	0.50
19:S:44:MET:O	19:S:62:ILE:HG21	2.11	0.50
1:A:1279:C:C6	7:G:114:ARG:NH1	2.79	0.50
5:E:5:ASP:CG	5:E:6:PHE:H	2.20	0.50
10:J:49:VAL:CG1	14:N:41:ARG:HB2	2.41	0.50
14:N:12:ARG:C	14:N:14:PRO:CD	2.85	0.50
1:A:516:A:O2'	1:A:517:U:OP1	2.29	0.50
1:A:985:C:O2	1:A:986:C:N3	2.45	0.50
1:A:1127:C:H1'	1:A:1128:A:C8	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1163:G:H4'	1:A:1164:A:H5''	1.94	0.50
1:A:1384:C:O2	1:A:1477:A:N1	2.45	0.50
2:B:142:LEU:O	2:B:142:LEU:HD23	2.11	0.50
3:C:58:GLU:N	3:C:65:ALA:HB3	2.26	0.50
3:C:134:ILE:CG2	3:C:168:ALA:HB3	2.42	0.50
3:C:203:PHE:C	3:C:204:LEU:HD23	2.36	0.50
6:F:12:PRO:HG3	6:F:55:ASP:CG	2.36	0.50
20:T:90:GLN:O	20:T:93:GLU:HB2	2.11	0.50
1:A:516:A:O2'	1:A:517:U:P	2.69	0.50
1:A:603:C:N1	4:D:135:LEU:HD13	2.26	0.50
1:A:937:U:O2'	1:A:1204:C:C5'	2.60	0.50
1:A:983:A:OP1	1:A:983:A:O3'	2.30	0.50
1:A:1111:C:O2'	1:A:1112:A:P	2.70	0.50
2:B:25:ASN:O	2:B:26:PRO:C	2.55	0.50
2:B:229:VAL:O	2:B:229:VAL:HG12	2.12	0.50
9:I:16:ARG:NE	9:I:64:THR:HG23	2.25	0.50
16:P:67:THR:HG22	16:P:68:ASP:H	1.75	0.50
20:T:57:ARG:CD	20:T:102:GLY:HA3	2.41	0.50
1:A:385:C:H2'	1:A:386:G:H8	1.75	0.50
1:A:1124:G:H2'	1:A:1125:G:C5'	2.34	0.50
1:A:1279:C:H2'	7:G:114:ARG:HH12	1.77	0.50
3:C:29:TYR:C	3:C:29:TYR:CD2	2.90	0.50
3:C:35:GLU:OE1	3:C:95:THR:HG23	2.12	0.50
13:M:19:LEU:HD11	13:M:34:LEU:HD21	1.93	0.50
16:P:8:ARG:HG2	16:P:17:TYR:CE2	2.47	0.50
17:Q:78:GLU:OE2	17:Q:81:ARG:HD2	2.11	0.50
20:T:65:LYS:O	20:T:68:LYS:HB2	2.12	0.50
1:A:450:C:H2'	1:A:451:C:C6	2.46	0.50
1:A:1311:U:OP1	13:M:23:TYR:O	2.29	0.50
2:B:142:LEU:HD23	2:B:142:LEU:C	2.37	0.50
4:D:62:GLN:NE2	4:D:65:ARG:NH1	2.58	0.50
4:D:150:GLU:O	4:D:153:ARG:HG3	2.11	0.50
6:F:91:VAL:HG11	18:R:72:ARG:NH1	2.27	0.50
9:I:10:ARG:HD2	9:I:75:ASP:HB3	1.94	0.50
10:J:34:VAL:HG22	10:J:74:ILE:HG22	1.93	0.50
11:K:126:ARG:O	11:K:127:LYS:CB	2.59	0.50
12:L:89:ARG:H	12:L:89:ARG:NE	2.09	0.50
17:Q:3:LYS:CB	17:Q:60:ILE:HD11	2.41	0.50
1:A:268:A:H1'	17:Q:16:GLN:HE21	1.76	0.50
1:A:294:G:H2'	1:A:295:A:C8	2.47	0.50
1:A:726:U:H2'	1:A:727:C:H6	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1073:U:O2	1:A:1075:A:C8	2.64	0.50
1:A:1186:U:H2'	1:A:1187:G:C8	2.47	0.50
1:A:1349:C:C5'	10:J:60:ARG:HH12	2.21	0.50
2:B:158:LEU:HD21	2:B:180:LEU:HD13	1.94	0.50
8:H:29:SER:OG	8:H:32:LYS:HG3	2.12	0.50
8:H:104:ARG:NH2	8:H:138:TRP:CH2	2.80	0.50
11:K:54:ARG:O	11:K:57:THR:CG2	2.49	0.50
1:A:48:C:O2'	1:A:49:U:OP1	2.29	0.49
1:A:371:G:P	16:P:67:THR:HG21	2.52	0.49
1:A:1003:U:H3'	1:A:1003:U:C6	2.47	0.49
1:A:1133:A:H2'	1:A:1134:A:C8	2.47	0.49
1:A:1159:G:N2	1:A:1161:A:H3'	2.27	0.49
1:A:1289:U:H5'	13:M:110:ARG:HH21	1.77	0.49
3:C:22:TRP:CE3	3:C:22:TRP:O	2.65	0.49
13:M:36:LYS:HD2	13:M:59:TYR:OH	2.12	0.49
21:V:7:ARG:O	21:V:7:ARG:HG3	2.12	0.49
1:A:114:C:H5'	1:A:115:G:OP1	2.11	0.49
1:A:154:A:C2	1:A:338:U:H4'	2.48	0.49
1:A:695:A:H2'	1:A:696:G:O4'	2.12	0.49
1:A:955:A:C1'	1:A:1303:C:O2	2.57	0.49
1:A:1182:A:H4'	1:A:1183:G:O5'	2.13	0.49
11:K:122:LYS:O	11:K:123:LYS:C	2.55	0.49
17:Q:76:LEU:HD23	17:Q:76:LEU:C	2.37	0.49
1:A:310:A:O2'	1:A:311:G:OP2	2.24	0.49
1:A:323:C:OP1	1:A:324:A:H5'	2.11	0.49
1:A:339:A:H5''	1:A:340:C:OP2	2.13	0.49
1:A:675:U:OP1	11:K:124:LYS:HE3	2.12	0.49
1:A:1042:C:O2	1:A:1179:G:C2	2.66	0.49
2:B:69:LEU:HD12	2:B:155:LEU:CD1	2.41	0.49
3:C:40:ARG:O	3:C:44:GLU:CB	2.60	0.49
4:D:64:LEU:HD23	4:D:64:LEU:C	2.37	0.49
7:G:136:LYS:O	7:G:140:ASP:HB2	2.12	0.49
9:I:10:ARG:NH1	9:I:11:LYS:HB2	2.27	0.49
19:S:13:ASP:HA	19:S:16:LEU:HB3	1.95	0.49
20:T:30:LYS:O	20:T:31:SER:C	2.55	0.49
21:V:5:ASP:HB3	21:V:8:THR:OG1	2.13	0.49
1:A:1258:C:C6	1:A:1258:C:C3'	2.92	0.49
12:L:89:ARG:HA	12:L:97:ARG:HA	1.94	0.49
15:O:65:ARG:HH11	15:O:65:ARG:HG3	1.77	0.49
16:P:21:VAL:HG21	16:P:59:TRP:CD1	2.47	0.49
1:A:79:U:C6	1:A:79:U:C3'	2.96	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:A:H2'	1:A:155:A:O4'	2.13	0.49
1:A:854:C:O2'	1:A:855:G:H5'	2.12	0.49
1:A:1461:C:H2'	1:A:1462:U:C5'	2.43	0.49
3:C:32:LEU:O	3:C:36:ASP:HB2	2.13	0.49
5:E:39:GLY:O	5:E:69:VAL:N	2.43	0.49
5:E:82:VAL:HG11	5:E:134:ALA:O	2.11	0.49
12:L:55:VAL:HG13	12:L:67:THR:HG23	1.94	0.49
13:M:84:ILE:C	13:M:86:CYS:N	2.71	0.49
20:T:90:GLN:HA	20:T:93:GLU:HG2	1.95	0.49
1:A:981:G:N1	1:A:982:A:N3	2.61	0.49
1:A:1098:C:O2'	1:A:1099:G:H5''	2.12	0.49
2:B:129:GLU:O	2:B:130:ARG:HB2	2.11	0.49
3:C:13:GLY:O	3:C:14:ILE:HD13	2.13	0.49
3:C:119:ARG:HE	3:C:140:ARG:HH12	1.60	0.49
3:C:134:ILE:HG21	3:C:168:ALA:HB3	1.94	0.49
6:F:91:VAL:HG12	6:F:92:LYS:O	2.12	0.49
11:K:13:GLN:HA	11:K:75:TYR:O	2.12	0.49
12:L:33:ARG:HE	12:L:62:SER:HB3	1.77	0.49
13:M:49:THR:HB	13:M:52:GLU:CG	2.41	0.49
13:M:79:LYS:HA	13:M:82:MET:HE3	1.94	0.49
19:S:46:GLY:N	19:S:62:ILE:HG23	2.27	0.49
1:A:175:G:H4'	1:A:176:U:C5'	2.43	0.49
1:A:530:A:OP2	4:D:2:GLY:HA3	2.13	0.49
1:A:775:A:H4'	1:A:776:U:H5''	1.95	0.49
1:A:959:U:H4'	1:A:960:A:O5'	2.13	0.49
1:A:1301:C:H2'	1:A:1302:C:O4'	2.13	0.49
1:A:1485:G:O2'	1:A:1486:C:H5'	2.13	0.49
2:B:114:ARG:HE	2:B:118:LEU:HD11	1.78	0.49
4:D:5:ILE:HG22	4:D:5:ILE:O	2.11	0.49
6:F:23:LYS:HD2	6:F:42:GLU:OE1	2.13	0.49
6:F:40:VAL:HG22	6:F:41:GLU:N	2.26	0.49
11:K:79:SER:HB2	11:K:104:GLN:HB3	1.93	0.49
13:M:117:VAL:HG12	13:M:118:ALA:N	2.22	0.49
1:A:562:G:C5'	1:A:711:A:H1'	2.37	0.49
1:A:635:U:O2'	1:A:636:A:O5'	2.30	0.49
1:A:919:G:C2	1:A:920:U:C6	3.01	0.49
1:A:1261:A:H5'	10:J:40:LEU:HD22	1.94	0.49
1:A:1436:C:O2'	1:A:1437:A:H5'	2.13	0.49
3:C:14:ILE:O	3:C:16:ARG:N	2.45	0.49
3:C:22:TRP:CZ3	3:C:32:LEU:HB2	2.48	0.49
9:I:36:TYR:HD2	9:I:37:PHE:CE2	2.31	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:60:LEU:HD21	12:L:85:ILE:HD12	1.93	0.49
17:Q:67:LYS:CA	17:Q:70:ARG:NH1	2.71	0.49
23:X:39:PSU:H2'	23:X:40:C:C5'	2.38	0.49
1:A:457:A:C4'	16:P:82:GLN:HE21	2.26	0.49
1:A:1458:U:H2'	1:A:1459:G:C5'	2.43	0.49
2:B:223:ILE:HG13	2:B:224:GLN:N	2.28	0.49
4:D:76:ARG:HG2	4:D:76:ARG:NH1	2.26	0.49
5:E:143:ARG:NH1	8:H:77:GLU:CD	2.71	0.49
6:F:21:LEU:O	6:F:25:ILE:HG13	2.13	0.49
7:G:15:ASP:OD2	7:G:18:TYR:N	2.34	0.49
10:J:12:ASP:O	10:J:15:THR:HG22	2.13	0.49
13:M:5:ALA:HB3	13:M:8:GLU:CG	2.41	0.49
13:M:37:THR:HG22	13:M:55:ARG:HD2	1.95	0.49
13:M:37:THR:HG23	13:M:55:ARG:HD2	1.95	0.49
15:O:33:THR:O	15:O:37:ASN:OD1	2.29	0.49
1:A:79:U:H3'	1:A:80:U:H5''	1.95	0.49
1:A:485:G:H4'	1:A:533:G:H4'	1.95	0.49
1:A:525:G:H5''	4:D:40:PRO:O	2.13	0.49
1:A:1042:C:H2'	1:A:1043:G:C8	2.41	0.49
1:A:1191:C:H2'	1:A:1192:U:O4'	2.13	0.49
1:A:1253:G:C2'	1:A:1254:G:H5'	2.43	0.49
3:C:91:LEU:HD23	3:C:99:VAL:CG2	2.43	0.49
3:C:167:TRP:O	3:C:168:ALA:HB3	2.12	0.49
4:D:175:SER:HB3	4:D:184:LYS:CB	2.43	0.49
5:E:64:ARG:O	5:E:65:ASN:HB3	2.12	0.49
12:L:83:VAL:CG2	12:L:100:ILE:HG23	2.43	0.49
13:M:23:TYR:HB2	13:M:67:GLU:OE2	2.12	0.49
13:M:34:LEU:CD1	13:M:41:PRO:HA	2.42	0.49
19:S:32:LYS:HA	19:S:50:ALA:O	2.12	0.49
1:A:469:G:O2'	1:A:470:U:P	2.71	0.48
1:A:795:C:H4'	1:A:796:U:C5'	2.41	0.48
1:A:1005:C:H2'	1:A:1006:C:C4	2.48	0.48
1:A:1121:G:H21	1:A:1125:G:N2	2.11	0.48
4:D:31:CYS:O	4:D:32:ALA:HB3	2.13	0.48
4:D:98:GLU:CD	4:D:107:ARG:HH21	2.20	0.48
9:I:3:GLN:OE1	9:I:20:ARG:NE	2.46	0.48
9:I:5:TYR:CG	9:I:6:GLY:N	2.80	0.48
9:I:17:VAL:HB	9:I:80:GLY:O	2.13	0.48
13:M:9:ILE:HD12	13:M:9:ILE:H	1.78	0.48
1:A:192:G:O2'	1:A:193:G:H5'	2.13	0.48
1:A:1184:C:H2'	1:A:1185:A:O4'	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1509:U:O2'	1:A:1510:C:H5'	2.13	0.48
2:B:170:GLU:O	2:B:173:ALA:HB3	2.13	0.48
5:E:8:GLU:HB3	5:E:34:VAL:HG22	1.95	0.48
5:E:122:GLU:O	5:E:123:LEU:HD23	2.13	0.48
8:H:2:LEU:HD12	8:H:2:LEU:N	2.28	0.48
10:J:32:ALA:HB3	10:J:75:ILE:HG13	1.94	0.48
14:N:23:ARG:C	14:N:33:VAL:HG11	2.37	0.48
15:O:54:ARG:O	15:O:58:MET:HG3	2.13	0.48
18:R:41:LYS:O	18:R:43:PHE:N	2.46	0.48
19:S:28:LYS:HB3	19:S:31:ILE:HD11	1.95	0.48
1:A:156:A:N7	1:A:157:C:H1'	2.28	0.48
1:A:513:G:O2'	1:A:514:U:OP2	2.30	0.48
1:A:1300:A:C4'	19:S:37:ARG:NH1	2.77	0.48
1:A:1472:U:H2'	1:A:1473:C:H6	1.78	0.48
2:B:27:LYS:O	2:B:194:PRO:HG3	2.13	0.48
7:G:73:MET:HG2	7:G:90:GLU:HA	1.94	0.48
9:I:20:ARG:O	9:I:21:PRO:C	2.56	0.48
9:I:118:LYS:HZ3	9:I:118:LYS:HB3	1.78	0.48
10:J:6:ILE:O	10:J:71:LEU:O	2.30	0.48
17:Q:76:LEU:HD21	17:Q:78:GLU:C	2.38	0.48
1:A:323:C:O2	1:A:323:C:C2'	2.61	0.48
1:A:667:A:N6	1:A:668:G:C6	2.81	0.48
1:A:1027:C:H2'	1:A:1028:A:O5'	2.14	0.48
2:B:69:LEU:C	2:B:69:LEU:HD23	2.39	0.48
2:B:100:GLY:O	2:B:104:ASN:N	2.43	0.48
3:C:35:GLU:O	3:C:36:ASP:C	2.56	0.48
4:D:190:ASP:O	4:D:191:ARG:C	2.56	0.48
6:F:9:VAL:HB	6:F:87:ARG:HB2	1.94	0.48
10:J:37:PRO:HA	10:J:72:VAL:H	1.78	0.48
11:K:77:MET:HE3	11:K:80:VAL:HG12	1.96	0.48
17:Q:26:GLN:O	17:Q:27:PHE:HB3	2.14	0.48
23:X:31:A:N3	23:X:31:A:C2'	2.74	0.48
1:A:1217:A:OP1	21:V:2:GLY:HA3	2.13	0.48
2:B:55:PHE:HE1	2:B:218:ALA:HA	1.77	0.48
2:B:213:LEU:HD23	2:B:217:ARG:CG	2.43	0.48
3:C:107:GLN:O	3:C:108:ASN:CB	2.61	0.48
5:E:10:MET:SD	5:E:13:ILE:HG23	2.53	0.48
5:E:30:ALA:O	5:E:45:PHE:HA	2.14	0.48
11:K:49:GLY:O	11:K:50:TYR:C	2.57	0.48
19:S:23:ASN:C	19:S:25:LYS:H	2.22	0.48
21:V:2:GLY:C	21:V:4:GLY:N	2.72	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:U:H4'	1:A:417:C:OP2	2.14	0.48
1:A:602:U:O2	4:D:133:VAL:HA	2.14	0.48
1:A:795:C:O2'	1:A:796:U:OP2	2.32	0.48
1:A:982:A:O2'	1:A:983:A:OP1	2.30	0.48
1:A:1236:G:H2'	1:A:1239:G:H21	1.77	0.48
5:E:76:ILE:HG23	5:E:142:LEU:CD1	2.43	0.48
9:I:3:GLN:HG3	9:I:4:TYR:N	2.28	0.48
9:I:50:LEU:O	9:I:53:VAL:HG22	2.13	0.48
17:Q:97:SER:HB2	17:Q:105:ALA:HB2	1.94	0.48
1:A:626:C:H4'	8:H:31:PHE:CE2	2.49	0.48
1:A:647:G:OP1	18:R:64:ARG:HD2	2.13	0.48
1:A:649:G:H5'	1:A:709:C:H1'	1.96	0.48
1:A:1114:C:O5'	1:A:1114:C:H6	1.97	0.48
1:A:1437:A:H2'	1:A:1438:G:O4'	2.13	0.48
1:A:1516:C:H41	7:G:82:GLY:HA2	1.78	0.48
3:C:5:ILE:O	3:C:5:ILE:HD12	2.14	0.48
3:C:16:ARG:HG3	3:C:16:ARG:NH1	2.19	0.48
4:D:60:GLU:HG2	4:D:202:LEU:HD12	1.94	0.48
17:Q:3:LYS:H	17:Q:3:LYS:HG2	1.51	0.48
18:R:37:VAL:HG22	18:R:78:LEU:HB3	1.96	0.48
20:T:39:LYS:HD2	20:T:55:ILE:HD12	1.93	0.48
1:A:238:A:H4'	1:A:239:U:O5'	2.13	0.48
1:A:948:G:H4'	1:A:949:C:OP2	2.14	0.48
1:A:1282:U:O2'	1:A:1283:U:OP1	2.28	0.48
2:B:52:GLU:O	2:B:56:ARG:HG3	2.14	0.48
2:B:185:ILE:HG23	2:B:199:TYR:HB2	1.95	0.48
3:C:8:ILE:O	3:C:11:ARG:N	2.34	0.48
3:C:35:GLU:O	3:C:38:ARG:N	2.46	0.48
4:D:14:ARG:HA	4:D:39:PRO:HB3	1.95	0.48
4:D:81:GLU:O	4:D:85:LYS:HG3	2.13	0.48
8:H:97:VAL:HG13	8:H:98:LYS:N	2.27	0.48
9:I:113:LYS:N	9:I:113:LYS:HD2	2.29	0.48
15:O:74:ASP:O	15:O:76:GLU:N	2.47	0.48
1:A:275:C:O5'	1:A:275:C:H6	1.97	0.48
1:A:507:G:H2'	1:A:508:C:C6	2.48	0.48
1:A:945:A:H4'	1:A:946:A:OP2	2.13	0.48
1:A:986:C:N4	1:A:1000:G:H22	2.11	0.48
1:A:1423:G:H4'	1:A:1424:G:C5	2.48	0.48
4:D:98:GLU:OE2	4:D:103:ASN:ND2	2.39	0.48
4:D:199:ASN:ND2	4:D:199:ASN:C	2.71	0.48
9:I:116:LYS:O	9:I:117:HIS:C	2.56	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:42:ARG:H	16:P:42:ARG:HG2	1.36	0.48
20:T:8:ARG:HH11	20:T:8:ARG:CB	2.05	0.48
20:T:45:GLN:HA	20:T:91:LEU:HD22	1.96	0.48
1:A:15:G:C4'	5:E:24:ARG:HH12	2.26	0.48
1:A:45:U:H2'	1:A:46:G:C8	2.49	0.48
1:A:450:C:H2'	1:A:451:C:H6	1.78	0.48
1:A:558:G:H4'	1:A:559:G:O5'	2.14	0.48
1:A:685:A:O2'	1:A:686:G:OP1	2.32	0.48
1:A:949:C:OP1	10:J:57:LYS:HD3	2.13	0.48
1:A:1098:C:C2'	1:A:1099:G:C5'	2.84	0.48
4:D:3:ARG:O	4:D:4:TYR:HB3	2.12	0.48
4:D:8:VAL:CG1	4:D:115:ARG:NH1	2.77	0.48
7:G:80:VAL:HG12	7:G:81:GLY:N	2.29	0.48
7:G:145:ALA:O	7:G:147:ALA:N	2.46	0.48
9:I:121:ARG:HG2	9:I:121:ARG:NH1	2.29	0.48
10:J:40:LEU:HD22	10:J:41:PRO:HD2	1.96	0.48
10:J:94:VAL:CG1	10:J:95:GLU:N	2.77	0.48
12:L:47:LYS:NZ	12:L:47:LYS:CB	2.77	0.48
1:A:407:A:C2	4:D:35:ARG:CG	2.97	0.47
1:A:966:C:O2'	1:A:967:C:H5'	2.14	0.47
2:B:41:ILE:HG13	2:B:41:ILE:O	2.13	0.47
4:D:13:ARG:NH1	4:D:38:TYR:O	2.47	0.47
8:H:119:LEU:HB3	8:H:123:GLU:HB2	1.95	0.47
9:I:4:TYR:CZ	9:I:88:TYR:HA	2.48	0.47
19:S:5:LEU:HD12	19:S:6:LYS:N	2.28	0.47
1:A:67:C:O2'	1:A:165:A:H1'	2.14	0.47
1:A:748:G:N2	1:A:795:C:O2'	2.47	0.47
1:A:876:C:O5'	1:A:876:C:H6	1.98	0.47
1:A:1345:A:H1'	1:A:1347:G:C8	2.49	0.47
1:A:1374:G:N2	1:A:1479:A:H8	2.12	0.47
1:A:1378:A:H4'	1:A:1379:C:H5''	1.95	0.47
1:A:1476:A:O2'	1:A:1477:A:H5'	2.13	0.47
4:D:31:CYS:C	4:D:33:MET:N	2.68	0.47
11:K:32:ILE:HG21	11:K:77:MET:HE2	1.96	0.47
17:Q:84:LEU:O	17:Q:85:VAL:C	2.57	0.47
17:Q:99:SER:OG	17:Q:100:LYS:N	2.44	0.47
1:A:563:U:H2'	1:A:564:G:O4'	2.14	0.47
1:A:1107:U:H3	10:J:5:ARG:NH2	2.12	0.47
2:B:7:VAL:HB	2:B:8:LYS:HZ2	1.78	0.47
2:B:71:VAL:O	2:B:165:VAL:HG22	2.14	0.47
2:B:87:ARG:HE	2:B:233:SER:HA	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:147:LYS:HE2	3:C:205:GLY:H	1.79	0.47
7:G:143:ARG:O	7:G:147:ALA:HB2	2.14	0.47
9:I:127:LYS:O	9:I:128:ARG:HB2	2.15	0.47
14:N:45:ARG:O	14:N:49:HIS:CD2	2.67	0.47
15:O:76:GLU:C	15:O:78:TYR:N	2.72	0.47
20:T:29:LYS:O	20:T:33:ILE:HG13	2.15	0.47
1:A:50:A:H3'	1:A:50:A:P	2.54	0.47
1:A:124:A:C8	17:Q:63:ARG:HG3	2.49	0.47
1:A:433:G:C4'	1:A:434:A:OP1	2.61	0.47
1:A:822:U:H5'	1:A:823:C:H5	1.79	0.47
1:A:986:C:N4	1:A:1000:G:N2	2.62	0.47
1:A:1047:U:O2'	1:A:1048:C:OP2	2.32	0.47
1:A:1487:U:H2'	1:A:1488:G:C8	2.49	0.47
4:D:70:ILE:HG22	4:D:71:SER:O	2.15	0.47
4:D:100:ARG:NH2	4:D:102:ASP:OD2	2.48	0.47
6:F:22:GLU:OE2	6:F:82:ARG:NE	2.40	0.47
13:M:58:GLU:HA	13:M:58:GLU:OE2	2.14	0.47
13:M:61:GLU:C	13:M:62:ASN:HD22	2.23	0.47
1:A:26:A:N6	1:A:541:G:H1'	2.29	0.47
1:A:423:G:O2'	1:A:424:U:OP2	2.31	0.47
1:A:660:U:H3	1:A:696:G:H22	1.62	0.47
1:A:1189:C:H2'	1:A:1190:C:H6	1.78	0.47
1:A:1211:C:H2'	1:A:1212:G:H8	1.80	0.47
2:B:158:LEU:HD23	2:B:182:ILE:HD11	1.96	0.47
2:B:158:LEU:CD2	2:B:180:LEU:HD13	2.45	0.47
12:L:83:VAL:HG22	12:L:84:LEU:N	2.29	0.47
1:A:96:C:P	20:T:17:ARG:HH11	2.37	0.47
1:A:176:U:H2'	1:A:177:G:O5'	2.15	0.47
1:A:446:A:H4'	16:P:72:ARG:HE	1.80	0.47
1:A:597:A:H2'	1:A:598:C:O4'	2.14	0.47
1:A:1174:G:O2'	1:A:1175:U:H5'	2.15	0.47
1:A:1197:G:H5''	14:N:5:ALA:CB	2.44	0.47
1:A:1502:G:O2'	1:A:1503:G:H5'	2.14	0.47
3:C:108:ASN:HD21	3:C:110:ASN:HB2	1.79	0.47
7:G:15:ASP:HB2	7:G:20:ASP:O	2.14	0.47
1:A:480:A:O2'	1:A:481:U:OP1	2.26	0.47
1:A:539:C:O2'	1:A:540:G:H5'	2.15	0.47
1:A:563:U:O2'	15:O:57:LEU:HG	2.15	0.47
1:A:639:C:O2'	15:O:28:GLN:OE1	2.20	0.47
1:A:720:A:H1'	6:F:73:ASN:HD21	1.79	0.47
1:A:823:C:H3'	1:A:823:C:OP2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:982:A:O2'	1:A:983:A:P	2.73	0.47
1:A:1035:G:O6	1:A:1180:U:H2'	2.15	0.47
1:A:1354:U:H2'	1:A:1355:G:O4'	2.14	0.47
2:B:114:ARG:O	2:B:117:GLU:HB3	2.15	0.47
2:B:181:PHE:HD2	8:H:70:GLN:HG2	1.79	0.47
4:D:140:VAL:CG1	4:D:146:ILE:HD11	2.43	0.47
6:F:60:PHE:CZ	18:R:78:LEU:HD21	2.50	0.47
7:G:15:ASP:HB3	7:G:20:ASP:N	2.30	0.47
13:M:109:THR:CG2	13:M:110:ARG:N	2.78	0.47
14:N:36:PHE:O	14:N:36:PHE:CD1	2.68	0.47
20:T:60:GLU:O	20:T:63:ILE:HB	2.13	0.47
1:A:31:G:H2'	1:A:48:C:N4	2.30	0.47
1:A:56:U:H2'	1:A:57:G:C8	2.50	0.47
1:A:173:A:H2'	1:A:174:U:H6	1.79	0.47
1:A:242:G:P	17:Q:99:SER:HG	2.38	0.47
1:A:953:G:H4'	1:A:954:A:OP1	2.14	0.47
1:A:1469:A:OP1	12:L:47:LYS:HA	2.15	0.47
1:A:1518:U:H3'	1:A:1518:U:C6	2.50	0.47
6:F:33:TYR:HA	6:F:71:ARG:HH21	1.80	0.47
18:R:41:LYS:C	18:R:43:PHE:H	2.23	0.47
18:R:47:THR:HG23	18:R:83:GLU:O	2.15	0.47
20:T:54:LYS:O	20:T:57:ARG:HB2	2.15	0.47
1:A:7:G:H21	5:E:121:LYS:HG2	1.79	0.47
1:A:241:A:N6	1:A:276:G:H1'	2.30	0.47
1:A:485:G:OP1	12:L:118:SER:CB	2.63	0.47
2:B:77:ALA:HB1	2:B:81:VAL:HG23	1.97	0.47
2:B:115:LEU:HD21	2:B:153:ARG:NH1	2.30	0.47
4:D:70:ILE:HD11	4:D:100:ARG:HD2	1.93	0.47
5:E:50:GLU:HG3	5:E:53:LEU:HB2	1.97	0.47
12:L:61:THR:C	12:L:63:GLY:H	2.22	0.47
12:L:83:VAL:HG21	12:L:100:ILE:CG2	2.44	0.47
13:M:106:ASN:O	13:M:107:ALA:CB	2.63	0.47
1:A:124:A:O2'	1:A:125:C:P	2.73	0.47
1:A:152:G:C6	1:A:158:U:O2	2.68	0.47
1:A:409:A:OP2	1:A:423:G:N2	2.46	0.47
1:A:645:G:H2'	1:A:646:A:C8	2.49	0.47
1:A:701:G:H1'	11:K:116:HIS:HA	1.95	0.47
1:A:1083:A:H8	2:B:172:ILE:HD13	1.79	0.47
1:A:1183:G:H2'	1:A:1184:C:O5'	2.14	0.47
5:E:102:ALA:HB2	5:E:120:THR:HB	1.96	0.47
11:K:34:ASP:OD2	11:K:38:ASN:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:21:VAL:HG21	16:P:59:TRP:CG	2.50	0.47
18:R:19:LYS:HG3	18:R:20:ALA:N	2.29	0.47
1:A:249:G:OP1	17:Q:67:LYS:O	2.33	0.46
1:A:494:C:O2'	1:A:495:U:O5'	2.33	0.46
1:A:705:A:H3'	1:A:705:A:N3	2.30	0.46
1:A:985:C:H2'	1:A:986:C:C5	2.48	0.46
1:A:1024:G:H2'	1:A:1025:C:C6	2.49	0.46
4:D:52:SER:O	4:D:54:TYR:N	2.49	0.46
4:D:63:LYS:O	4:D:67:ILE:HG13	2.14	0.46
5:E:135:THR:O	5:E:138:ALA:HB3	2.15	0.46
16:P:4:ILE:HG13	16:P:64:ALA:HB1	1.97	0.46
1:A:432:U:O2'	4:D:123:HIS:CD2	2.68	0.46
1:A:652:U:H2'	1:A:653:G:H8	1.80	0.46
6:F:47:ARG:HA	6:F:57:GLN:HG2	1.97	0.46
7:G:70:LYS:HB3	7:G:96:GLN:HG2	1.98	0.46
10:J:3:LYS:C	10:J:4:ILE:HD12	2.40	0.46
12:L:55:VAL:HG11	12:L:67:THR:HG23	1.97	0.46
14:N:25:VAL:HG13	14:N:26:ARG:N	2.30	0.46
17:Q:4:LYS:HD2	17:Q:6:LEU:CD2	2.45	0.46
18:R:36:ASN:OD1	18:R:38:GLU:HG2	2.15	0.46
19:S:40:ILE:HG21	19:S:62:ILE:CD1	2.45	0.46
1:A:1288:U:H2'	1:A:1289:U:C6	2.51	0.46
3:C:119:ARG:HG3	3:C:123:GLN:HE21	1.79	0.46
5:E:76:ILE:HG23	5:E:77:PRO:HD2	1.96	0.46
9:I:3:GLN:HB2	9:I:19:LEU:O	2.15	0.46
1:A:31:G:N1	1:A:48:C:H5''	2.31	0.46
1:A:801:G:O2'	1:A:802:A:H5''	2.15	0.46
4:D:199:ASN:HD21	4:D:201:GLN:CB	2.26	0.46
7:G:64:GLN:HG2	7:G:128:ALA:HB1	1.97	0.46
8:H:25:ASP:OD2	8:H:60:ARG:NH1	2.46	0.46
10:J:45:ARG:NH1	10:J:45:ARG:HG2	2.30	0.46
12:L:50:SER:O	12:L:51:ALA:HB2	2.15	0.46
17:Q:67:LYS:C	17:Q:69:LYS:H	2.22	0.46
1:A:238:A:N6	1:A:276:G:O2'	2.47	0.46
1:A:1162:G:O2'	1:A:1163:G:C5'	2.64	0.46
1:A:1352:G:O2'	1:A:1353:G:H5'	2.15	0.46
2:B:82:ARG:O	2:B:86:GLU:HG3	2.15	0.46
3:C:82:GLU:HG3	3:C:83:ARG:N	2.31	0.46
5:E:79:GLU:O	8:H:104:ARG:CZ	2.63	0.46
5:E:144:THR:O	5:E:145:LYS:C	2.58	0.46
9:I:15:ALA:HB2	9:I:65:VAL:HG23	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:43:ALA:O	9:I:44:VAL:C	2.58	0.46
11:K:45:GLY:C	11:K:55:LYS:HG2	2.41	0.46
15:O:39:LEU:HD23	15:O:43:LEU:HG	1.97	0.46
17:Q:45:HIS:NE2	17:Q:47:PRO:HG3	2.30	0.46
17:Q:90:ILE:O	17:Q:93:GLN:N	2.48	0.46
1:A:537:C:H2'	1:A:538:C:C6	2.51	0.46
1:A:906:G:H2'	1:A:907:C:O4'	2.16	0.46
1:A:1153:C:H2'	1:A:1154:G:H8	1.80	0.46
1:A:1231:A:H2'	1:A:1232:A:C8	2.51	0.46
1:A:1328:G:HO2'	1:A:1355:G:H1	1.64	0.46
7:G:28:ASN:HD21	7:G:36:LYS:HE3	1.79	0.46
9:I:99:LEU:HB3	9:I:101:PHE:CE1	2.50	0.46
13:M:54:VAL:O	13:M:58:GLU:HG2	2.15	0.46
15:O:74:ASP:C	15:O:76:GLU:N	2.73	0.46
17:Q:81:ARG:HB2	17:Q:83:ASP:OD1	2.15	0.46
23:X:30:G:H2'	23:X:31:A:C8	2.51	0.46
1:A:453:G:C3'	1:A:454:A:H5''	2.45	0.46
1:A:1108:U:H2'	1:A:1109:G:O5'	2.16	0.46
1:A:1378:A:O2'	1:A:1379:C:OP2	2.26	0.46
2:B:91:PRO:CG	2:B:154:LEU:HB3	2.36	0.46
10:J:9:ARG:HB3	10:J:9:ARG:NH1	2.30	0.46
12:L:10:LEU:O	12:L:14:GLY:N	2.48	0.46
15:O:42:HIS:O	15:O:45:VAL:O	2.34	0.46
1:A:189:U:O2'	1:A:190:G:OP1	2.28	0.46
1:A:404:G:H2'	1:A:405:G:O5'	2.15	0.46
1:A:1099:G:H4'	9:I:104:ARG:NH1	2.31	0.46
1:A:1338:A:N7	1:A:1339:U:C5	2.84	0.46
8:H:6:ILE:HB	8:H:85:ARG:HH12	1.80	0.46
8:H:36:LEU:CD1	8:H:59:LEU:HD13	2.46	0.46
15:O:69:TYR:O	15:O:73:GLU:HG2	2.15	0.46
18:R:37:VAL:HG12	18:R:41:LYS:HD3	1.97	0.46
1:A:669:U:H2'	1:A:670:A:O5'	2.16	0.46
1:A:1023:A:H2'	1:A:1023:A:N3	2.31	0.46
1:A:1217:A:O2'	1:A:1285:G:H4'	2.16	0.46
1:A:1406:C:C2'	1:A:1407:U:H5'	2.46	0.46
2:B:18:GLY:O	2:B:19:HIS:C	2.59	0.46
12:L:53:ARG:HH12	12:L:92:ASP:CB	2.29	0.46
12:L:110:VAL:O	12:L:122:THR:CG2	2.63	0.46
23:X:36:U:O2'	23:X:37:12A:H5''	2.16	0.46
1:A:143:A:H2'	1:A:144:C:H6	1.81	0.46
1:A:485:G:C2	1:A:486:C:C2	3.04	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:777:A:H2'	1:A:778:C:O4'	2.16	0.46
1:A:926:A:C2	1:A:1214:G:N3	2.84	0.46
1:A:1285:G:C6	1:A:1286:G:N1	2.83	0.46
1:A:1299:A:H4'	19:S:10:PHE:CD1	2.51	0.46
1:A:1463:G:H2'	1:A:1464:G:O4'	2.15	0.46
2:B:20:GLU:O	2:B:21:ARG:C	2.59	0.46
3:C:15:THR:HB	3:C:181:ASN:HB2	1.98	0.46
3:C:108:ASN:OD1	3:C:144:SER:HB2	2.15	0.46
8:H:20:TYR:CE1	8:H:76:PRO:HD2	2.51	0.46
10:J:8:LEU:HB2	10:J:70:ARG:CB	2.29	0.46
10:J:35:SER:HB3	10:J:72:VAL:O	2.16	0.46
12:L:33:ARG:HB3	12:L:60:LEU:HD12	1.97	0.46
12:L:82:VAL:HG22	12:L:106:ASP:OD1	2.16	0.46
13:M:59:TYR:O	13:M:63:THR:CG2	2.63	0.46
20:T:41:VAL:O	20:T:45:GLN:HB2	2.16	0.46
20:T:54:LYS:H	20:T:100:ILE:HD12	1.79	0.46
1:A:238:A:C2	1:A:241:A:C8	3.04	0.45
1:A:919:G:O2'	1:A:920:U:H5'	2.16	0.45
1:A:1294:U:H5	19:S:4:SER:HB2	1.81	0.45
1:A:1461:C:H3'	1:A:1461:C:H6	1.80	0.45
2:B:55:PHE:CE1	2:B:218:ALA:HA	2.50	0.45
3:C:34:LEU:HD23	3:C:34:LEU:O	2.14	0.45
3:C:108:ASN:ND2	3:C:110:ASN:HB2	2.31	0.45
6:F:67:MET:HE1	6:F:75:LEU:CB	2.46	0.45
10:J:38:ILE:HB	10:J:71:LEU:CB	2.46	0.45
13:M:29:ARG:HB3	13:M:64:TRP:CH2	2.51	0.45
20:T:50:GLU:HG2	20:T:100:ILE:HG12	1.97	0.45
1:A:246:G:H5'	1:A:247:U:OP1	2.16	0.45
1:A:315:C:H2'	1:A:316:A:C8	2.51	0.45
1:A:438:C:H2'	1:A:439:G:H8	1.82	0.45
1:A:516:A:C2	1:A:519:C:C5	3.04	0.45
1:A:1042:C:H4'	10:J:52:GLY:H	1.81	0.45
1:A:1288:U:C5'	13:M:109:THR:HG21	2.47	0.45
2:B:7:VAL:CG1	2:B:221:LEU:HD11	2.47	0.45
2:B:50:GLU:HB3	2:B:200:ILE:O	2.16	0.45
3:C:19:GLU:OE1	14:N:52:GLN:HG3	2.16	0.45
4:D:24:GLU:OE1	4:D:25:ARG:N	2.45	0.45
4:D:64:LEU:HD23	4:D:64:LEU:O	2.15	0.45
4:D:127:THR:OG1	4:D:130:GLY:O	2.35	0.45
4:D:200:GLU:OE1	4:D:200:GLU:N	2.43	0.45
6:F:1:MET:HE2	6:F:1:MET:CA	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:78:ILE:HG22	13:M:82:MET:HE2	1.98	0.45
13:M:114:ARG:HG2	13:M:114:ARG:HH11	1.81	0.45
21:V:3:LYS:H	21:V:3:LYS:CD	2.28	0.45
1:A:41:G:H2'	1:A:42:G:H8	1.80	0.45
1:A:424:U:HO2'	1:A:425:A:P	2.39	0.45
1:A:1049:A:C4'	1:A:1050:G:O5'	2.59	0.45
1:A:1082:C:H6	1:A:1082:C:C3'	2.24	0.45
1:A:1217:A:H4'	1:A:1285:G:H4'	1.97	0.45
1:A:1237:A:H2'	1:A:1238:U:C5'	2.45	0.45
1:A:1297:G:H22	1:A:1299:A:H3'	1.80	0.45
1:A:1349:C:C5'	10:J:60:ARG:NH1	2.79	0.45
4:D:201:GLN:OE1	4:D:201:GLN:HA	2.16	0.45
8:H:91:ARG:CG	12:L:7:ILE:HG13	2.44	0.45
11:K:21:ILE:HD13	11:K:94:ALA:HB3	1.99	0.45
12:L:53:ARG:HH12	12:L:92:ASP:HB2	1.81	0.45
13:M:8:GLU:C	13:M:9:ILE:HG13	2.40	0.45
13:M:98:VAL:C	13:M:100:GLY:H	2.25	0.45
16:P:53:VAL:O	16:P:57:ARG:HG3	2.17	0.45
20:T:43:LEU:HB3	20:T:48:LYS:HB2	1.97	0.45
20:T:91:LEU:C	20:T:93:GLU:N	2.74	0.45
1:A:190:G:H4'	1:A:191:G:OP2	2.17	0.45
1:A:198:U:C1'	20:T:103:GLY:HA2	2.43	0.45
1:A:408:G:H2'	1:A:423:G:N2	2.32	0.45
1:A:504:G:OP1	12:L:73:GLU:O	2.34	0.45
1:A:568:G:N3	1:A:856:C:H4'	2.31	0.45
1:A:689:A:O4'	11:K:29:ILE:HD11	2.16	0.45
1:A:965:G:H22	1:A:1199:C:H1'	1.81	0.45
5:E:92:LYS:HB3	5:E:119:LEU:HB2	1.99	0.45
7:G:23:VAL:HG13	7:G:43:PHE:CE2	2.52	0.45
9:I:4:TYR:CE1	9:I:88:TYR:HD1	2.35	0.45
12:L:7:ILE:O	12:L:11:VAL:HG23	2.16	0.45
13:M:33:ALA:HA	13:M:59:TYR:CE2	2.50	0.45
1:A:160:G:H2'	1:A:161:G:H8	1.82	0.45
1:A:297:G:H5''	12:L:17:LYS:CE	2.44	0.45
1:A:743:G:O2'	17:Q:98:LEU:HD22	2.17	0.45
1:A:824:U:H6	1:A:825:C:H1'	1.81	0.45
1:A:1112:A:O2'	9:I:3:GLN:NE2	2.50	0.45
2:B:8:LYS:HB2	2:B:9:GLU:H	1.46	0.45
2:B:19:HIS:HA	2:B:39:ILE:CG2	2.46	0.45
2:B:71:VAL:O	2:B:71:VAL:HG23	2.17	0.45
3:C:33:LEU:HD21	14:N:53:LEU:HD22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:56:LEU:O	15:O:60:VAL:HG23	2.16	0.45
17:Q:15:MET:HE1	17:Q:43:LEU:HD22	1.99	0.45
18:R:29:PHE:CE1	18:R:31:LEU:HG	2.51	0.45
20:T:23:ARG:HH22	20:T:27:LYS:HZ3	1.63	0.45
20:T:77:ALA:O	20:T:80:ARG:HB2	2.17	0.45
1:A:903:G:H3'	1:A:1482:G:N2	2.31	0.45
1:A:1030:G:H5''	14:N:3:ARG:HG3	1.97	0.45
1:A:1371:C:H2'	1:A:1372:U:O4'	2.17	0.45
2:B:131:PRO:O	2:B:135:GLN:HB2	2.16	0.45
6:F:23:LYS:NZ	6:F:42:GLU:OE2	2.40	0.45
9:I:3:GLN:HB3	9:I:20:ARG:HB3	1.98	0.45
9:I:5:TYR:CD1	9:I:6:GLY:N	2.84	0.45
10:J:50:ILE:HG12	10:J:60:ARG:HE	1.81	0.45
10:J:53:PRO:HA	14:N:41:ARG:NH2	2.29	0.45
13:M:96:LEU:HB3	13:M:97:PRO:HD2	1.98	0.45
1:A:268:A:N6	1:A:269:A:C6	2.85	0.45
1:A:278:C:O2'	1:A:279:G:H5'	2.17	0.45
1:A:431:C:H2'	1:A:432:U:C6	2.52	0.45
1:A:1086:G:OP1	2:B:111:ARG:HD2	2.17	0.45
1:A:1133:A:H4'	1:A:1134:A:OP1	2.17	0.45
1:A:1509:U:H2'	1:A:1510:C:C4'	2.47	0.45
3:C:19:GLU:OE2	3:C:54:ARG:HD2	2.17	0.45
5:E:31:LEU:HD23	5:E:45:PHE:HB2	1.98	0.45
6:F:15:ASP:OD1	6:F:18:GLN:HB2	2.16	0.45
6:F:69:GLU:C	6:F:71:ARG:H	2.25	0.45
7:G:15:ASP:CB	7:G:20:ASP:N	2.80	0.45
11:K:101:SER:C	11:K:103:LEU:H	2.24	0.45
14:N:44:LEU:HD12	14:N:44:LEU:C	2.42	0.45
17:Q:78:GLU:CD	17:Q:81:ARG:HD2	2.41	0.45
23:X:31:A:H3'	23:X:32:C:C6	2.51	0.45
1:A:337:C:H2'	1:A:338:U:C5'	2.45	0.45
1:A:501:C:C4	1:A:513:G:C2	3.04	0.45
1:A:562:G:H2'	1:A:563:U:C6	2.51	0.45
1:A:562:G:H1	1:A:745:C:H42	1.65	0.45
1:A:705:A:O2'	1:A:706:U:H3'	2.16	0.45
1:A:934:U:H3	1:A:937:U:H5''	1.80	0.45
1:A:1133:A:O2'	1:A:1134:A:C8	2.70	0.45
6:F:9:VAL:HA	6:F:59:TYR:O	2.16	0.45
7:G:36:LYS:O	7:G:39:ALA:HB3	2.17	0.45
8:H:104:ARG:O	8:H:106:GLY:N	2.49	0.45
19:S:40:ILE:O	19:S:67:VAL:O	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:24:LEU:HD12	20:T:27:LYS:HE3	1.97	0.45
1:A:83:A:H2'	1:A:84:C:H5'	1.98	0.45
1:A:123:G:C5	1:A:191:G:H1'	2.51	0.45
1:A:484:C:O3'	12:L:118:SER:HB2	2.16	0.45
1:A:707:G:O2'	1:A:708:G:H5'	2.16	0.45
1:A:801:G:O2'	1:A:803:U:H5	2.00	0.45
1:A:1297:G:C2	1:A:1299:A:H5''	2.52	0.45
2:B:27:LYS:HD3	2:B:195:ASP:OD2	2.17	0.45
3:C:33:LEU:HD11	14:N:53:LEU:HD23	1.99	0.45
3:C:84:ILE:HG13	3:C:88:ARG:CZ	2.47	0.45
9:I:43:ALA:N	9:I:74:ILE:HD13	2.32	0.45
13:M:20:THR:C	13:M:22:ILE:H	2.23	0.45
17:Q:67:LYS:HG2	17:Q:68:ARG:N	2.32	0.45
18:R:41:LYS:C	18:R:43:PHE:N	2.74	0.45
19:S:42:PRO:O	19:S:44:MET:N	2.50	0.45
1:A:5:U:O2'	1:A:6:G:OP2	2.30	0.45
1:A:257:A:C6	1:A:258:A:C6	3.04	0.45
1:A:591:A:H2'	1:A:592:A:H5'	1.99	0.45
1:A:731:C:H4'	1:A:732:C:O5'	2.17	0.45
3:C:7:PRO:HG2	3:C:184:TYR:HB2	2.00	0.45
4:D:31:CYS:O	4:D:33:MET:N	2.46	0.45
7:G:62:PHE:HD1	7:G:124:LEU:HD21	1.82	0.45
9:I:59:PHE:HZ	9:I:88:TYR:CG	2.35	0.45
12:L:44:THR:HA	12:L:45:PRO:HD3	1.85	0.45
16:P:19:ILE:HG22	16:P:36:ILE:CG1	2.47	0.45
19:S:9:VAL:CG1	19:S:10:PHE:N	2.80	0.45
20:T:50:GLU:HG2	20:T:100:ILE:CG1	2.47	0.45
1:A:64:G:O2'	1:A:65:U:OP2	2.29	0.44
1:A:261:G:H5'	1:A:262:C:OP1	2.17	0.44
1:A:378:A:H2'	1:A:379:G:H5'	2.00	0.44
1:A:740:U:H2'	1:A:741:G:O4'	2.16	0.44
1:A:922:G:H21	1:A:1315:G:H4'	1.81	0.44
1:A:982:A:N7	1:A:1019:C:C2	2.86	0.44
1:A:1043:G:H1'	10:J:56:HIS:CE1	2.52	0.44
2:B:39:ILE:HG22	2:B:40:HIS:N	2.32	0.44
5:E:20:GLN:O	5:E:21:ALA:C	2.59	0.44
5:E:81:GLU:OE1	5:E:88:LYS:HE2	2.17	0.44
17:Q:13:ASP:C	17:Q:15:MET:N	2.75	0.44
17:Q:63:ARG:O	17:Q:65:ILE:HD12	2.17	0.44
20:T:57:ARG:HD2	20:T:102:GLY:HA3	1.99	0.44
1:A:398:C:O2'	1:A:399:U:H5'	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:898:U:O2'	5:E:19:MET:O	2.29	0.44
1:A:984:C:C2'	1:A:985:C:C6	2.75	0.44
1:A:1006:C:N4	1:A:1007:C:C4	2.85	0.44
1:A:1301:C:C2	19:S:72:GLY:HA3	2.52	0.44
2:B:101:MET:O	2:B:105:PHE:HA	2.17	0.44
2:B:102:LEU:N	2:B:102:LEU:CD1	2.80	0.44
3:C:51:GLY:O	3:C:52:LEU:HB3	2.16	0.44
4:D:28:SER:O	4:D:30:LYS:N	2.51	0.44
5:E:145:LYS:HA	8:H:107:LEU:CD2	2.46	0.44
9:I:55:ALA:O	9:I:56:LEU:HB2	2.17	0.44
13:M:11:ARG:CG	13:M:12:ASN:N	2.78	0.44
15:O:66:LEU:O	15:O:67:LEU:C	2.61	0.44
20:T:12:ALA:O	20:T:15:ARG:HB2	2.18	0.44
1:A:100:G:C3'	1:A:101:G:H5''	2.47	0.44
1:A:362:U:C6	1:A:389:G:N2	2.85	0.44
1:A:565:U:C2	1:A:743:G:C6	3.05	0.44
1:A:630:C:H2'	1:A:631:A:H8	1.83	0.44
1:A:1126:G:C8	1:A:1126:G:C3'	3.00	0.44
1:A:1134:A:H2'	1:A:1135:C:H6	1.82	0.44
1:A:1218:C:H4'	1:A:1315:G:N2	2.31	0.44
1:A:1231:A:H5''	9:I:68:GLY:N	2.32	0.44
2:B:7:VAL:HG21	2:B:8:LYS:HZ3	1.81	0.44
2:B:15:VAL:HG12	2:B:209:ARG:O	2.17	0.44
4:D:199:ASN:C	4:D:199:ASN:HD22	2.26	0.44
5:E:75:THR:HG23	5:E:76:ILE:O	2.18	0.44
7:G:61:VAL:HG23	7:G:62:PHE:N	2.33	0.44
10:J:9:ARG:C	10:J:16:LEU:HD11	2.41	0.44
12:L:60:LEU:CD2	12:L:66:VAL:HG22	2.47	0.44
17:Q:66:SER:OG	17:Q:69:LYS:HB2	2.17	0.44
1:A:167:U:H5''	1:A:203:A:O4'	2.18	0.44
1:A:501:C:OP2	1:A:513:G:H1'	2.17	0.44
1:A:915:A:N6	1:A:916:G:C6	2.86	0.44
1:A:1095:C:H1'	3:C:178:LEU:HD21	1.99	0.44
1:A:1163:G:C8	1:A:1163:G:O5'	2.70	0.44
1:A:1168:G:OP1	9:I:113:LYS:NZ	2.51	0.44
1:A:1203:G:P	19:S:77:THR:HG21	2.57	0.44
2:B:115:LEU:HD21	2:B:153:ARG:CZ	2.48	0.44
2:B:213:LEU:HD23	2:B:213:LEU:C	2.42	0.44
3:C:64:VAL:HG12	3:C:66:VAL:CG2	2.44	0.44
4:D:60:GLU:OE2	4:D:198:VAL:HA	2.17	0.44
5:E:74:GLY:HA3	5:E:116:THR:HG22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:137:GLU:HG2	5:E:140:ARG:HH12	1.82	0.44
6:F:10:LEU:H	6:F:10:LEU:HG	1.65	0.44
7:G:28:ASN:O	7:G:31:MET:HB3	2.18	0.44
8:H:64:LYS:HG2	8:H:79:VAL:CG2	2.41	0.44
11:K:87:THR:HG23	11:K:91:ARG:HH22	1.79	0.44
12:L:47:LYS:HB3	12:L:48:PRO:HD3	1.99	0.44
13:M:60:VAL:HG12	13:M:66:LEU:HD11	1.98	0.44
18:R:59:SER:O	18:R:61:LYS:N	2.51	0.44
19:S:12:ASP:HB3	19:S:14:HIS:CD2	2.52	0.44
1:A:175:G:H4'	1:A:176:U:H5'	1.97	0.44
1:A:364:C:O2	1:A:388:A:C2	2.70	0.44
1:A:407:A:C2	4:D:35:ARG:HG3	2.52	0.44
1:A:408:G:N2	1:A:423:G:H1'	2.32	0.44
1:A:801:G:C3'	1:A:802:A:H5'	2.48	0.44
1:A:1068:U:H3	1:A:1081:G:H22	1.65	0.44
1:A:1238:U:O2'	1:A:1239:G:P	2.76	0.44
2:B:43:ASP:O	2:B:44:LEU:C	2.60	0.44
2:B:61:LEU:CD2	2:B:66:GLY:HA3	2.47	0.44
3:C:113:ALA:N	3:C:114:PRO:CD	2.81	0.44
3:C:113:ALA:HB3	3:C:114:PRO:HD3	2.00	0.44
3:C:126:ARG:HG3	3:C:126:ARG:NH1	2.32	0.44
6:F:61:LEU:O	6:F:62:TRP:HB2	2.16	0.44
7:G:18:TYR:HD1	7:G:59:LEU:HD22	1.80	0.44
8:H:75:ARG:HA	8:H:76:PRO:HD3	1.78	0.44
9:I:3:GLN:CB	9:I:20:ARG:HB3	2.48	0.44
9:I:55:ALA:C	9:I:57:GLY:N	2.76	0.44
10:J:24:VAL:HG13	10:J:28:ARG:HH12	1.83	0.44
10:J:34:VAL:HG13	10:J:74:ILE:HG22	1.99	0.44
12:L:53:ARG:HG2	12:L:53:ARG:NH1	2.33	0.44
1:A:470:U:O2'	1:A:471:A:H5'	2.17	0.44
1:A:492:A:H5'	4:D:54:TYR:HD2	1.81	0.44
1:A:502:C:H2'	1:A:503:A:O4'	2.17	0.44
1:A:731:C:H1'	1:A:732:C:H5	1.83	0.44
1:A:1037:A:H5'	1:A:1037:A:H8	1.83	0.44
1:A:1426:A:O2'	1:A:1427:G:OP1	2.35	0.44
2:B:145:LEU:O	2:B:149:LEU:HB2	2.18	0.44
3:C:8:ILE:C	3:C:10:PHE:N	2.74	0.44
3:C:178:LEU:O	3:C:179:ARG:HB2	2.18	0.44
5:E:82:VAL:HB	5:E:138:ALA:HB2	1.99	0.44
7:G:21:VAL:HG23	7:G:22:LEU:N	2.32	0.44
8:H:123:GLU:O	8:H:127:LEU:HD23	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:19:LEU:HB3	9:I:59:PHE:CD2	2.53	0.44
10:J:47:PHE:CE2	14:N:37:PHE:CE1	2.98	0.44
1:A:55:A:O2'	1:A:56:U:H5'	2.18	0.44
1:A:350:C:O4'	1:A:383:G:O2'	2.31	0.44
1:A:1112:A:H3'	1:A:1113:G:C8	2.52	0.44
1:A:1210:A:H2'	1:A:1211:C:C6	2.52	0.44
2:B:81:VAL:O	2:B:85:ALA:HB2	2.18	0.44
3:C:108:ASN:C	3:C:108:ASN:HD22	2.26	0.44
3:C:182:ILE:HA	3:C:202:ILE:O	2.17	0.44
4:D:3:ARG:O	4:D:4:TYR:CB	2.66	0.44
4:D:166:LYS:HG3	4:D:178:VAL:HG11	1.98	0.44
5:E:69:VAL:HG21	5:E:113:ALA:HB1	1.99	0.44
16:P:6:LEU:HD12	16:P:6:LEU:N	2.33	0.44
18:R:59:SER:O	18:R:60:GLY:C	2.60	0.44
1:A:82:U:H3'	1:A:82:U:H6	1.83	0.44
1:A:209:U:C4'	1:A:210:U:OP1	2.65	0.44
1:A:520:G:H5''	12:L:113:ARG:HH21	1.82	0.44
1:A:565:U:OP1	15:O:64:ARG:NH1	2.51	0.44
1:A:1083:A:C8	2:B:172:ILE:HD13	2.53	0.44
1:A:1091:C:OP2	3:C:176:HIS:CD2	2.71	0.44
3:C:10:PHE:CZ	3:C:178:LEU:HD13	2.53	0.44
10:J:87:THR:O	10:J:88:LEU:HG	2.17	0.44
12:L:83:VAL:HG22	12:L:84:LEU:H	1.82	0.44
13:M:108:ARG:O	13:M:112:GLY:N	2.51	0.44
14:N:27:CYS:SG	14:N:29:ARG:HB2	2.58	0.44
15:O:82:ILE:O	15:O:83:GLU:C	2.61	0.44
21:V:14:TRP:C	21:V:16:GLY:N	2.73	0.44
23:X:36:U:C2'	23:X:37:12A:C5'	2.86	0.44
1:A:457:A:O4'	16:P:82:GLN:NE2	2.38	0.44
1:A:635:U:HO2'	1:A:636:A:P	2.41	0.44
1:A:1008:C:H2'	1:A:1009:G:C8	2.53	0.44
2:B:91:PRO:HG2	2:B:155:LEU:HG	2.00	0.44
3:C:191:THR:HG22	3:C:192:THR:N	2.32	0.44
9:I:27:THR:HG22	9:I:28:VAL:N	2.32	0.44
9:I:58:ARG:HH11	9:I:58:ARG:HG3	1.83	0.44
10:J:16:LEU:O	10:J:17:ASP:C	2.61	0.44
14:N:45:ARG:HH11	14:N:45:ARG:HG3	1.82	0.44
14:N:61:TRP:N	14:N:61:TRP:CE3	2.85	0.44
17:Q:65:ILE:N	17:Q:65:ILE:CD1	2.81	0.44
20:T:14:LYS:HE2	20:T:18:GLN:NE2	2.32	0.44
1:A:117:G:C6	1:A:118:U:C4	3.06	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:C:H2'	1:A:291:U:O4'	2.17	0.43
1:A:324:A:H4'	1:A:325:C:OP1	2.18	0.43
1:A:349:G:N3	1:A:349:G:H2'	2.33	0.43
1:A:463:C:H2'	1:A:464:U:O4'	2.18	0.43
1:A:505:C:H41	12:L:53:ARG:HH22	1.61	0.43
1:A:953:G:H8	1:A:1339:U:O2'	2.01	0.43
1:A:1139:A:O2'	1:A:1140:C:OP2	2.28	0.43
2:B:92:TYR:CD2	2:B:151:GLY:HA3	2.53	0.43
4:D:121:VAL:O	4:D:134:ASP:HA	2.18	0.43
5:E:12:LEU:HD13	5:E:12:LEU:C	2.43	0.43
6:F:12:PRO:HG3	6:F:55:ASP:OD1	2.18	0.43
9:I:33:PHE:CZ	9:I:47:LEU:HD21	2.53	0.43
9:I:127:LYS:HE2	9:I:127:LYS:HB2	1.73	0.43
11:K:63:LEU:O	11:K:64:ALA:C	2.60	0.43
12:L:52:LEU:O	12:L:54:LYS:HD2	2.18	0.43
12:L:86:ARG:HG3	12:L:86:ARG:NH1	2.32	0.43
13:M:108:ARG:NE	13:M:108:ARG:HA	2.32	0.43
14:N:37:PHE:CD2	14:N:53:LEU:HD13	2.53	0.43
17:Q:48:GLU:O	17:Q:49:GLU:C	2.61	0.43
18:R:55:ARG:HB3	18:R:55:ARG:HH11	1.79	0.43
23:X:32:C:H2'	23:X:33:U:O4'	2.18	0.43
1:A:259:U:O2'	17:Q:64:PRO:HB2	2.18	0.43
1:A:570:G:O2'	1:A:571:G:O5'	2.36	0.43
1:A:831:G:C6	1:A:832:G:N7	2.86	0.43
1:A:872:G:H2'	1:A:873:C:C6	2.52	0.43
1:A:1046:G:H4'	1:A:1047:U:OP1	2.17	0.43
1:A:1049:A:O2'	1:A:1050:G:C8	2.68	0.43
1:A:1221:U:HO2'	1:A:1222:G:P	2.39	0.43
1:A:1259:U:H5''	1:A:1260:A:O4'	2.17	0.43
1:A:1461:C:C6	1:A:1461:C:C3'	3.00	0.43
4:D:187:ARG:HG3	4:D:188:LEU:N	2.34	0.43
5:E:121:LYS:HA	5:E:121:LYS:HD2	1.79	0.43
6:F:101:ALA:CB	18:R:28:GLU:HG3	2.46	0.43
14:N:3:ARG:O	14:N:4:LYS:C	2.61	0.43
15:O:17:ARG:NH2	15:O:77:ARG:HD3	2.33	0.43
18:R:47:THR:HG22	18:R:48:GLY:H	1.83	0.43
19:S:22:LEU:HD21	19:S:28:LYS:HB2	2.00	0.43
1:A:169:C:O2'	1:A:170:C:H5'	2.19	0.43
1:A:513:G:OP1	1:A:514:U:H5''	2.18	0.43
1:A:670:A:HO2'	1:A:671:G:P	2.42	0.43
1:A:1220:A:H2'	1:A:1279:C:H42	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1259:U:C5'	1:A:1260:A:O4'	2.66	0.43
3:C:65:ALA:O	3:C:66:VAL:CB	2.67	0.43
7:G:99:LEU:HD23	7:G:99:LEU:HA	1.90	0.43
9:I:113:LYS:H	9:I:119:ALA:HA	1.83	0.43
20:T:100:ILE:O	20:T:101:GLY:C	2.59	0.43
1:A:82:U:C6	1:A:82:U:C3'	3.00	0.43
1:A:627:G:C5	1:A:628:C:C5	3.07	0.43
1:A:670:A:O2'	1:A:671:G:OP2	2.35	0.43
1:A:832:G:H2'	1:A:833:C:C6	2.54	0.43
1:A:859:C:O2'	1:A:860:C:H5'	2.19	0.43
1:A:926:A:N7	13:M:106:ASN:ND2	2.66	0.43
3:C:31:HIS:C	3:C:33:LEU:N	2.77	0.43
3:C:68:VAL:HG12	3:C:70:VAL:HG13	2.01	0.43
3:C:132:ARG:HA	3:C:135:LYS:HD3	1.99	0.43
9:I:40:LEU:O	9:I:42:ARG:N	2.51	0.43
9:I:45:ALA:O	9:I:48:GLU:N	2.38	0.43
11:K:70:LYS:O	11:K:71:LYS:C	2.60	0.43
11:K:115:PRO:C	11:K:117:ASN:H	2.26	0.43
12:L:89:ARG:HD2	12:L:89:ARG:N	2.33	0.43
14:N:29:ARG:HH22	14:N:41:ARG:NH1	2.15	0.43
1:A:114:C:C4'	1:A:115:G:OP1	2.65	0.43
1:A:333:A:H2	1:A:346:G:H22	1.67	0.43
1:A:392:A:H3'	1:A:392:A:N3	2.34	0.43
1:A:752:G:H4'	1:A:1490:A:H4'	1.99	0.43
1:A:1109:G:H21	1:A:1128:A:N6	2.13	0.43
1:A:1133:A:O2'	1:A:1134:A:P	2.77	0.43
1:A:1374:G:N2	1:A:1479:A:C8	2.86	0.43
2:B:231:GLU:HB3	2:B:232:PRO:HD2	2.01	0.43
3:C:157:ILE:HB	3:C:164:ARG:NH2	2.32	0.43
7:G:58:PRO:C	7:G:60:LYS:H	2.26	0.43
7:G:58:PRO:HA	7:G:61:VAL:HG22	2.00	0.43
10:J:75:ILE:O	10:J:76:ASN:CB	2.66	0.43
12:L:89:ARG:CD	12:L:89:ARG:N	2.81	0.43
12:L:113:ARG:O	12:L:117:ARG:HG2	2.18	0.43
13:M:6:GLY:O	13:M:7:VAL:HG22	2.18	0.43
20:T:16:HIS:NE2	20:T:20:LEU:HD21	2.34	0.43
20:T:94:ALA:O	20:T:95:ALA:HB3	2.19	0.43
1:A:53:A:N6	1:A:54:C:C4	2.85	0.43
1:A:143:A:H2'	1:A:144:C:C6	2.53	0.43
1:A:484:C:H2'	1:A:485:G:C8	2.52	0.43
1:A:985:C:O5'	1:A:985:C:H6	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1167:G:H21	14:N:61:TRP:C	2.26	0.43
1:A:1281:G:O2'	1:A:1282:U:P	2.75	0.43
2:B:208:ILE:C	2:B:210:SER:N	2.77	0.43
3:C:108:ASN:C	3:C:110:ASN:H	2.26	0.43
13:M:65:LYS:HD3	13:M:69:GLU:HG2	1.99	0.43
1:A:270:G:H5'	17:Q:14:LYS:HB3	2.00	0.43
1:A:608:G:H2'	1:A:609:U:C6	2.54	0.43
1:A:723:U:O2'	1:A:724:G:H5'	2.18	0.43
1:A:736:A:C4'	1:A:737:C:O5'	2.58	0.43
1:A:780:C:OP1	11:K:124:LYS:CE	2.64	0.43
1:A:1216:U:H2'	1:A:1217:A:O4'	2.19	0.43
1:A:1384:C:C5	1:A:1385:C:C5	3.07	0.43
1:A:1504:C:O2'	1:A:1505:U:H5'	2.19	0.43
2:B:61:LEU:O	2:B:61:LEU:HD22	2.18	0.43
2:B:69:LEU:HD22	2:B:71:VAL:HG13	1.99	0.43
3:C:70:VAL:C	3:C:106:VAL:HG23	2.42	0.43
4:D:34:GLU:O	4:D:35:ARG:CB	2.60	0.43
5:E:35:GLY:HA2	5:E:40:ARG:O	2.19	0.43
5:E:83:GLU:HG3	5:E:88:LYS:HG3	2.00	0.43
12:L:65:GLU:N	12:L:65:GLU:OE1	2.52	0.43
15:O:82:ILE:O	15:O:85:LEU:N	2.51	0.43
16:P:74:LEU:CG	16:P:79:VAL:HG21	2.41	0.43
19:S:11:VAL:HG13	19:S:38:SER:HB2	1.99	0.43
1:A:129:C:O2	16:P:1:MET:N	2.51	0.43
1:A:501:C:O2'	12:L:50:SER:HB3	2.18	0.43
1:A:636:A:OP1	8:H:56:LYS:NZ	2.49	0.43
1:A:888:U:H2'	1:A:889:C:C6	2.53	0.43
1:A:1029:G:C2'	1:A:1030:G:H5'	2.49	0.43
2:B:114:ARG:NE	2:B:118:LEU:HD11	2.34	0.43
3:C:23:TYR:CG	3:C:24:ALA:N	2.86	0.43
3:C:73:PRO:O	3:C:75:VAL:N	2.51	0.43
4:D:149:ALA:HB3	4:D:152:SER:HB2	2.01	0.43
5:E:36:ASP:OD2	5:E:40:ARG:HD3	2.18	0.43
7:G:64:GLN:HG3	7:G:68:ASN:ND2	2.34	0.43
15:O:33:THR:HG23	15:O:63:ARG:NH1	2.34	0.43
17:Q:60:ILE:HD13	17:Q:60:ILE:C	2.44	0.43
18:R:48:GLY:O	18:R:74:ARG:NH2	2.52	0.43
19:S:40:ILE:HD13	19:S:62:ILE:HD13	2.00	0.43
19:S:43:GLU:HG2	19:S:43:GLU:O	2.18	0.43
1:A:385:C:O3'	16:P:28:ARG:NH2	2.52	0.43
1:A:399:U:H2'	1:A:400:U:C6	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:562:G:H5'	1:A:711:A:C1'	2.42	0.43
1:A:625:A:N7	8:H:115:SER:HA	2.34	0.43
1:A:915:A:C6	1:A:916:G:C5	3.07	0.43
1:A:1133:A:C2'	1:A:1134:A:C8	3.02	0.43
2:B:76:GLN:O	2:B:208:ILE:HG12	2.19	0.43
2:B:81:VAL:O	2:B:81:VAL:CG1	2.66	0.43
2:B:111:ARG:HB3	2:B:149:LEU:HD11	2.00	0.43
2:B:209:ARG:NH1	2:B:239:VAL:HG21	2.34	0.43
3:C:15:THR:O	3:C:16:ARG:CB	2.58	0.43
5:E:28:PHE:O	5:E:47:LYS:HA	2.18	0.43
7:G:148:ASN:HD22	7:G:148:ASN:N	2.08	0.43
9:I:14:VAL:O	9:I:65:VAL:HG23	2.18	0.43
11:K:123:LYS:O	11:K:124:LYS:C	2.62	0.43
12:L:8:ASN:OD1	17:Q:34:LYS:HE2	2.19	0.43
12:L:119:LYS:O	12:L:120:TYR:CB	2.67	0.43
13:M:15:VAL:HG21	13:M:48:LEU:HD21	2.00	0.43
18:R:59:SER:C	18:R:61:LYS:H	2.26	0.43
20:T:67:ALA:O	20:T:73:HIS:CE1	2.72	0.43
1:A:126:C:HO2'	1:A:127:U:H5'	1.84	0.43
1:A:198:U:H1'	20:T:103:GLY:CA	2.45	0.43
1:A:328:G:O2'	1:A:329:C:H5'	2.19	0.43
1:A:340:C:H4'	1:A:341:G:O5'	2.18	0.43
1:A:402:G:H2'	1:A:403:A:H8	1.83	0.43
1:A:407:A:C2	4:D:35:ARG:HB3	2.54	0.43
1:A:757:G:H2'	1:A:758:G:O4'	2.19	0.43
1:A:867:G:O2'	1:A:868:U:OP2	2.23	0.43
1:A:869:A:C2	1:A:884:A:C4	3.07	0.43
1:A:1099:G:O3'	9:I:104:ARG:NH1	2.52	0.43
1:A:1293:G:O6	19:S:4:SER:HB3	2.18	0.43
1:A:1298:C:H2'	1:A:1299:A:O4'	2.18	0.43
2:B:92:TYR:O	2:B:151:GLY:HA3	2.19	0.43
8:H:4:ASP:C	8:H:4:ASP:OD1	2.62	0.43
8:H:104:ARG:O	8:H:107:LEU:N	2.46	0.43
9:I:89:ASN:O	9:I:92:TYR:HB2	2.18	0.43
13:M:5:ALA:O	13:M:6:GLY:C	2.61	0.43
14:N:24:CYS:SG	14:N:40:CYS:N	2.92	0.43
16:P:19:ILE:HG22	16:P:36:ILE:HG13	2.01	0.43
1:A:100:G:H3'	1:A:101:G:H5''	2.01	0.42
1:A:156:A:C5	1:A:157:C:H1'	2.54	0.42
1:A:221:G:O2'	1:A:222:G:H5'	2.19	0.42
1:A:239:U:H4'	1:A:240:C:O5'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:A:H1'	1:A:548:U:O2	2.19	0.42
1:A:951:A:OP2	14:N:41:ARG:NH1	2.51	0.42
1:A:985:C:N3	1:A:986:C:N4	2.66	0.42
1:A:1076:G:O2'	1:A:1077:U:OP2	2.34	0.42
1:A:1339:U:H3'	1:A:1340:C:C6	2.54	0.42
2:B:217:ARG:HA	2:B:220:ASP:OD2	2.19	0.42
7:G:46:ALA:O	7:G:50:ILE:HG13	2.19	0.42
7:G:62:PHE:HA	7:G:124:LEU:HD23	2.01	0.42
7:G:89:MET:O	7:G:90:GLU:C	2.62	0.42
8:H:104:ARG:O	8:H:105:ARG:C	2.61	0.42
9:I:10:ARG:HD2	9:I:75:ASP:CB	2.48	0.42
10:J:45:ARG:HG2	10:J:45:ARG:HH11	1.83	0.42
11:K:109:VAL:HG22	18:R:86:VAL:HG22	2.00	0.42
14:N:29:ARG:HB3	14:N:40:CYS:CB	2.49	0.42
16:P:42:ARG:O	16:P:43:LYS:C	2.62	0.42
16:P:45:THR:C	16:P:47:ASP:N	2.73	0.42
19:S:5:LEU:O	19:S:6:LYS:CB	2.66	0.42
1:A:415:U:H2'	1:A:417:C:C4	2.54	0.42
1:A:1092:A:H8	1:A:1092:A:O5'	2.02	0.42
1:A:1240:C:O2	1:A:1264:G:H1'	2.19	0.42
3:C:29:TYR:CE1	14:N:54:PRO:HG2	2.54	0.42
6:F:14:LEU:HB3	6:F:18:GLN:CB	2.46	0.42
10:J:47:PHE:CZ	14:N:37:PHE:HE1	2.37	0.42
13:M:84:ILE:HG13	13:M:86:CYS:HB2	2.00	0.42
13:M:94:ARG:HH12	19:S:81:ARG:CD	2.15	0.42
14:N:8:GLU:OE2	14:N:11:LYS:HD2	2.19	0.42
17:Q:43:LEU:HD12	17:Q:68:ARG:HB3	2.01	0.42
17:Q:86:GLU:O	17:Q:90:ILE:HG13	2.19	0.42
18:R:53:ARG:C	18:R:55:ARG:H	2.27	0.42
1:A:401:G:C4	1:A:479:A:C5	3.08	0.42
1:A:925:C:O2'	1:A:926:A:H5'	2.19	0.42
1:A:936:A:C5'	1:A:937:U:OP2	2.55	0.42
1:A:952:A:H4'	1:A:953:G:OP2	2.18	0.42
1:A:1003:U:C6	1:A:1003:U:C3'	3.01	0.42
1:A:1039:G:H5''	3:C:154:SER:CB	2.49	0.42
1:A:1221:U:O2'	1:A:1222:G:OP1	2.28	0.42
1:A:1282:U:O2'	1:A:1283:U:P	2.77	0.42
1:A:1335:C:O2'	1:A:1336:G:H5'	2.19	0.42
2:B:88:ALA:HB2	2:B:219:VAL:HG13	2.01	0.42
2:B:230:VAL:CG1	2:B:231:GLU:H	2.27	0.42
6:F:36:ARG:NH1	6:F:38:GLU:HG2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:41:PRO:O	16:P:43:LYS:HG3	2.19	0.42
20:T:67:ALA:HA	20:T:73:HIS:H	1.83	0.42
1:A:412:C:H6	1:A:412:C:O5'	2.02	0.42
1:A:469:G:HO2'	1:A:470:U:P	2.35	0.42
1:A:630:C:H2'	1:A:631:A:C8	2.54	0.42
1:A:878:A:C5	1:A:879:G:H1'	2.55	0.42
1:A:984:C:H3'	1:A:984:C:H6	1.85	0.42
1:A:1094:C:N3	3:C:178:LEU:N	2.61	0.42
2:B:61:LEU:HD21	2:B:66:GLY:HA3	2.01	0.42
3:C:8:ILE:O	3:C:9:GLY:C	2.62	0.42
5:E:36:ASP:OD1	5:E:40:ARG:HB2	2.19	0.42
6:F:100:ASN:ND2	18:R:23:LYS:HZ2	2.16	0.42
10:J:79:ARG:HG2	10:J:79:ARG:HH11	1.84	0.42
12:L:47:LYS:HB2	12:L:47:LYS:HZ2	1.81	0.42
1:A:102:A:C6	1:A:321:G:C6	3.07	0.42
1:A:578:G:H22	1:A:626:C:H41	1.66	0.42
1:A:724:G:H5''	15:O:39:LEU:HD12	2.00	0.42
1:A:936:A:C3'	1:A:937:U:C5'	2.92	0.42
1:A:1280:A:C5	1:A:1282:U:O2	2.72	0.42
1:A:1296:U:H2'	1:A:1297:G:O4'	2.19	0.42
2:B:18:GLY:O	2:B:40:HIS:HB3	2.20	0.42
2:B:88:ALA:CB	2:B:90:MET:HG2	2.49	0.42
3:C:11:ARG:C	3:C:13:GLY:N	2.78	0.42
3:C:122:GLU:HG2	3:C:126:ARG:HH21	1.85	0.42
3:C:149:ALA:HA	3:C:201:TYR:O	2.19	0.42
4:D:107:ARG:C	4:D:109:GLY:N	2.76	0.42
5:E:13:ILE:C	5:E:13:ILE:CD1	2.93	0.42
5:E:107:ARG:HG2	5:E:108:ALA:N	2.35	0.42
7:G:51:GLN:C	7:G:53:LYS:H	2.27	0.42
11:K:33:THR:HB	11:K:38:ASN:C	2.45	0.42
11:K:51:LYS:C	11:K:51:LYS:HD3	2.44	0.42
14:N:11:LYS:O	14:N:12:ARG:C	2.62	0.42
17:Q:81:ARG:HG3	17:Q:81:ARG:O	2.19	0.42
1:A:85:U:O5'	1:A:85:U:H6	2.03	0.42
1:A:242:G:P	17:Q:99:SER:OG	2.77	0.42
1:A:337:C:C2'	1:A:338:U:H5'	2.47	0.42
1:A:377:A:C2	1:A:378:A:C4	3.08	0.42
1:A:399:U:H5'	4:D:122:ARG:HD2	2.01	0.42
1:A:936:A:HO2'	1:A:961:C:HO2'	1.68	0.42
3:C:76:VAL:O	3:C:83:ARG:O	2.38	0.42
6:F:76:ALA:O	6:F:77:ARG:C	2.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:62:ASN:O	13:M:63:THR:HB	2.19	0.42
15:O:21:ASP:CG	15:O:24:SER:HB3	2.45	0.42
20:T:59:ALA:O	20:T:60:GLU:C	2.61	0.42
1:A:451:C:H2'	1:A:452:C:H6	1.83	0.42
1:A:465:G:C2'	1:A:467:C:N4	2.79	0.42
1:A:523:G:H2'	1:A:524:G:O4'	2.19	0.42
1:A:720:A:H2'	1:A:721:C:O4'	2.20	0.42
1:A:959:U:OP1	1:A:959:U:C6	2.69	0.42
1:A:1077:U:H2'	1:A:1078:C:C6	2.55	0.42
1:A:1163:G:H4'	1:A:1164:A:C5'	2.50	0.42
1:A:1213:U:H2'	1:A:1214:G:O4'	2.20	0.42
1:A:1269:A:C2	1:A:1270:A:C4	3.08	0.42
1:A:1501:C:OP1	11:K:120:ARG:NH1	2.52	0.42
2:B:114:ARG:HG2	2:B:114:ARG:HH11	1.83	0.42
3:C:73:PRO:C	3:C:75:VAL:N	2.75	0.42
3:C:116:VAL:HG21	3:C:202:ILE:HD11	2.02	0.42
4:D:105:VAL:HG13	4:D:110:PHE:HB2	2.02	0.42
5:E:51:VAL:HB	5:E:52:PRO:CD	2.46	0.42
6:F:10:LEU:CD1	6:F:59:TYR:HD2	2.33	0.42
7:G:15:ASP:HB2	7:G:20:ASP:H	1.82	0.42
11:K:44:SER:H	11:K:47:VAL:HB	1.83	0.42
12:L:93:LEU:HB2	12:L:96:VAL:CG2	2.49	0.42
16:P:29:ASP:OD2	16:P:29:ASP:N	2.53	0.42
18:R:47:THR:HG22	18:R:48:GLY:N	2.35	0.42
20:T:50:GLU:HA	20:T:100:ILE:HG13	2.01	0.42
20:T:56:MET:HE3	20:T:88:VAL:HG11	2.02	0.42
1:A:813:G:H2'	1:A:814:U:O4'	2.20	0.42
1:A:1095:C:H1'	3:C:178:LEU:CD2	2.48	0.42
1:A:1187:G:C6	1:A:1188:G:C5	3.08	0.42
1:A:1520:C:C2'	1:A:1521:U:H5'	2.50	0.42
2:B:118:LEU:C	2:B:120:ALA:N	2.75	0.42
4:D:36:ARG:H	4:D:37:PRO:HD3	1.85	0.42
4:D:64:LEU:C	4:D:64:LEU:CD2	2.93	0.42
5:E:143:ARG:HD3	5:E:143:ARG:HA	1.78	0.42
6:F:1:MET:O	6:F:2:ARG:HG3	2.19	0.42
6:F:11:ASN:HD21	6:F:13:ASN:CG	2.27	0.42
6:F:30:LEU:HD23	6:F:75:LEU:HD21	2.01	0.42
6:F:36:ARG:HH12	6:F:38:GLU:HG2	1.84	0.42
13:M:16:ASP:OD1	13:M:16:ASP:N	2.50	0.42
16:P:14:ASN:N	16:P:15:PRO:CD	2.83	0.42
19:S:16:LEU:CA	19:S:19:VAL:HG12	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:A:N1	1:A:896:A:H2	2.18	0.42
1:A:29:G:H5'	1:A:291:U:OP1	2.20	0.42
1:A:970:G:O2'	1:A:971:A:OP1	2.30	0.42
1:A:1113:G:C8	1:A:1113:G:C3'	3.03	0.42
1:A:1331:A:C2	1:A:1332:U:C2	3.08	0.42
2:B:16:HIS:C	2:B:17:PHE:O	2.61	0.42
5:E:24:ARG:HH11	5:E:24:ARG:CG	2.33	0.42
17:Q:17:LYS:HA	17:Q:46:ASP:O	2.19	0.42
20:T:65:LYS:O	20:T:68:LYS:CB	2.68	0.42
1:A:157:C:C2'	1:A:158:U:H5'	2.50	0.42
1:A:246:G:C4'	1:A:247:U:H5'	2.42	0.42
1:A:669:U:C2'	1:A:670:A:O5'	2.68	0.42
1:A:825:C:H3'	1:A:825:C:H6	1.80	0.42
1:A:837:A:H2'	1:A:838:G:O4'	2.20	0.42
1:A:849:A:C4'	1:A:850:A:OP1	2.60	0.42
1:A:951:A:OP2	14:N:32:SER:OG	2.37	0.42
1:A:1207:C:C4'	1:A:1208:A:OP1	2.60	0.42
2:B:177:ALA:O	2:B:180:LEU:N	2.45	0.42
4:D:15:GLU:CD	4:D:59:ARG:HH21	2.28	0.42
7:G:58:PRO:C	7:G:60:LYS:N	2.77	0.42
9:I:10:ARG:HH11	9:I:11:LYS:HB2	1.85	0.42
9:I:71:SER:HA	9:I:74:ILE:HB	2.01	0.42
13:M:40:ASN:ND2	13:M:40:ASN:C	2.78	0.42
18:R:29:PHE:HE1	18:R:31:LEU:HG	1.84	0.42
19:S:77:THR:HG22	19:S:78:ARG:N	2.33	0.42
1:A:218:U:H2'	1:A:219:C:O4'	2.20	0.41
1:A:576:G:O2'	1:A:577:G:H5'	2.20	0.41
1:A:936:A:C3'	1:A:937:U:H5''	2.30	0.41
1:A:961:C:H2'	1:A:962:C:C6	2.55	0.41
1:A:1506:G:C4'	1:A:1507:G:OP2	2.68	0.41
25:A:1783:PAR:H43	25:A:1783:PAR:N64	2.35	0.41
2:B:76:GLN:HB3	2:B:211:ILE:HD11	2.01	0.41
7:G:38:LEU:HA	7:G:41:ARG:CD	2.47	0.41
10:J:55:LYS:O	10:J:56:HIS:HB2	2.18	0.41
14:N:13:THR:N	14:N:14:PRO:CD	2.83	0.41
14:N:22:THR:HB	14:N:33:VAL:CG2	2.47	0.41
14:N:39:LEU:CD1	14:N:47:LEU:HD12	2.50	0.41
19:S:7:LYS:O	19:S:7:LYS:CD	2.53	0.41
19:S:15:LEU:O	19:S:19:VAL:N	2.53	0.41
19:S:63:THR:OG1	19:S:66:MET:HE3	2.19	0.41
23:X:37:12A:N1	23:X:37:12A:N	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:G:C8	17:Q:96:GLN:NE2	2.88	0.41
1:A:699:A:O2'	1:A:700:C:H5'	2.20	0.41
1:A:714:G:H5'	1:A:749:A:H4'	2.02	0.41
1:A:854:C:O2	8:H:3:THR:OG1	2.33	0.41
1:A:1049:A:H1'	1:A:1050:G:O4'	2.21	0.41
1:A:1092:A:N6	1:A:1093:A:C6	2.88	0.41
1:A:1131:C:OP1	9:I:14:VAL:HG11	2.20	0.41
1:A:1193:U:H2'	1:A:1194:A:OP2	2.21	0.41
1:A:1247:G:N2	1:A:1251:C:N3	2.67	0.41
1:A:1323:C:O2'	9:I:124:GLN:HB2	2.20	0.41
1:A:1341:A:H2'	1:A:1342:G:O4'	2.20	0.41
1:A:1420:G:H2'	1:A:1421:C:C6	2.55	0.41
1:A:1509:U:H2'	1:A:1510:C:H4'	2.02	0.41
4:D:52:SER:C	4:D:54:TYR:N	2.76	0.41
5:E:126:ARG:CG	5:E:126:ARG:HH11	2.33	0.41
7:G:120:ILE:O	7:G:124:LEU:HD13	2.20	0.41
8:H:81:HIS:ND1	8:H:81:HIS:N	2.66	0.41
13:M:73:GLU:O	13:M:77:ASN:HB2	2.20	0.41
15:O:45:VAL:HG12	15:O:46:HIS:ND1	2.35	0.41
1:A:65:U:O2'	1:A:66:G:OP2	2.32	0.41
1:A:84:C:H2'	1:A:85:U:O4'	2.21	0.41
1:A:436:C:H2'	1:A:437:C:C6	2.55	0.41
1:A:591:A:C2'	1:A:592:A:H5'	2.50	0.41
1:A:816:U:H2'	1:A:817:C:H6	1.83	0.41
1:A:954:A:H2'	1:A:954:A:N3	2.34	0.41
1:A:986:C:C4	1:A:1000:G:N2	2.87	0.41
1:A:1269:A:H2'	1:A:1270:A:H8	1.85	0.41
2:B:164:VAL:HB	2:B:186:ALA:HB2	2.01	0.41
3:C:11:ARG:C	3:C:13:GLY:H	2.27	0.41
3:C:84:ILE:HG13	3:C:88:ARG:NH2	2.36	0.41
4:D:120:LEU:O	4:D:126:ILE:HG12	2.20	0.41
5:E:103:GLY:O	5:E:104:ALA:C	2.61	0.41
7:G:31:MET:SD	7:G:34:GLY:HA2	2.61	0.41
9:I:99:LEU:CB	9:I:101:PHE:CE1	3.03	0.41
10:J:4:ILE:N	10:J:4:ILE:CD1	2.83	0.41
12:L:28:LYS:O	12:L:29:GLY:C	2.62	0.41
17:Q:87:LYS:O	17:Q:88:TYR:C	2.62	0.41
1:A:304:G:O2'	1:A:305:G:H5'	2.20	0.41
1:A:669:U:O4	1:A:670:A:N6	2.53	0.41
1:A:1202:G:OP1	1:A:1302:C:N3	2.53	0.41
3:C:191:THR:HG21	3:C:193:TYR:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:195:VAL:O	3:C:196:LEU:HD23	2.19	0.41
4:D:111:ALA:HB2	4:D:120:LEU:HD12	2.02	0.41
4:D:157:LEU:HD23	4:D:157:LEU:C	2.46	0.41
5:E:118:ILE:HG12	5:E:119:LEU:N	2.35	0.41
7:G:15:ASP:HB3	7:G:19:GLY:H	1.79	0.41
8:H:112:LEU:HD12	8:H:112:LEU:H	1.81	0.41
9:I:19:LEU:HB3	9:I:59:PHE:HD2	1.85	0.41
13:M:35:GLU:O	13:M:37:THR:N	2.53	0.41
15:O:65:ARG:HG3	15:O:65:ARG:NH1	2.34	0.41
15:O:70:LEU:HD12	15:O:78:TYR:HA	2.02	0.41
23:X:39:PSU:HO2'	23:X:40:C:H5'	1.83	0.41
1:A:31:G:H1	1:A:48:C:H5''	1.86	0.41
1:A:44:G:O2'	1:A:45:U:H5'	2.20	0.41
1:A:249:G:OP1	17:Q:68:ARG:HB2	2.20	0.41
1:A:588:U:H2'	1:A:589:G:O4'	2.20	0.41
1:A:735:G:H4'	15:O:69:TYR:OH	2.21	0.41
1:A:838:G:C2'	1:A:839:C:H5'	2.50	0.41
1:A:1077:U:P	1:A:1090:G:H1	2.44	0.41
1:A:1134:A:H5'	10:J:13:HIS:HB2	2.02	0.41
1:A:1193:U:C2'	1:A:1194:A:OP2	2.69	0.41
1:A:1231:A:H5'	9:I:68:GLY:O	2.19	0.41
1:A:1317:C:H4'	1:A:1318:G:OP2	2.20	0.41
2:B:177:ALA:O	2:B:178:ARG:C	2.64	0.41
5:E:19:MET:O	5:E:20:GLN:NE2	2.46	0.41
6:F:27:GLN:HE21	6:F:27:GLN:HB3	1.57	0.41
7:G:113:GLU:CG	7:G:119:ARG:HG2	2.51	0.41
11:K:24:SER:C	11:K:26:ASN:N	2.79	0.41
11:K:77:MET:CE	11:K:80:VAL:HG12	2.51	0.41
11:K:95:ILE:CG2	11:K:108:ILE:HD13	2.51	0.41
12:L:76:ASN:O	12:L:76:ASN:ND2	2.54	0.41
15:O:86:GLY:C	15:O:87:ILE:HG13	2.46	0.41
17:Q:101:ARG:HG2	17:Q:101:ARG:HH11	1.86	0.41
1:A:750:A:H2'	1:A:751:A:O4'	2.20	0.41
1:A:982:A:HO2'	1:A:983:A:P	2.43	0.41
1:A:1123:C:C2'	1:A:1124:G:H5'	2.43	0.41
1:A:1189:C:H2'	1:A:1190:C:C6	2.55	0.41
1:A:1460:A:C2'	1:A:1461:C:O5'	2.69	0.41
2:B:30:ARG:H	2:B:30:ARG:HG2	1.57	0.41
4:D:76:ARG:NH1	4:D:80:GLU:OE1	2.53	0.41
4:D:131:ARG:HE	4:D:131:ARG:HB2	1.68	0.41
15:O:87:ILE:O	15:O:88:ARG:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:34:GLU:OE1	16:P:55:ARG:NH1	2.53	0.41
16:P:52:ASP:OD1	16:P:52:ASP:C	2.63	0.41
19:S:17:GLU:HA	19:S:20:LEU:HG	2.03	0.41
1:A:494:C:O2'	1:A:495:U:C5'	2.69	0.41
1:A:735:G:O2'	1:A:736:A:OP2	2.38	0.41
1:A:1111:C:OP1	9:I:62:TYR:OH	2.38	0.41
1:A:1113:G:H8	1:A:1113:G:O5'	2.04	0.41
1:A:1264:G:O2'	1:A:1265:C:H5'	2.21	0.41
1:A:1357:A:H2'	1:A:1358:U:O4'	2.21	0.41
1:A:1382:C:C4'	1:A:1383:G:OP2	2.68	0.41
2:B:9:GLU:CD	2:B:9:GLU:N	2.78	0.41
2:B:72:GLY:HA2	2:B:165:VAL:CG2	2.50	0.41
4:D:102:ASP:OD1	4:D:103:ASN:N	2.54	0.41
9:I:43:ALA:HA	9:I:74:ILE:HD13	2.03	0.41
10:J:76:ASN:O	10:J:78:ASN:N	2.51	0.41
11:K:58:PRO:O	11:K:61:ALA:HB3	2.21	0.41
17:Q:76:LEU:HD23	17:Q:77:VAL:C	2.46	0.41
20:T:54:LYS:N	20:T:100:ILE:HD12	2.36	0.41
20:T:69:GLY:O	20:T:73:HIS:CD2	2.73	0.41
1:A:278:C:C2'	1:A:279:G:H5'	2.50	0.41
1:A:387:G:C4	1:A:388:A:C8	3.09	0.41
1:A:705:A:O2'	1:A:706:U:O5'	2.38	0.41
1:A:743:G:H2'	1:A:744:G:H5'	2.02	0.41
1:A:899:G:H5'	5:E:20:GLN:HE22	1.82	0.41
1:A:959:U:H5''	14:N:3:ARG:HH22	1.86	0.41
1:A:1194:A:HO2'	1:A:1195:C:P	2.42	0.41
1:A:1502:G:P	11:K:120:ARG:HH22	2.44	0.41
2:B:82:ARG:NH1	2:B:83:MET:CE	2.83	0.41
2:B:144:ARG:C	2:B:146:GLN:N	2.78	0.41
3:C:29:TYR:C	3:C:29:TYR:HD2	2.29	0.41
3:C:85:ARG:HA	3:C:88:ARG:HH21	1.86	0.41
3:C:139:GLN:NE2	3:C:139:GLN:CA	2.76	0.41
5:E:79:GLU:O	8:H:104:ARG:NH1	2.54	0.41
5:E:126:ARG:HG3	5:E:126:ARG:HH11	1.84	0.41
10:J:8:LEU:CD2	10:J:96:ILE:HG12	2.50	0.41
11:K:70:LYS:HA	11:K:73:MET:HG3	2.02	0.41
17:Q:74:LEU:O	17:Q:74:LEU:HD23	2.19	0.41
19:S:22:LEU:HD22	19:S:26:GLY:O	2.20	0.41
23:X:36:U:H2'	23:X:37:12A:H5'	1.99	0.41
1:A:44:G:C2	1:A:45:U:H1'	2.56	0.41
1:A:157:C:H2'	1:A:158:U:H5'	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:C:H2'	1:A:335:U:C6	2.55	0.41
1:A:446:A:O2'	1:A:447:A:H8	2.03	0.41
1:A:492:A:H5'	4:D:54:TYR:CD2	2.56	0.41
1:A:505:C:H2'	1:A:506:A:O4'	2.21	0.41
1:A:635:U:O2'	1:A:636:A:C5'	2.69	0.41
1:A:657:G:H2'	1:A:658:A:C8	2.55	0.41
1:A:658:A:H1'	11:K:116:HIS:CG	2.56	0.41
1:A:659:A:O2'	1:A:660:U:H5'	2.20	0.41
1:A:739:C:C4	1:A:740:U:C4	3.09	0.41
1:A:914:A:C2	1:A:1361:G:O6	2.74	0.41
1:A:919:G:N3	1:A:920:U:C6	2.89	0.41
1:A:932:U:O2'	1:A:933:U:H5'	2.21	0.41
1:A:960:A:H3'	1:A:960:A:N3	2.36	0.41
1:A:981:G:O2'	1:A:982:A:OP1	2.30	0.41
1:A:1009:G:O5'	1:A:1009:G:H8	2.04	0.41
1:A:1127:C:O2'	1:A:1128:A:P	2.79	0.41
1:A:1203:G:OP1	19:S:77:THR:HG21	2.20	0.41
1:A:1395:A:H2'	1:A:1396:U:O4'	2.21	0.41
1:A:1426:A:O2'	1:A:1427:G:P	2.79	0.41
2:B:28:PHE:HE1	2:B:188:ALA:HB1	1.85	0.41
2:B:84:GLU:OE1	2:B:216:SER:HA	2.19	0.41
2:B:220:ASP:O	2:B:224:GLN:HB2	2.20	0.41
2:B:239:VAL:HG12	2:B:240:GLN:NE2	2.36	0.41
3:C:122:GLU:HG2	3:C:126:ARG:NH2	2.36	0.41
4:D:196:LEU:HA	4:D:196:LEU:HD23	1.80	0.41
5:E:101:ILE:HD12	5:E:119:LEU:HD23	2.03	0.41
7:G:138:LYS:HE2	7:G:142:GLU:OE1	2.20	0.41
9:I:16:ARG:O	9:I:63:ILE:HG23	2.21	0.41
11:K:84:VAL:CG2	11:K:110:ASP:HA	2.42	0.41
15:O:29:VAL:HG11	15:O:67:LEU:HD21	2.03	0.41
20:T:93:GLU:HA	20:T:93:GLU:OE2	2.21	0.41
21:V:3:LYS:HG2	21:V:14:TRP:CD1	2.56	0.41
1:A:280:G:O2'	1:A:281:G:H5'	2.21	0.41
1:A:404:G:C2'	1:A:405:G:O5'	2.68	0.41
1:A:408:G:N2	1:A:423:G:O2'	2.54	0.41
1:A:539:C:C2'	1:A:540:G:H5'	2.50	0.41
1:A:1025:C:H2'	1:A:1026:A:OP2	2.20	0.41
1:A:1085:C:H2'	1:A:1086:G:O4'	2.22	0.41
1:A:1170:C:C5'	1:A:1171:G:OP2	2.60	0.41
1:A:1171:G:C2'	1:A:1172:A:OP2	2.69	0.41
2:B:54:THR:O	2:B:58:ILE:HG13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:68:GLU:O	5:E:70:PRO:HD3	2.21	0.41
8:H:11:THR:O	8:H:12:ARG:C	2.63	0.41
10:J:34:VAL:HG12	10:J:35:SER:N	2.36	0.41
10:J:54:PHE:O	10:J:55:LYS:HG2	2.21	0.41
13:M:49:THR:O	13:M:50:GLU:C	2.61	0.41
15:O:26:GLU:HA	15:O:81:LEU:HD11	2.04	0.41
17:Q:86:GLU:O	17:Q:89:LEU:HB2	2.21	0.41
1:A:110:G:O6	1:A:284:G:H1'	2.21	0.40
1:A:370:U:O2	16:P:28:ARG:NE	2.51	0.40
1:A:669:U:O2	11:K:42:TRP:CZ2	2.73	0.40
1:A:670:A:H2	1:A:683:G:N3	2.20	0.40
1:A:942:A:O2'	1:A:943:G:OP2	2.39	0.40
1:A:1042:C:OP1	14:N:45:ARG:NH2	2.54	0.40
1:A:1103:U:H2'	1:A:1104:U:C6	2.56	0.40
1:A:1127:C:O2'	1:A:1128:A:O5'	2.32	0.40
1:A:1237:A:O2'	1:A:1238:U:H4'	2.19	0.40
1:A:1286:G:O2'	1:A:1287:A:O5'	2.39	0.40
1:A:1484:A:C2	1:A:1485:G:C4	3.09	0.40
1:A:1506:G:C5'	1:A:1507:G:OP2	2.67	0.40
5:E:91:LEU:HD22	5:E:118:ILE:CD1	2.51	0.40
6:F:19:LEU:O	6:F:22:GLU:N	2.54	0.40
7:G:18:TYR:HB3	7:G:59:LEU:HD22	2.03	0.40
10:J:8:LEU:HD23	10:J:96:ILE:HG12	2.02	0.40
10:J:63:PHE:HA	14:N:57:ARG:O	2.21	0.40
12:L:88:GLY:C	12:L:97:ARG:O	2.64	0.40
15:O:78:TYR:C	15:O:80:ALA:N	2.77	0.40
16:P:18:ARG:O	16:P:20:VAL:HG12	2.20	0.40
17:Q:15:MET:HB2	17:Q:18:THR:O	2.22	0.40
1:A:245:A:O4'	1:A:247:U:C6	2.74	0.40
1:A:457:A:H4'	16:P:80:PHE:O	2.21	0.40
1:A:847:U:H4'	1:A:848:U:O5'	2.21	0.40
1:A:931:G:H2'	1:A:932:U:C6	2.56	0.40
1:A:1023:A:C6	1:A:1024:G:N7	2.89	0.40
1:A:1044:U:H2'	1:A:1045:C:C6	2.55	0.40
1:A:1311:U:C2'	1:A:1312:G:H5'	2.51	0.40
1:A:1422:C:H2'	1:A:1423:G:H5'	2.02	0.40
1:A:1424:G:N3	1:A:1424:G:H2'	2.37	0.40
1:A:1483:U:O2'	1:A:1484:A:OP1	2.38	0.40
4:D:49:ARG:O	4:D:51:PRO:HD3	2.20	0.40
5:E:79:GLU:O	5:E:80:ILE:HG23	2.19	0.40
7:G:64:GLN:O	7:G:67:GLU:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:25:ILE:HD11	13:M:60:VAL:HG13	2.02	0.40
13:M:37:THR:HG22	13:M:37:THR:O	2.21	0.40
19:S:15:LEU:H	19:S:15:LEU:HD23	1.86	0.40
1:A:82:U:H2'	1:A:83:A:C8	2.56	0.40
1:A:701:G:O6	18:R:74:ARG:NH1	2.55	0.40
1:A:775:A:O2'	1:A:776:U:OP2	2.39	0.40
1:A:808:G:N2	8:H:11:THR:HG21	2.36	0.40
1:A:1008:C:H2'	1:A:1009:G:H8	1.85	0.40
1:A:1084:A:H2'	1:A:1085:C:C6	2.57	0.40
1:A:1123:C:H2'	1:A:1123:C:O2	2.21	0.40
1:A:1188:G:H2'	1:A:1189:C:H6	1.86	0.40
4:D:196:LEU:HD23	4:D:197:PRO:HD2	2.04	0.40
5:E:126:ARG:NH1	5:E:126:ARG:CG	2.85	0.40
6:F:10:LEU:O	6:F:11:ASN:C	2.64	0.40
8:H:31:PHE:CZ	8:H:134:ILE:HD13	2.57	0.40
9:I:11:LYS:O	9:I:12:GLU:HB3	2.21	0.40
10:J:8:LEU:O	10:J:69:ASN:HA	2.21	0.40
13:M:114:ARG:HG2	13:M:114:ARG:NH1	2.37	0.40
14:N:23:ARG:NH1	14:N:30:ALA:HB2	2.36	0.40
17:Q:81:ARG:HB2	17:Q:81:ARG:HE	1.75	0.40
19:S:10:PHE:C	19:S:11:VAL:HG23	2.47	0.40
20:T:38:LYS:O	20:T:39:LYS:C	2.64	0.40
1:A:9:G:N7	1:A:541:G:O2'	2.51	0.40
1:A:124:A:H1'	1:A:258:A:O2'	2.21	0.40
1:A:434:A:C4	1:A:480:A:C2	3.09	0.40
1:A:592:A:C2'	1:A:593:G:H5'	2.51	0.40
1:A:952:A:H4'	1:A:953:G:C5'	2.45	0.40
1:A:1326:U:O2'	1:A:1327:A:OP2	2.34	0.40
1:A:1509:U:C2'	1:A:1510:C:C5'	2.88	0.40
2:B:55:PHE:HE1	2:B:218:ALA:CA	2.33	0.40
3:C:11:ARG:HG3	3:C:11:ARG:HH11	1.86	0.40
3:C:29:TYR:OH	14:N:54:PRO:CD	2.70	0.40
3:C:134:ILE:O	3:C:138:VAL:HG23	2.22	0.40
12:L:83:VAL:HG21	12:L:100:ILE:HG21	2.03	0.40
12:L:98:TYR:CD1	12:L:98:TYR:N	2.89	0.40
13:M:66:LEU:O	13:M:67:GLU:C	2.63	0.40
15:O:11:VAL:HG21	15:O:34:LEU:HD22	2.03	0.40
19:S:29:ARG:O	19:S:30:LEU:HB2	2.22	0.40
21:V:5:ASP:HB3	21:V:8:THR:CG2	2.52	0.40
21:V:6:ARG:HG2	21:V:15:ARG:HH11	1.84	0.40
1:A:109:A:H61	1:A:308:A:H1'	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:G:H2'	1:A:329:C:H6	1.87	0.40
1:A:545:C:H4'	1:A:546:A:O5'	2.21	0.40
1:A:1425:G:H5''	1:A:1426:A:C5'	2.48	0.40
1:A:1478:C:C5	1:A:1481:G:C4	3.09	0.40
6:F:8:ILE:CD1	6:F:79:LEU:HD22	2.52	0.40
7:G:37:ASN:O	7:G:38:LEU:C	2.65	0.40
8:H:86:ILE:O	8:H:87:SER:C	2.63	0.40
8:H:104:ARG:C	8:H:106:GLY:N	2.78	0.40
10:J:38:ILE:CG1	10:J:71:LEU:HB3	2.51	0.40
10:J:89:ASP:O	10:J:90:LEU:HD23	2.22	0.40
11:K:59:TYR:O	11:K:60:ALA:C	2.64	0.40
13:M:15:VAL:CG2	13:M:48:LEU:HD21	2.51	0.40
16:P:26:ARG:HG2	16:P:27:LYS:H	1.87	0.40
18:R:24:ALA:O	18:R:26:LEU:N	2.55	0.40
18:R:45:SER:C	18:R:47:THR:N	2.77	0.40
20:T:57:ARG:NH2	20:T:100:ILE:CG2	2.84	0.40
21:V:15:ARG:O	21:V:17:THR:HG23	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	232/256 (91%)	165 (71%)	47 (20%)	20 (9%)	0	3
3	C	204/239 (85%)	151 (74%)	33 (16%)	20 (10%)	0	2
4	D	206/209 (99%)	171 (83%)	29 (14%)	6 (3%)	3	18
5	E	148/162 (91%)	135 (91%)	13 (9%)	0	100	100
6	F	99/101 (98%)	78 (79%)	16 (16%)	5 (5%)	1	9
7	G	153/156 (98%)	120 (78%)	27 (18%)	6 (4%)	2	13
8	H	136/138 (99%)	121 (89%)	12 (9%)	3 (2%)	5	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	125/128 (98%)	93 (74%)	24 (19%)	8 (6%)	1	6
10	J	96/105 (91%)	69 (72%)	18 (19%)	9 (9%)	0	3
11	K	117/129 (91%)	94 (80%)	17 (14%)	6 (5%)	1	9
12	L	122/132 (92%)	93 (76%)	22 (18%)	7 (6%)	1	7
13	M	123/126 (98%)	90 (73%)	23 (19%)	10 (8%)	1	4
14	N	58/61 (95%)	40 (69%)	12 (21%)	6 (10%)	0	2
15	O	86/89 (97%)	68 (79%)	14 (16%)	4 (5%)	2	10
16	P	81/88 (92%)	64 (79%)	14 (17%)	3 (4%)	2	14
17	Q	102/105 (97%)	82 (80%)	16 (16%)	4 (4%)	2	13
18	R	71/88 (81%)	57 (80%)	9 (13%)	5 (7%)	1	5
19	S	78/93 (84%)	60 (77%)	10 (13%)	8 (10%)	0	2
20	T	97/106 (92%)	70 (72%)	20 (21%)	7 (7%)	1	4
21	V	22/27 (82%)	15 (68%)	5 (23%)	2 (9%)	0	3
All	All	2356/2538 (93%)	1836 (78%)	381 (16%)	139 (6%)	1	7

All (139) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	15	VAL
2	B	20	GLU
2	B	190	THR
3	C	15	THR
3	C	16	ARG
3	C	20	SER
3	C	24	ALA
3	C	65	ALA
3	C	179	ARG
3	C	189	ALA
4	D	30	LYS
6	F	98	LEU
7	G	5	ARG
7	G	7	ALA
9	I	117	HIS
10	J	34	VAL
10	J	39	PRO
10	J	51	ARG
10	J	54	PHE

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Mol	Chain	Res	Type
11	K	12	ARG
11	K	127	LYS
12	L	27	LEU
12	L	116	SER
13	M	63	THR
13	M	67	GLU
13	M	107	ALA
18	R	87	ARG
19	S	5	LEU
19	S	9	VAL
21	V	3	LYS
2	B	19	HIS
2	B	108	ILE
2	B	209	ARG
2	B	230	VAL
3	C	61	ALA
3	C	74	GLY
3	C	167	TRP
3	C	168	ALA
4	D	4	TYR
4	D	29	PRO
4	D	31	CYS
8	H	105	ARG
9	I	41	VAL
10	J	90	LEU
11	K	50	TYR
11	K	128	ALA
12	L	29	GLY
12	L	115	LYS
13	M	36	LYS
13	M	85	GLY
13	M	106	ASN
13	M	120	LYS
13	M	124	PRO
14	N	8	GLU
14	N	23	ARG
17	Q	99	SER
18	R	25	THR
19	S	6	LYS
2	B	78	GLN
2	B	87	ARG
3	C	4	LYS

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Mol	Chain	Res	Type
3	C	66	VAL
3	C	82	GLU
3	C	108	ASN
3	C	130	VAL
3	C	154	SER
6	F	70	ASP
7	G	4	ARG
7	G	9	VAL
7	G	90	GLU
8	H	91	ARG
9	I	119	ALA
9	I	127	LYS
10	J	40	LEU
10	J	73	ASP
11	K	25	TYR
13	M	23	TYR
14	N	29	ARG
14	N	32	SER
15	O	88	ARG
17	Q	68	ARG
18	R	42	ARG
18	R	45	SER
19	S	43	GLU
19	S	44	MET
20	T	54	LYS
20	T	73	HIS
20	T	94	ALA
2	B	64	ARG
2	B	95	GLN
3	C	188	LEU
4	D	53	ASP
4	D	88	VAL
6	F	62	TRP
6	F	99	ALA
10	J	60	ARG
10	J	72	VAL
12	L	41	ARG
12	L	51	ALA
14	N	13	THR
14	N	31	ARG
16	P	52	ASP
19	S	8	GLY

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Mol	Chain	Res	Type
19	S	30	LEU
20	T	49	ALA
20	T	102	GLY
2	B	10	LEU
2	B	52	GLU
2	B	97	TRP
2	B	131	PRO
3	C	53	ALA
9	I	12	GLU
11	K	35	PRO
13	M	117	VAL
15	O	13	GLN
15	O	24	SER
18	R	28	GLU
19	S	69	HIS
20	T	9	ASN
21	V	15	ARG
2	B	45	GLN
2	B	121	LEU
6	F	37	VAL
9	I	24	GLY
15	O	75	PRO
16	P	10	GLY
2	B	130	ARG
7	G	80	VAL
20	T	96	GLY
8	H	83	ILE
2	B	202	PRO
3	C	84	ILE
9	I	21	PRO
17	Q	33	GLY
2	B	232	PRO
9	I	44	VAL
12	L	121	GLY
16	P	19	ILE
17	Q	64	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	202/220 (92%)	183 (91%)	19 (9%)	8	29
3	C	160/188 (85%)	139 (87%)	21 (13%)	4	17
4	D	180/181 (99%)	165 (92%)	15 (8%)	10	34
5	E	115/123 (94%)	103 (90%)	12 (10%)	7	25
6	F	90/90 (100%)	86 (96%)	4 (4%)	25	54
7	G	126/127 (99%)	113 (90%)	13 (10%)	7	26
8	H	119/119 (100%)	106 (89%)	13 (11%)	6	23
9	I	98/99 (99%)	89 (91%)	9 (9%)	8	30
10	J	87/92 (95%)	80 (92%)	7 (8%)	11	35
11	K	90/99 (91%)	84 (93%)	6 (7%)	15	41
12	L	104/109 (95%)	91 (88%)	13 (12%)	4	18
13	M	100/101 (99%)	94 (94%)	6 (6%)	17	45
14	N	49/50 (98%)	44 (90%)	5 (10%)	7	26
15	O	79/80 (99%)	74 (94%)	5 (6%)	16	43
16	P	72/74 (97%)	64 (89%)	8 (11%)	6	22
17	Q	96/97 (99%)	90 (94%)	6 (6%)	16	43
18	R	64/77 (83%)	56 (88%)	8 (12%)	4	18
19	S	71/80 (89%)	65 (92%)	6 (8%)	10	33
20	T	76/82 (93%)	65 (86%)	11 (14%)	3	13
21	V	19/22 (86%)	18 (95%)	1 (5%)	20	49
All	All	1997/2110 (95%)	1809 (91%)	188 (9%)	8	29

All (188) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	8	LYS
2	B	9	GLU
2	B	15	VAL
2	B	16	HIS
2	B	37	ASN
2	B	40	HIS
2	B	67	THR
2	B	96	ARG

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Mol	Chain	Res	Type
2	B	102	LEU
2	B	139	LYS
2	B	144	ARG
2	B	154	LEU
2	B	170	GLU
2	B	172	ILE
2	B	178	ARG
2	B	187	LEU
2	B	200	ILE
2	B	232	PRO
2	B	236	TYR
3	C	3	ASN
3	C	5	ILE
3	C	6	HIS
3	C	16	ARG
3	C	21	ARG
3	C	33	LEU
3	C	36	ASP
3	C	37	GLN
3	C	39	ILE
3	C	42	LEU
3	C	56	ASP
3	C	83	ARG
3	C	89	GLU
3	C	91	LEU
3	C	104	GLN
3	C	139	GLN
3	C	167	TRP
3	C	188	LEU
3	C	192	THR
3	C	196	LEU
3	C	204	LEU
4	D	3	ARG
4	D	9	CYS
4	D	21	LEU
4	D	33	MET
4	D	35	ARG
4	D	47	ARG
4	D	53	ASP
4	D	58	LEU
4	D	65	ARG
4	D	66	ARG

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Mol	Chain	Res	Type
4	D	76	ARG
4	D	96	LEU
4	D	122	ARG
4	D	127	THR
4	D	134	ASP
5	E	12	LEU
5	E	15	ARG
5	E	16	THR
5	E	24	ARG
5	E	38	GLN
5	E	41	VAL
5	E	53	LEU
5	E	79	GLU
5	E	82	VAL
5	E	89	ILE
5	E	126	ARG
5	E	137	GLU
6	F	10	LEU
6	F	47	ARG
6	F	54	LYS
6	F	98	LEU
7	G	4	ARG
7	G	11	GLN
7	G	12	LEU
7	G	16	LEU
7	G	22	LEU
7	G	38	LEU
7	G	45	ASP
7	G	76	ARG
7	G	96	GLN
7	G	113	GLU
7	G	124	LEU
7	G	140	ASP
7	G	144	MET
8	H	22	GLU
8	H	26	VAL
8	H	39	LEU
8	H	63	LEU
8	H	68	ARG
8	H	69	ARG
8	H	84	ARG
8	H	85	ARG

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Mol	Chain	Res	Type
8	H	88	LYS
8	H	91	ARG
8	H	102	ARG
8	H	127	LEU
8	H	133	LEU
9	I	14	VAL
9	I	20	ARG
9	I	35	GLU
9	I	47	LEU
9	I	56	LEU
9	I	64	THR
9	I	75	ASP
9	I	118	LYS
9	I	121	ARG
10	J	3	LYS
10	J	4	ILE
10	J	28	ARG
10	J	46	ARG
10	J	65	LEU
10	J	71	LEU
10	J	98	ILE
11	K	29	ILE
11	K	35	PRO
11	K	48	ILE
11	K	73	MET
11	K	81	ASP
11	K	92	GLU
12	L	12	ARG
12	L	19	ARG
12	L	41	ARG
12	L	46	LYS
12	L	47	LYS
12	L	65	GLU
12	L	79	GLU
12	L	85	ILE
12	L	89	ARG
12	L	91	LYS
12	L	99	HIS
12	L	113	ARG
12	L	126	LYS
13	M	9	ILE
13	M	45	VAL

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Mol	Chain	Res	Type
13	M	70	LEU
13	M	77	ASN
13	M	105	THR
13	M	121	LYS
14	N	8	GLU
14	N	16	PHE
14	N	22	THR
14	N	33	VAL
14	N	44	LEU
15	O	6	GLU
15	O	24	SER
15	O	31	LEU
15	O	40	SER
15	O	81	LEU
16	P	1	MET
16	P	2	VAL
16	P	8	ARG
16	P	28	ARG
16	P	42	ARG
16	P	45	THR
16	P	76	GLN
16	P	80	PHE
17	Q	3	LYS
17	Q	38	ARG
17	Q	60	ILE
17	Q	65	ILE
17	Q	74	LEU
17	Q	92	ARG
18	R	26	LEU
18	R	28	GLU
18	R	39	VAL
18	R	46	GLU
18	R	53	ARG
18	R	54	ARG
18	R	69	THR
18	R	87	ARG
19	S	7	LYS
19	S	13	ASP
19	S	22	LEU
19	S	42	PRO
19	S	53	ASN
19	S	78	ARG

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Mol	Chain	Res	Type
20	T	8	ARG
20	T	10	LEU
20	T	39	LYS
20	T	42	GLN
20	T	56	MET
20	T	57	ARG
20	T	68	LYS
20	T	73	HIS
20	T	75	ASN
20	T	83	ARG
20	T	84	LEU
21	V	3	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	37	ASN
2	B	146	GLN
2	B	204	ASN
2	B	240	GLN
3	C	28	GLN
3	C	31	HIS
3	C	108	ASN
3	C	110	ASN
3	C	118	GLN
3	C	123	GLN
3	C	139	GLN
3	C	176	HIS
4	D	42	GLN
4	D	45	GLN
4	D	62	GLN
4	D	123	HIS
4	D	161	ASN
4	D	199	ASN
5	E	20	GLN
5	E	65	ASN
5	E	73	ASN
6	F	11	ASN
6	F	27	GLN
6	F	57	GLN
6	F	64	GLN
6	F	73	ASN

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Mol	Chain	Res	Type
6	F	100	ASN
7	G	11	GLN
7	G	13	GLN
7	G	28	ASN
7	G	56	GLN
7	G	148	ASN
9	I	23	ASN
9	I	29	ASN
9	I	38	GLN
9	I	73	GLN
9	I	124	GLN
10	J	13	HIS
10	J	62	HIS
10	J	69	ASN
10	J	78	ASN
10	J	84	GLN
11	K	62	GLN
11	K	99	GLN
11	K	117	ASN
12	L	75	HIS
13	M	12	ASN
13	M	40	ASN
13	M	62	ASN
13	M	101	GLN
14	N	52	GLN
15	O	13	GLN
15	O	37	ASN
16	P	14	ASN
16	P	76	GLN
17	Q	16	GLN
19	S	14	HIS
19	S	53	ASN
20	T	9	ASN
20	T	73	HIS
20	T	90	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1513/1513 (100%)	347 (22%)	188 (12%)
22	W	2/3 (66%)	0	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
23	X	10/11 (90%)	6 (60%)	2 (20%)
All	All	1525/1527 (99%)	353 (23%)	190 (12%)

All (353) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	G
1	A	8	A
1	A	9	G
1	A	13	U
1	A	14	U
1	A	26	A
1	A	31	G
1	A	32	A
1	A	39	G
1	A	47	C
1	A	48	C
1	A	49	U
1	A	50	A
1	A	51	A
1	A	52	G
1	A	61	G
1	A	65	U
1	A	66	G
1	A	80	U
1	A	94	A
1	A	101	G
1	A	102	A
1	A	103	C
1	A	109	A
1	A	113	A
1	A	114	C
1	A	115	G
1	A	123	G
1	A	124	A
1	A	125	C
1	A	157	C
1	A	167	U
1	A	168	C
1	A	176	U
1	A	177	G
1	A	189	U

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Mol	Chain	Res	Type
1	A	190	G
1	A	191	G
1	A	203	A
1	A	204	G
1	A	208	U
1	A	209	U
1	A	210	U
1	A	239	U
1	A	240	C
1	A	242	G
1	A	246	G
1	A	247	U
1	A	248	U
1	A	261	G
1	A	262	C
1	A	270	G
1	A	274	A
1	A	275	C
1	A	276	G
1	A	277	A
1	A	284	G
1	A	292	G
1	A	293	A
1	A	301	G
1	A	311	G
1	A	316	A
1	A	323	C
1	A	324	A
1	A	325	C
1	A	327	G
1	A	339	A
1	A	340	C
1	A	341	G
1	A	342	G
1	A	347	C
1	A	348	A
1	A	349	G
1	A	362	U
1	A	363	U
1	A	368	A
1	A	384	A
1	A	392	A

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Mol	Chain	Res	Type
1	A	393	C
1	A	405	G
1	A	406	A
1	A	407	A
1	A	408	G
1	A	417	C
1	A	418	G
1	A	419	G
1	A	423	G
1	A	424	U
1	A	425	A
1	A	434	A
1	A	446	A
1	A	447	A
1	A	454	A
1	A	455	C
1	A	456	G
1	A	465	G
1	A	466	A
1	A	468	G
1	A	469	G
1	A	470	U
1	A	480	A
1	A	481	U
1	A	483	G
1	A	491	C
1	A	492	A
1	A	494	C
1	A	495	U
1	A	501	C
1	A	502	C
1	A	510	G
1	A	513	G
1	A	514	U
1	A	515	A
1	A	516	A
1	A	517	U
1	A	519	C
1	A	531	G
1	A	533	G
1	A	542	A
1	A	543	U

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Mol	Chain	Res	Type
1	A	544	U
1	A	545	C
1	A	546	A
1	A	549	G
1	A	550	G
1	A	555	A
1	A	556	A
1	A	558	G
1	A	559	G
1	A	560	G
1	A	571	G
1	A	578	G
1	A	579	C
1	A	602	U
1	A	624	U
1	A	625	A
1	A	636	A
1	A	637	G
1	A	648	A
1	A	670	A
1	A	671	G
1	A	684	C
1	A	685	A
1	A	686	G
1	A	687	A
1	A	701	G
1	A	704	G
1	A	705	A
1	A	706	U
1	A	707	G
1	A	714	G
1	A	716	A
1	A	717	G
1	A	732	C
1	A	736	A
1	A	737	C
1	A	738	G
1	A	760	A
1	A	764	A
1	A	770	A
1	A	775	A
1	A	776	U

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Mol	Chain	Res	Type
1	A	777	A
1	A	796	U
1	A	798	A
1	A	799	A
1	A	800	C
1	A	801	G
1	A	802	A
1	A	803	U
1	A	804	G
1	A	811	A
1	A	822	U
1	A	823	C
1	A	824	U
1	A	825	C
1	A	826	C
1	A	835	G
1	A	848	U
1	A	849	A
1	A	850	A
1	A	851	G
1	A	862	G
1	A	866	A
1	A	867	G
1	A	868	U
1	A	879	G
1	A	891	A
1	A	899	G
1	A	903	G
1	A	904	G
1	A	911	C
1	A	912	A
1	A	922	G
1	A	936	A
1	A	937	U
1	A	938	U
1	A	943	G
1	A	945	A
1	A	946	A
1	A	948	G
1	A	949	C
1	A	951	A
1	A	952	A

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Mol	Chain	Res	Type
1	A	953	G
1	A	954	A
1	A	955	A
1	A	959	U
1	A	960	A
1	A	961	C
1	A	969	U
1	A	970	G
1	A	971	A
1	A	981	G
1	A	982	A
1	A	983	A
1	A	984	C
1	A	986	C
1	A	987	G
1	A	988	G
1	A	1002	G
1	A	1003	U
1	A	1004	G
1	A	1007	C
1	A	1010	C
1	A	1025	C
1	A	1026	A
1	A	1028	A
1	A	1032	G
1	A	1036	C
1	A	1037	A
1	A	1047	U
1	A	1048	C
1	A	1049	A
1	A	1050	G
1	A	1067	U
1	A	1068	U
1	A	1076	G
1	A	1082	C
1	A	1083	A
1	A	1084	A
1	A	1099	G
1	A	1106	G
1	A	1107	U
1	A	1109	G
1	A	1111	C

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Mol	Chain	Res	Type
1	A	1112	A
1	A	1115	G
1	A	1117	U
1	A	1118	U
1	A	1119	C
1	A	1120	G
1	A	1121	G
1	A	1122	C
1	A	1128	A
1	A	1134	A
1	A	1139	A
1	A	1140	C
1	A	1141	U
1	A	1142	G
1	A	1164	A
1	A	1165	G
1	A	1172	A
1	A	1177	U
1	A	1178	G
1	A	1181	C
1	A	1182	A
1	A	1183	G
1	A	1184	C
1	A	1192	U
1	A	1193	U
1	A	1194	A
1	A	1195	C
1	A	1196	G
1	A	1206	A
1	A	1207	C
1	A	1208	A
1	A	1217	A
1	A	1219	A
1	A	1221	U
1	A	1222	G
1	A	1237	A
1	A	1238	U
1	A	1239	G
1	A	1241	C
1	A	1243	C
1	A	1260	A
1	A	1261	A

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Mol	Chain	Res	Type
1	A	1262	U
1	A	1263	C
1	A	1266	A
1	A	1267	A
1	A	1268	A
1	A	1279	C
1	A	1280	A
1	A	1281	G
1	A	1282	U
1	A	1283	U
1	A	1284	C
1	A	1287	A
1	A	1300	A
1	A	1301	C
1	A	1313	A
1	A	1317	C
1	A	1318	G
1	A	1327	A
1	A	1328	G
1	A	1329	U
1	A	1334	G
1	A	1344	C
1	A	1345	A
1	A	1346	U
1	A	1347	G
1	A	1361	G
1	A	1363	U
1	A	1376	A
1	A	1377	C
1	A	1379	C
1	A	1380	A
1	A	1382	C
1	A	1383	G
1	A	1424	G
1	A	1426	A
1	A	1427	G
1	A	1432	C
1	A	1433	G
1	A	1460	A
1	A	1461	C
1	A	1467	C
1	A	1469	A

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Mol	Chain	Res	Type
1	A	1474	G
1	A	1475	U
1	A	1476	A
1	A	1479	A
1	A	1480	A
1	A	1481	G
1	A	1482	G
1	A	1483	U
1	A	1484	A
1	A	1494	G
1	A	1496	A
1	A	1497	G
1	A	1506	G
1	A	1507	G
1	A	1510	C
1	A	1511	A
1	A	1516	C
23	X	32	C
23	X	34	70U
23	X	37	12A
23	X	38	A
23	X	39	PSU
23	X	40	C

All (190) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	5	U
1	A	7	G
1	A	8	A
1	A	13	U
1	A	30	U
1	A	31	G
1	A	47	C
1	A	48	C
1	A	49	U
1	A	50	A
1	A	51	A
1	A	60	A
1	A	64	G
1	A	65	U
1	A	102	A

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Mol	Chain	Res	Type
1	A	108	G
1	A	112	A
1	A	114	C
1	A	123	G
1	A	124	A
1	A	167	U
1	A	175	G
1	A	188	U
1	A	189	U
1	A	190	G
1	A	203	A
1	A	208	U
1	A	209	U
1	A	211	G
1	A	238	A
1	A	239	U
1	A	241	A
1	A	245	A
1	A	246	G
1	A	261	G
1	A	269	A
1	A	274	A
1	A	275	C
1	A	276	G
1	A	300	G
1	A	310	A
1	A	322	A
1	A	323	C
1	A	324	A
1	A	339	A
1	A	340	C
1	A	346	G
1	A	361	C
1	A	362	U
1	A	367	C
1	A	383	G
1	A	407	A
1	A	416	U
1	A	417	C
1	A	423	G
1	A	424	U
1	A	433	G

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Mol	Chain	Res	Type
1	A	445	A
1	A	446	A
1	A	454	A
1	A	455	C
1	A	465	G
1	A	468	G
1	A	469	G
1	A	479	A
1	A	480	A
1	A	482	A
1	A	491	C
1	A	494	C
1	A	500	G
1	A	501	C
1	A	513	G
1	A	516	A
1	A	518	A
1	A	530	A
1	A	542	A
1	A	544	U
1	A	545	C
1	A	549	G
1	A	558	G
1	A	559	G
1	A	570	G
1	A	578	G
1	A	624	U
1	A	635	U
1	A	636	A
1	A	670	A
1	A	684	C
1	A	685	A
1	A	686	G
1	A	700	C
1	A	704	G
1	A	705	A
1	A	716	A
1	A	731	C
1	A	735	G
1	A	736	A
1	A	775	A
1	A	776	U

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Mol	Chain	Res	Type
1	A	795	C
1	A	798	A
1	A	800	C
1	A	801	G
1	A	802	A
1	A	803	U
1	A	823	C
1	A	847	U
1	A	848	U
1	A	849	A
1	A	850	A
1	A	861	U
1	A	866	A
1	A	867	G
1	A	890	A
1	A	911	C
1	A	937	U
1	A	942	A
1	A	945	A
1	A	948	G
1	A	951	A
1	A	952	A
1	A	953	G
1	A	959	U
1	A	969	U
1	A	970	G
1	A	982	A
1	A	1031	U
1	A	1047	U
1	A	1049	A
1	A	1067	U
1	A	1083	A
1	A	1106	G
1	A	1111	C
1	A	1121	G
1	A	1127	C
1	A	1133	A
1	A	1139	A
1	A	1141	U
1	A	1163	G
1	A	1164	A
1	A	1171	G

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Mol	Chain	Res	Type
1	A	1177	U
1	A	1181	C
1	A	1182	A
1	A	1194	A
1	A	1195	C
1	A	1205	G
1	A	1206	A
1	A	1207	C
1	A	1220	A
1	A	1221	U
1	A	1238	U
1	A	1259	U
1	A	1261	A
1	A	1262	U
1	A	1266	A
1	A	1278	C
1	A	1279	C
1	A	1281	G
1	A	1282	U
1	A	1283	U
1	A	1286	G
1	A	1312	G
1	A	1316	C
1	A	1317	C
1	A	1326	U
1	A	1327	A
1	A	1328	G
1	A	1345	A
1	A	1346	U
1	A	1362	U
1	A	1376	A
1	A	1378	A
1	A	1379	C
1	A	1381	C
1	A	1382	C
1	A	1426	A
1	A	1431	A
1	A	1432	C
1	A	1475	U
1	A	1479	A
1	A	1480	A
1	A	1481	G

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Mol	Chain	Res	Type
1	A	1482	G
1	A	1483	U
1	A	1505	U
1	A	1506	G
1	A	1510	C
23	X	31	A
23	X	39	PSU

5.4 Non-standard residues in protein, DNA, RNA chains

3 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$
23	PSU	X	39	23	18,21,22	1.32	1 (5%)	21,30,33	2.27	3 (14%)
23	12A	X	37	23	33,36,37	1.03	3 (9%)	46,52,55	2.12	14 (30%)
23	70U	X	34	23,22	22,26,27	0.52	0	27,37,40	0.67	0

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
23	PSU	X	39	23	-	1/7/25/26	0/2/2/2
23	12A	X	37	23	-	0/25/43/44	0/3/3/3
23	70U	X	34	23,22	-	4/13/31/32	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	X	39	PSU	C6-C5	4.50	1.40	1.35
23	X	37	12A	CA-N	2.51	1.51	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	X	37	12A	C5-C4	2.36	1.43	1.39
23	X	37	12A	C5-N7	-2.06	1.35	1.39

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	X	39	PSU	C6-C5-C4	-7.28	113.26	118.17
23	X	37	12A	C5-C4-N3	-6.65	120.18	127.18
23	X	39	PSU	C3'-C2'-C1'	5.14	107.75	101.69
23	X	37	12A	N3-C4-N9	4.79	133.07	126.99
23	X	37	12A	CA-N-CC	4.78	129.95	121.99
23	X	37	12A	N6-CC-N	3.80	119.00	113.77
23	X	37	12A	C5-N7-C8	3.58	109.08	103.45
23	X	37	12A	C2-N3-C4	3.28	120.89	112.29
23	X	37	12A	C4-C5-N7	-3.22	106.90	110.58
23	X	37	12A	C6-C5-N7	3.15	135.87	132.43
23	X	37	12A	N3-C2-N1	-2.94	121.64	127.00
23	X	37	12A	C2-N1-C6	2.65	122.57	117.54
23	X	37	12A	OO-CC-N6	-2.55	119.10	123.64
23	X	39	PSU	C4-N3-C2	-2.34	123.14	126.37
23	X	37	12A	N9-C8-N7	-2.23	110.78	113.94
23	X	37	12A	O4'-C1'-N9	2.16	112.24	108.09
23	X	37	12A	OXT-C-CA	2.11	121.45	114.15

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	X	34	70U	C4-C5-C5M-C8
23	X	34	70U	C6-C5-C5M-C8
23	X	34	70U	O4'-C4'-C5'-O5'
23	X	39	PSU	C3'-C4'-C5'-O5'
23	X	34	70U	C3'-C4'-C5'-O5'

There are no ring outliers.

3 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	X	39	PSU	10	0
23	X	37	12A	11	0
23	X	34	70U	5	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 188 ligands modelled in this entry, 187 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	1783	-	44,45,45	0.66	0	63,67,67	1.33	7 (11%)

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	1783	-	-	7/18/94/94	0/4/4/4

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	1783	PAR	C14-O33-C33	-4.38	107.60	117.98
25	A	1783	PAR	O54-C54-C64	4.25	114.23	106.07
25	A	1783	PAR	C11-O11-C42	-3.28	110.21	117.98
25	A	1783	PAR	C13-O52-C52	-2.91	111.08	117.98
25	A	1783	PAR	C11-O51-C51	-2.34	109.14	113.72
25	A	1783	PAR	C64-C54-C44	-2.34	107.33	112.80
25	A	1783	PAR	C23-C33-C43	-2.31	99.20	103.24

There are no chirality outliers.

All (7) torsion outliers are listed below:

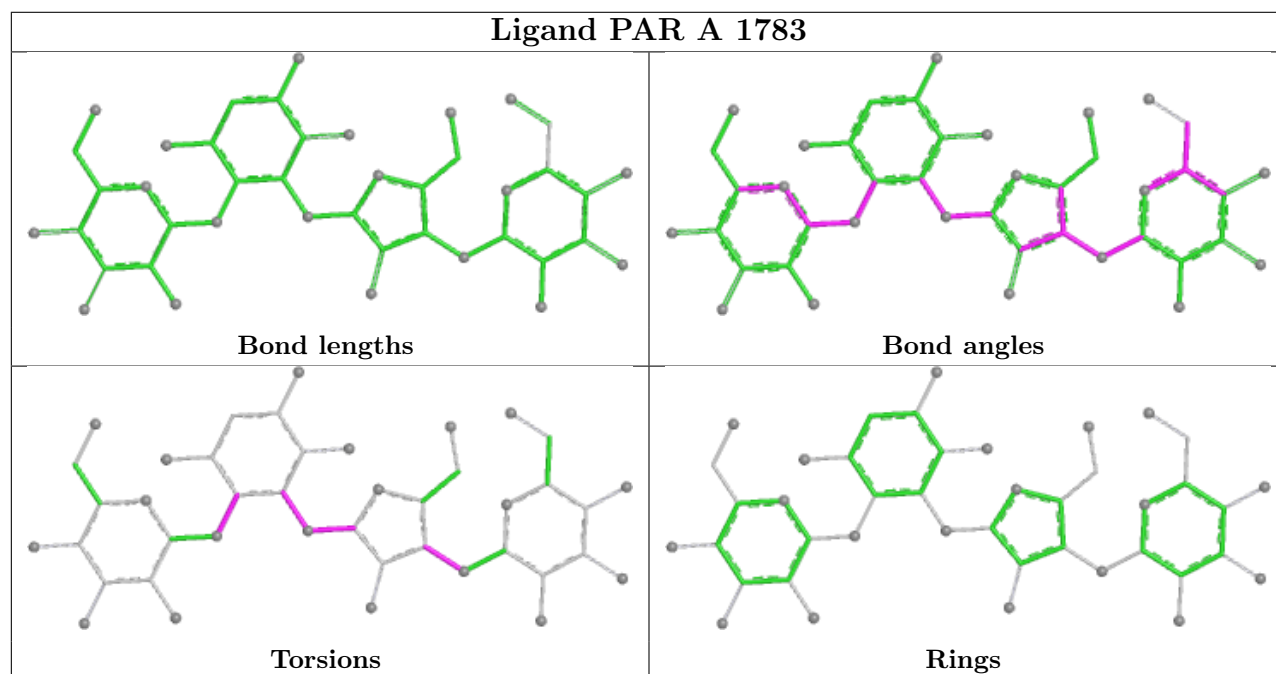
Mol	Chain	Res	Type	Atoms
25	A	1783	PAR	C52-C42-O11-C11
25	A	1783	PAR	C42-C52-O52-C13
25	A	1783	PAR	C23-C13-O52-C52
25	A	1783	PAR	C62-C52-O52-C13
25	A	1783	PAR	O43-C13-O52-C52
25	A	1783	PAR	C43-C33-O33-C14
25	A	1783	PAR	C23-C33-O33-C14

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	A	1783	PAR	5	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	1512/1513 (99%)	0.56	159 (10%) 11 6	29, 58, 125, 178	0
2	B	234/256 (91%)	1.41	54 (23%) 2 1	50, 92, 137, 145	0
3	C	206/239 (86%)	1.12	32 (15%) 5 2	57, 83, 119, 125	0
4	D	208/209 (99%)	0.76	29 (13%) 6 3	45, 66, 101, 106	0
5	E	150/162 (92%)	0.16	4 (2%) 56 35	33, 51, 67, 82	0
6	F	101/101 (100%)	0.78	8 (7%) 18 10	64, 85, 102, 106	0
7	G	155/156 (99%)	0.74	13 (8%) 17 9	51, 75, 110, 123	0
8	H	138/138 (100%)	-0.04	1 (0%) 84 68	30, 47, 61, 70	0
9	I	127/128 (99%)	1.17	21 (16%) 4 2	44, 85, 102, 108	0
10	J	98/105 (93%)	2.15	49 (50%) 0 0	57, 116, 139, 143	0
11	K	119/129 (92%)	0.48	7 (5%) 28 15	42, 58, 84, 97	0
12	L	124/132 (93%)	0.57	11 (8%) 15 8	19, 57, 70, 96	0
13	M	125/126 (99%)	1.04	21 (16%) 4 2	59, 71, 129, 157	0
14	N	60/61 (98%)	1.39	13 (21%) 2 1	58, 74, 109, 114	0
15	O	88/89 (98%)	0.27	3 (3%) 48 28	39, 61, 87, 104	0
16	P	83/88 (94%)	-0.08	0 100 100	38, 47, 59, 83	0
17	Q	104/105 (99%)	0.41	11 (10%) 11 6	33, 50, 108, 131	0
18	R	73/88 (82%)	0.71	7 (9%) 13 7	49, 70, 111, 129	0
19	S	80/93 (86%)	1.43	18 (22%) 2 1	80, 93, 112, 115	0
20	T	99/106 (93%)	0.52	5 (5%) 33 18	40, 55, 80, 86	0
21	V	24/27 (88%)	1.16	4 (16%) 4 2	49, 63, 79, 89	0
22	W	3/3 (100%)	0.44	0 100 100	57, 57, 62, 63	0
23	X	8/11 (72%)	1.94	4 (50%) 0 0	67, 101, 127, 137	0
All	All	3919/4065 (96%)	0.71	474 (12%) 8 5	19, 64, 121, 178	0

All (474) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	M	124	PRO	8.3
13	M	119	GLY	7.7
7	G	156	TRP	7.4
13	M	125	ARG	6.8
20	T	103	GLY	6.8
13	M	121	LYS	6.6
17	Q	96	GLN	6.6
4	D	21	LEU	6.2
1	A	1003	U	6.2
1	A	513	G	6.1
13	M	120	LYS	6.1
10	J	74	ILE	5.8
14	N	2	ALA	5.7
19	S	3	ARG	5.7
13	M	123	ALA	5.5
1	A	1109	G	5.5
19	S	37	ARG	5.4
1	A	1517	U	5.4
1	A	1107	U	5.3
2	B	39	ILE	5.3
10	J	23	ILE	5.3
9	I	128	ARG	5.2
2	B	16	HIS	5.2
1	A	1112	A	5.2
1	A	1108	U	5.2
1	A	1518	U	5.1
13	M	122	LYS	5.1
14	N	13	THR	5.1
17	Q	103	GLY	5.0
11	K	128	ALA	5.0
3	C	26	LYS	5.0
10	J	75	ILE	4.9
2	B	17	PHE	4.9
1	A	1018	G	4.9
1	A	1111	C	4.7
2	B	38	GLY	4.7
1	A	983	A	4.7
2	B	13	ALA	4.6
1	A	1110	C	4.6
1	A	1510	C	4.6
19	S	2	PRO	4.6
12	L	47	LYS	4.5

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Mol	Chain	Res	Type	RSRZ
23	X	40	C	4.5
1	A	1005	C	4.5
19	S	4	SER	4.4
13	M	126	LYS	4.4
1	A	1122	C	4.4
1	A	408	G	4.4
2	B	133	LYS	4.4
4	D	75	PHE	4.4
9	I	70	LYS	4.4
4	D	26	CYS	4.4
2	B	234	PRO	4.4
4	D	2	GLY	4.3
1	A	1027	C	4.3
1	A	1516	C	4.3
2	B	229	VAL	4.3
1	A	1116	G	4.3
20	T	68	LYS	4.3
21	V	25	LYS	4.3
7	G	5	ARG	4.3
2	B	136	VAL	4.3
1	A	1519	U	4.2
2	B	76	GLN	4.2
10	J	57	LYS	4.2
6	F	36	ARG	4.2
1	A	1128	A	4.2
10	J	72	VAL	4.2
2	B	19	HIS	4.2
9	I	92	TYR	4.1
1	A	1127	C	4.1
2	B	35	GLU	4.1
1	A	1113	G	4.1
18	R	16	PRO	4.1
3	C	54	ARG	4.1
2	B	29	ALA	4.1
1	A	969	U	4.0
1	A	981	G	4.0
2	B	10	LEU	4.0
1	A	1036	C	4.0
2	B	77	ALA	3.9
2	B	123	ALA	3.9
2	B	230	VAL	3.8
4	D	8	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
10	J	5	ARG	3.8
1	A	1114	C	3.8
19	S	33	THR	3.8
11	K	129	SER	3.8
10	J	7	LYS	3.8
2	B	239	VAL	3.8
1	A	1455	C	3.7
1	A	1004	G	3.7
4	D	31	CYS	3.7
2	B	7	VAL	3.7
17	Q	99	SER	3.7
1	A	1020	C	3.7
1	A	1121	G	3.7
23	X	30	G	3.7
2	B	34	ALA	3.7
20	T	74	LYS	3.7
1	A	1239	G	3.6
4	D	9	CYS	3.6
3	C	100	ALA	3.6
1	A	1228	U	3.6
17	Q	101	ARG	3.6
7	G	85	TYR	3.6
2	B	44	LEU	3.6
3	C	58	GLU	3.6
9	I	19	LEU	3.6
1	A	1142	G	3.5
10	J	100	THR	3.5
11	K	36	ASP	3.5
21	V	6	ARG	3.5
1	A	984	C	3.5
1	A	1010	C	3.5
1	A	1082	C	3.5
1	A	1123	C	3.5
1	A	1115	G	3.5
17	Q	105	ALA	3.5
3	C	28	GLN	3.5
1	A	1002	G	3.5
7	G	80	VAL	3.4
10	J	24	VAL	3.4
4	D	74	GLN	3.4
10	J	73	ASP	3.4
1	A	970	G	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	1035	G	3.4
1	A	1259	U	3.4
2	B	21	ARG	3.4
1	A	998	U	3.4
13	M	118	ALA	3.4
12	L	26	ALA	3.4
10	J	6	ILE	3.4
3	C	2	GLY	3.3
10	J	98	ILE	3.3
2	B	240	GLN	3.3
1	A	1258	C	3.3
1	A	968	U	3.3
10	J	30	SER	3.3
4	D	49	ARG	3.3
18	R	46	GLU	3.3
3	C	155	GLY	3.3
2	B	125	PRO	3.2
6	F	98	LEU	3.2
3	C	110	ASN	3.2
2	B	81	VAL	3.2
10	J	85	LEU	3.2
1	A	515	A	3.2
2	B	223	ILE	3.2
2	B	131	PRO	3.2
2	B	183	PRO	3.2
7	G	77	SER	3.2
21	V	10	ARG	3.2
7	G	83	ALA	3.2
1	A	1117	U	3.1
1	A	1106	G	3.1
10	J	35	SER	3.1
10	J	17	ASP	3.1
11	K	51	LYS	3.1
3	C	76	VAL	3.1
3	C	21	ARG	3.1
12	L	19	ARG	3.1
1	A	516	A	3.1
1	A	1199	C	3.1
17	Q	17	LYS	3.1
1	A	1124	G	3.1
9	I	61	ALA	3.1
17	Q	102	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
3	C	207	VAL	3.1
1	A	1129	C	3.0
1	A	1302	C	3.0
1	A	1099	G	3.0
3	C	30	ARG	3.0
1	A	517	U	3.0
4	D	29	PRO	3.0
10	J	4	ILE	3.0
10	J	90	LEU	3.0
1	A	1508	A	3.0
1	A	1241	C	3.0
4	D	27	TYR	3.0
10	J	27	ALA	3.0
18	R	20	ALA	3.0
2	B	18	GLY	3.0
4	D	23	GLY	3.0
1	A	1021	C	3.0
13	M	7	VAL	3.0
1	A	1163	G	2.9
1	A	1205	G	2.9
3	C	94	LEU	2.9
19	S	77	THR	2.9
7	G	151	TYR	2.9
14	N	60	SER	2.9
10	J	11	PHE	2.9
1	A	407	A	2.9
1	A	1237	A	2.9
12	L	17	LYS	2.9
2	B	144	ARG	2.9
9	I	17	VAL	2.9
1	A	433	G	2.9
9	I	127	LYS	2.9
5	E	20	GLN	2.8
11	K	78	GLN	2.8
3	C	151	VAL	2.8
10	J	34	VAL	2.8
2	B	40	HIS	2.8
1	A	154	A	2.8
1	A	1426	A	2.8
1	A	1459	G	2.8
10	J	37	PRO	2.8
10	J	91	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
10	J	88	LEU	2.8
2	B	134	GLU	2.8
1	A	1229	A	2.8
2	B	206	ASP	2.8
1	A	825	C	2.8
1	A	987	G	2.8
9	I	114	TYR	2.8
10	J	41	PRO	2.8
10	J	96	ILE	2.8
4	D	6	GLY	2.8
1	A	1509	U	2.8
19	S	14	HIS	2.8
1	A	1025	C	2.8
1	A	1240	C	2.8
17	Q	104	LYS	2.8
2	B	15	VAL	2.8
3	C	77	ILE	2.8
1	A	208	U	2.7
1	A	1118	U	2.7
2	B	20	GLU	2.7
9	I	126	SER	2.7
10	J	8	LEU	2.7
1	A	47	C	2.7
1	A	1303	C	2.7
19	S	53	ASN	2.7
19	S	5	LEU	2.7
1	A	1076	G	2.7
1	A	1460	A	2.7
19	S	13	ASP	2.7
1	A	997	C	2.7
5	E	114	GLY	2.7
1	A	991	G	2.7
1	A	1120	G	2.7
10	J	59	SER	2.7
19	S	7	LYS	2.6
4	D	28	SER	2.6
10	J	44	VAL	2.6
14	N	18	VAL	2.6
20	T	100	ILE	2.6
10	J	36	GLY	2.6
14	N	30	ALA	2.6
1	A	976	C	2.6

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Mol	Chain	Res	Type	RSRZ
9	I	11	LYS	2.6
21	V	24	ARG	2.6
10	J	93	GLY	2.6
1	A	1403	G	2.6
3	C	70	VAL	2.6
3	C	73	PRO	2.6
10	J	33	GLN	2.6
6	F	14	LEU	2.6
9	I	12	GLU	2.6
1	A	1022	U	2.6
1	A	1141	U	2.6
2	B	36	ARG	2.6
1	A	980	G	2.6
1	A	995	G	2.6
4	D	4	TYR	2.6
13	M	10	PRO	2.6
3	C	96	GLY	2.6
1	A	1230	C	2.6
2	B	139	LYS	2.6
2	B	226	ARG	2.6
7	G	155	ARG	2.6
5	E	5	ASP	2.5
10	J	22	LYS	2.5
1	A	1023	A	2.5
2	B	42	ILE	2.5
14	N	22	THR	2.5
1	A	1019	C	2.5
10	J	77	PRO	2.5
9	I	94	ALA	2.5
13	M	35	GLU	2.5
9	I	63	ILE	2.5
9	I	115	GLY	2.5
2	B	235	SER	2.5
6	F	101	ALA	2.5
6	F	66	GLU	2.5
2	B	236	TYR	2.5
19	S	81	ARG	2.5
1	A	1280	A	2.5
1	A	988	G	2.5
12	L	51	ALA	2.5
10	J	38	ILE	2.5
1	A	1008	C	2.5

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Mol	Chain	Res	Type	RSRZ
7	G	6	ARG	2.5
2	B	26	PRO	2.5
10	J	20	ALA	2.4
2	B	52	GLU	2.4
10	J	3	LYS	2.4
3	C	167	TRP	2.4
1	A	1165	G	2.4
1	A	1198	C	2.4
8	H	2	LEU	2.4
3	C	84	ILE	2.4
14	N	9	LYS	2.4
14	N	57	ARG	2.4
19	S	36	ARG	2.4
7	G	16	LEU	2.4
5	E	86	ALA	2.4
10	J	18	ALA	2.4
1	A	1011	G	2.4
1	A	1125	G	2.4
1	A	1126	G	2.4
1	A	1247	G	2.4
1	A	1262	U	2.4
14	N	7	ILE	2.4
13	M	94	ARG	2.4
14	N	4	LYS	2.4
19	S	6	LYS	2.4
15	O	76	GLU	2.4
18	R	72	ARG	2.4
2	B	232	PRO	2.4
13	M	106	ASN	2.4
15	O	2	PRO	2.4
3	C	80	GLY	2.4
1	A	245	A	2.4
1	A	982	A	2.4
1	A	1017	A	2.4
1	A	514	U	2.4
4	D	72	GLU	2.4
1	A	405	G	2.4
1	A	1016	G	2.4
1	A	1236	G	2.4
10	J	53	PRO	2.4
10	J	67	THR	2.4
12	L	25	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
6	F	13	ASN	2.4
3	C	88	ARG	2.4
2	B	122	PHE	2.4
7	G	59	LEU	2.4
23	X	31	A	2.4
1	A	1402	C	2.3
1	A	1461	C	2.3
10	J	15	THR	2.3
10	J	92	THR	2.3
4	D	77	ASN	2.3
1	A	1255	G	2.3
4	D	201	GLN	2.3
7	G	79	ARG	2.3
10	J	82	ILE	2.3
14	N	5	ALA	2.3
17	Q	46	ASP	2.3
13	M	8	GLU	2.3
18	R	83	GLU	2.3
1	A	1162	G	2.3
13	M	117	VAL	2.3
9	I	119	ALA	2.3
1	A	1028	A	2.3
1	A	1267	A	2.3
1	A	1299	A	2.3
1	A	1193	U	2.3
1	A	1079	C	2.3
10	J	45	ARG	2.3
9	I	71	SER	2.3
1	A	614	G	2.3
13	M	50	GLU	2.3
1	A	1458	U	2.3
2	B	227	GLY	2.3
3	C	51	GLY	2.3
9	I	68	GLY	2.3
1	A	487	C	2.3
1	A	985	C	2.3
19	S	32	LYS	2.3
10	J	89	ASP	2.3
2	B	89	GLY	2.2
1	A	1177	U	2.2
2	B	11	LEU	2.2
1	A	1140	C	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	1195	C	2.2
11	K	54	ARG	2.2
17	Q	98	LEU	2.2
10	J	66	ARG	2.2
1	A	344	A	2.2
1	A	1261	A	2.2
4	D	42	GLN	2.2
4	D	24	GLU	2.2
3	C	42	LEU	2.2
6	F	58	GLY	2.2
19	S	8	GLY	2.2
4	D	35	ARG	2.2
13	M	11	ARG	2.2
2	B	140	HIS	2.2
10	J	19	SER	2.2
1	A	1238	U	2.2
1	A	343	G	2.2
1	A	978	A	2.2
4	D	11	LEU	2.2
12	L	48	PRO	2.2
2	B	22	LYS	2.2
1	A	455	C	2.2
1	A	986	C	2.2
1	A	1207	C	2.2
3	C	55	VAL	2.2
7	G	61	VAL	2.2
4	D	5	ILE	2.2
4	D	19	LEU	2.2
2	B	37	ASN	2.2
20	T	87	LYS	2.2
1	A	954	A	2.2
1	A	972	C	2.1
1	A	1007	C	2.1
1	A	1080	C	2.1
19	S	64	GLU	2.1
9	I	67	GLY	2.1
12	L	31	PRO	2.1
1	A	1185	A	2.1
3	C	43	LEU	2.1
1	A	1001	G	2.1
1	A	1015	G	2.1
3	C	83	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	497	C	2.1
9	I	29	ASN	2.1
3	C	69	HIS	2.1
4	D	43	HIS	2.1
1	A	432	U	2.1
3	C	67	THR	2.1
13	M	13	LYS	2.1
1	A	973	A	2.1
2	B	65	GLY	2.1
3	C	81	GLY	2.1
15	O	89	GLY	2.1
3	C	108	ASN	2.1
10	J	69	ASN	2.1
1	A	391	G	2.1
1	A	1009	G	2.1
1	A	1197	G	2.1
1	A	1203	G	2.1
1	A	1263	C	2.1
14	N	3	ARG	2.1
1	A	79	U	2.1
1	A	1067	U	2.1
2	B	132	LYS	2.1
13	M	9	ILE	2.1
11	K	111	ASP	2.1
9	I	7	THR	2.1
13	M	21	TYR	2.1
1	A	1098	C	2.1
1	A	1401	G	2.1
1	A	1425	G	2.1
4	D	32	ALA	2.1
17	Q	100	LYS	2.0
4	D	137	SER	2.0
3	C	178	LEU	2.0
2	B	48	MET	2.0
1	A	1231	A	2.0
12	L	32	PHE	2.0
1	A	730	C	2.0
1	A	1101	C	2.0
1	A	1348	C	2.0
12	L	20	LYS	2.0
6	F	46	ARG	2.0
1	A	5	U	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	706	U	2.0
23	X	33	U	2.0
19	S	39	THR	2.0
9	I	37	PHE	2.0
4	D	30	LYS	2.0
12	L	91	LYS	2.0
14	N	17	LYS	2.0
18	R	19	LYS	2.0
1	A	1479	A	2.0
4	D	73	ARG	2.0
10	J	94	VAL	2.0
18	R	54	ARG	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
23	PSU	X	39	20/21	0.82	0.15	86,86,88,88	0
23	70U	X	34	25/26	0.85	0.18	68,81,93,97	0
23	12A	X	37	34/35	0.86	0.13	71,71,71,71	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	A	1635	1/1	-0.07	0.56	14,14,14,14	1
24	MG	A	1706	1/1	0.01	0.87	2,2,2,2	1
24	MG	A	1722	1/1	0.09	1.74	24,24,24,24	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	MG	A	1754	1/1	0.13	1.63	1,1,1,1	1
24	MG	A	1625	1/1	0.17	0.69	1,1,1,1	1
24	MG	A	1694	1/1	0.21	0.56	26,26,26,26	1
24	MG	A	1644	1/1	0.27	0.53	23,23,23,23	1
24	MG	A	1743	1/1	0.28	2.35	1,1,1,1	1
24	MG	A	1693	1/1	0.28	1.14	34,34,34,34	1
24	MG	A	1756	1/1	0.29	1.55	30,30,30,30	1
24	MG	A	1718	1/1	0.31	0.72	1,1,1,1	1
24	MG	A	1766	1/1	0.41	0.91	1,1,1,1	1
24	MG	A	1774	1/1	0.44	2.81	35,35,35,35	1
24	MG	S	101	1/1	0.45	0.45	67,67,67,67	1
24	MG	A	1739	1/1	0.46	0.79	14,14,14,14	1
24	MG	A	1602	1/1	0.52	0.28	118,118,118,118	0
24	MG	A	1617	1/1	0.53	1.24	56,56,56,56	1
24	MG	A	1737	1/1	0.59	0.28	22,22,22,22	1
24	MG	A	1729	1/1	0.59	0.65	1,1,1,1	1
24	MG	A	1701	1/1	0.60	1.18	76,76,76,76	1
24	MG	A	1698	1/1	0.61	0.39	1,1,1,1	1
24	MG	A	1695	1/1	0.61	0.52	2,2,2,2	1
24	MG	A	1724	1/1	0.65	0.38	15,15,15,15	1
24	MG	A	1652	1/1	0.65	0.95	49,49,49,49	1
24	MG	A	1703	1/1	0.66	1.40	1,1,1,1	1
24	MG	A	1699	1/1	0.66	1.67	30,30,30,30	1
24	MG	A	1700	1/1	0.67	1.63	44,44,44,44	1
24	MG	A	1614	1/1	0.68	0.43	55,55,55,55	1
24	MG	A	1713	1/1	0.68	0.70	42,42,42,42	1
24	MG	A	1628	1/1	0.69	0.31	37,37,37,37	1
24	MG	A	1604	1/1	0.70	0.79	122,122,122,122	0
24	MG	A	1678	1/1	0.70	0.73	6,6,6,6	1
24	MG	A	1621	1/1	0.71	0.56	1,1,1,1	1
24	MG	A	1707	1/1	0.73	1.49	47,47,47,47	1
24	MG	A	1683	1/1	0.73	0.49	27,27,27,27	1
24	MG	A	1622	1/1	0.74	0.40	47,47,47,47	1
24	MG	A	1721	1/1	0.75	0.48	1,1,1,1	1
24	MG	A	1646	1/1	0.76	0.50	24,24,24,24	1
24	MG	A	1704	1/1	0.76	0.82	1,1,1,1	1
24	MG	A	1664	1/1	0.77	0.34	3,3,3,3	1
24	MG	A	1666	1/1	0.77	0.51	14,14,14,14	1
24	MG	A	1725	1/1	0.77	0.49	1,1,1,1	1
24	MG	A	1608	1/1	0.77	0.34	40,40,40,40	1
24	MG	A	1638	1/1	0.78	0.43	11,11,11,11	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	MG	A	1773	1/1	0.78	0.38	31,31,31,31	1
24	MG	A	1639	1/1	0.80	2.26	59,59,59,59	1
24	MG	L	201	1/1	0.80	0.47	1,1,1,1	1
24	MG	A	1748	1/1	0.80	0.88	3,3,3,3	1
24	MG	A	1732	1/1	0.81	0.30	4,4,4,4	1
24	MG	A	1692	1/1	0.81	0.56	28,28,28,28	1
24	MG	A	1740	1/1	0.82	0.36	1,1,1,1	1
24	MG	A	1658	1/1	0.82	0.42	31,31,31,31	1
24	MG	A	1767	1/1	0.82	1.16	26,26,26,26	1
24	MG	A	1747	1/1	0.82	0.46	26,26,26,26	1
24	MG	A	1669	1/1	0.82	1.25	1,1,1,1	1
24	MG	A	1750	1/1	0.82	0.67	10,10,10,10	1
24	MG	A	1671	1/1	0.82	0.45	20,20,20,20	1
24	MG	A	1711	1/1	0.83	0.41	5,5,5,5	1
24	MG	A	1710	1/1	0.83	0.57	47,47,47,47	1
24	MG	A	1631	1/1	0.84	0.27	45,45,45,45	1
24	MG	A	1757	1/1	0.84	0.74	9,9,9,9	1
24	MG	A	1751	1/1	0.84	0.78	42,42,42,42	1
24	MG	A	1610	1/1	0.84	0.26	56,56,56,56	0
24	MG	A	1772	1/1	0.85	0.31	1,1,1,1	1
24	MG	A	1603	1/1	0.85	0.23	58,58,58,58	0
24	MG	A	1601	1/1	0.85	0.09	34,34,34,34	0
24	MG	A	1779	1/1	0.85	0.49	24,24,24,24	1
24	MG	A	1619	1/1	0.85	0.83	46,46,46,46	1
24	MG	A	1715	1/1	0.85	0.40	1,1,1,1	1
24	MG	A	1728	1/1	0.86	0.34	1,1,1,1	1
24	MG	A	1605	1/1	0.86	0.44	36,36,36,36	1
24	MG	A	1717	1/1	0.87	0.69	7,7,7,7	1
24	MG	A	1632	1/1	0.87	0.87	28,28,28,28	1
24	MG	A	1720	1/1	0.87	0.58	16,16,16,16	1
24	MG	A	1777	1/1	0.87	1.21	41,41,41,41	1
24	MG	A	1764	1/1	0.87	0.49	40,40,40,40	1
24	MG	A	1727	1/1	0.87	0.17	14,14,14,14	1
24	MG	A	1626	1/1	0.87	0.46	36,36,36,36	1
24	MG	A	1641	1/1	0.88	0.17	1,1,1,1	1
24	MG	A	1630	1/1	0.88	0.43	87,87,87,87	1
24	MG	A	1708	1/1	0.88	0.25	8,8,8,8	1
24	MG	A	1623	1/1	0.88	0.48	46,46,46,46	1
24	MG	A	1753	1/1	0.88	0.35	5,5,5,5	1
24	MG	A	1667	1/1	0.88	0.62	1,1,1,1	1
24	MG	A	1723	1/1	0.88	0.51	1,1,1,1	1
24	MG	A	1613	1/1	0.88	0.34	30,30,30,30	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	MG	A	1656	1/1	0.88	0.33	1,1,1,1	1
24	MG	A	1662	1/1	0.89	0.29	1,1,1,1	1
24	MG	A	1618	1/1	0.89	0.54	41,41,41,41	1
24	MG	A	1607	1/1	0.89	0.29	62,62,62,62	1
24	MG	A	1731	1/1	0.89	0.29	9,9,9,9	1
24	MG	A	1620	1/1	0.89	0.29	52,52,52,52	1
24	MG	A	1763	1/1	0.89	0.35	11,11,11,11	1
24	MG	A	1749	1/1	0.89	0.91	17,17,17,17	1
24	MG	A	1684	1/1	0.89	0.85	28,28,28,28	1
24	MG	A	1762	1/1	0.90	0.15	18,18,18,18	1
24	MG	A	1677	1/1	0.90	0.53	2,2,2,2	1
24	MG	A	1633	1/1	0.90	0.60	36,36,36,36	1
24	MG	A	1696	1/1	0.90	0.23	28,28,28,28	1
24	MG	B	301	1/1	0.90	0.18	9,9,9,9	1
24	MG	A	1673	1/1	0.90	0.18	1,1,1,1	1
24	MG	A	1709	1/1	0.90	0.31	1,1,1,1	1
25	PAR	A	1783	42/42	0.90	0.16	43,53,68,70	0
24	MG	A	1778	1/1	0.91	0.28	4,4,4,4	1
24	MG	A	1651	1/1	0.91	0.48	2,2,2,2	1
24	MG	A	1734	1/1	0.91	0.63	1,1,1,1	1
24	MG	A	1687	1/1	0.91	0.46	11,11,11,11	1
24	MG	A	1738	1/1	0.91	0.60	15,15,15,15	1
24	MG	A	1627	1/1	0.91	0.15	1,1,1,1	1
24	MG	A	1616	1/1	0.92	0.39	23,23,23,23	1
24	MG	A	1670	1/1	0.92	0.56	1,1,1,1	1
24	MG	A	1675	1/1	0.92	0.22	8,8,8,8	1
24	MG	A	1676	1/1	0.92	0.23	20,20,20,20	1
24	MG	A	1761	1/1	0.92	0.34	8,8,8,8	1
24	MG	A	1733	1/1	0.93	0.79	13,13,13,13	1
24	MG	A	1645	1/1	0.93	0.23	7,7,7,7	1
24	MG	A	1769	1/1	0.93	0.41	15,15,15,15	1
24	MG	A	1780	1/1	0.93	0.43	1,1,1,1	1
24	MG	A	1629	1/1	0.93	0.47	1,1,1,1	1
24	MG	A	1705	1/1	0.93	1.33	1,1,1,1	1
24	MG	A	1679	1/1	0.93	0.29	9,9,9,9	1
24	MG	A	1775	1/1	0.93	0.23	1,1,1,1	1
24	MG	A	1746	1/1	0.94	0.44	22,22,22,22	1
24	MG	A	1726	1/1	0.94	0.29	1,1,1,1	1
24	MG	A	1712	1/1	0.94	0.17	23,23,23,23	1
24	MG	A	1771	1/1	0.94	0.74	19,19,19,19	1
24	MG	A	1690	1/1	0.94	0.13	14,14,14,14	1
24	MG	A	1714	1/1	0.94	0.26	2,2,2,2	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	MG	A	1691	1/1	0.94	0.15	16,16,16,16	1
24	MG	A	1637	1/1	0.94	0.36	21,21,21,21	1
24	MG	A	1776	1/1	0.94	0.87	1,1,1,1	1
24	MG	A	1654	1/1	0.94	0.28	13,13,13,13	1
24	MG	A	1640	1/1	0.94	0.21	66,66,66,66	1
24	MG	A	1634	1/1	0.94	0.38	23,23,23,23	1
24	MG	A	1660	1/1	0.94	0.22	14,14,14,14	1
24	MG	A	1649	1/1	0.94	0.24	3,3,3,3	1
24	MG	A	1643	1/1	0.94	0.58	37,37,37,37	1
24	MG	A	1689	1/1	0.94	0.44	1,1,1,1	1
24	MG	A	1765	1/1	0.94	0.63	8,8,8,8	1
26	ZN	D	301	1/1	0.94	0.34	97,97,97,97	0
24	MG	A	1770	1/1	0.95	0.21	1,1,1,1	1
24	MG	A	1702	1/1	0.95	0.33	9,9,9,9	1
24	MG	A	1735	1/1	0.95	0.41	1,1,1,1	1
24	MG	A	1736	1/1	0.95	0.17	5,5,5,5	1
24	MG	A	1755	1/1	0.95	0.68	3,3,3,3	1
24	MG	A	1648	1/1	0.95	0.20	11,11,11,11	0
24	MG	A	1688	1/1	0.95	0.23	16,16,16,16	1
24	MG	A	1759	1/1	0.95	0.16	7,7,7,7	1
24	MG	A	1665	1/1	0.95	0.17	7,7,7,7	1
24	MG	A	1697	1/1	0.95	0.11	10,10,10,10	1
24	MG	A	1716	1/1	0.95	0.45	6,6,6,6	1
24	MG	A	1636	1/1	0.95	0.18	26,26,26,26	1
24	MG	A	1680	1/1	0.95	0.51	15,15,15,15	1
24	MG	A	1719	1/1	0.95	0.59	19,19,19,19	1
24	MG	A	1642	1/1	0.95	0.22	22,22,22,22	1
24	MG	A	1663	1/1	0.95	0.23	21,21,21,21	1
24	MG	A	1768	1/1	0.96	0.42	9,9,9,9	1
24	MG	A	1760	1/1	0.96	0.25	1,1,1,1	1
24	MG	A	1672	1/1	0.96	0.44	1,1,1,1	1
24	MG	A	1661	1/1	0.96	0.33	4,4,4,4	1
24	MG	A	1782	1/1	0.96	0.48	1,1,1,1	1
24	MG	A	1674	1/1	0.96	0.29	24,24,24,24	1
24	MG	A	1647	1/1	0.96	0.69	39,39,39,39	1
24	MG	A	1657	1/1	0.96	0.58	1,1,1,1	1
24	MG	A	1609	1/1	0.96	0.31	35,35,35,35	1
24	MG	A	1615	1/1	0.96	0.23	1,1,1,1	0
24	MG	A	1741	1/1	0.97	0.58	5,5,5,5	1
24	MG	A	1752	1/1	0.97	0.49	19,19,19,19	1
24	MG	A	1685	1/1	0.97	0.67	25,25,25,25	1
24	MG	A	1781	1/1	0.97	0.69	1,1,1,1	1

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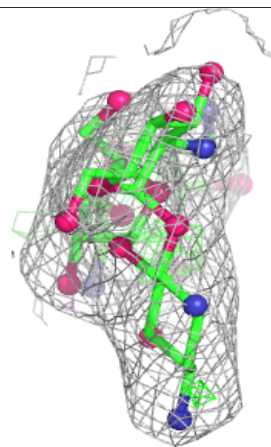
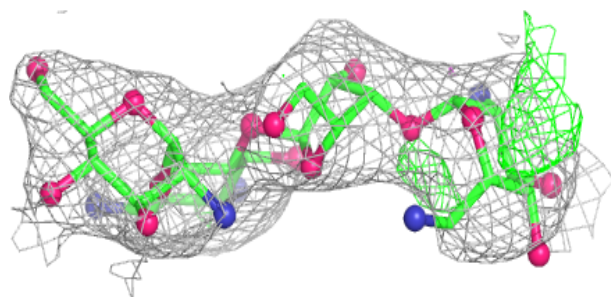
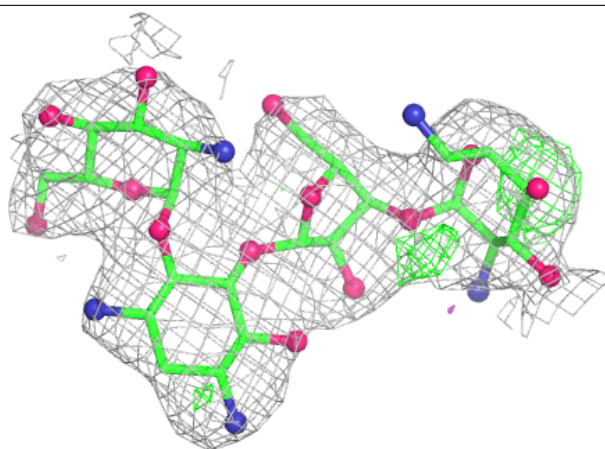
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	MG	A	1612	1/1	0.97	0.18	8,8,8,8	1
24	MG	A	1668	1/1	0.97	0.22	1,1,1,1	1
24	MG	A	1681	1/1	0.97	0.16	11,11,11,11	1
24	MG	A	1659	1/1	0.97	0.12	7,7,7,7	1
24	MG	A	1758	1/1	0.97	0.46	12,12,12,12	1
24	MG	A	1624	1/1	0.97	0.07	39,39,39,39	1
24	MG	A	1606	1/1	0.98	0.36	29,29,29,29	1
24	MG	A	1682	1/1	0.98	0.29	16,16,16,16	1
24	MG	A	1611	1/1	0.98	0.30	18,18,18,18	0
24	MG	A	1653	1/1	0.98	0.42	5,5,5,5	1
24	MG	A	1742	1/1	0.98	0.38	22,22,22,22	1
24	MG	A	1650	1/1	0.98	0.35	18,18,18,18	1
24	MG	A	1744	1/1	0.98	0.16	8,8,8,8	1
24	MG	A	1745	1/1	0.98	0.51	11,11,11,11	1
24	MG	A	1686	1/1	0.98	0.12	1,1,1,1	1
24	MG	A	1655	1/1	0.98	0.38	6,6,6,6	1
24	MG	A	1730	1/1	0.99	0.51	1,1,1,1	1
26	ZN	N	101	1/1	0.99	0.04	69,69,69,69	0

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

Electron density around PAR A 1783:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.