



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 21, 2026 – 07:14 am BST

PDB ID : 2UUC / pdb_00002uuc
Title : Structure of the *Thermus thermophilus* 30S ribosomal subunit complexed with a Valine-ASL with cmo5U in position 34 bound to an mRNA with a GUA-codon in the A-site and paromomycin.
Authors : Weixlbaumer, A.; Murphy, F.V.; Dziergowska, A.; Malkiewicz, A.; Vendeix, F.A.P.; Agris, P.F.; Ramakrishnan, V.
Deposited on : 2007-03-01
Resolution : 3.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

The following versions of software and data (see [references](#) ①) were used in the production of this report:

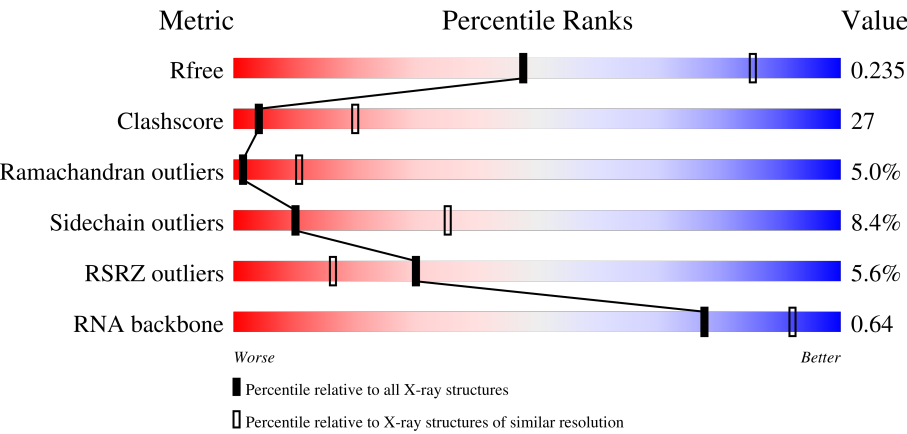
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)
RNA backbone	3983	1022 (3.32-2.88)

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

Mol	Chain	Length	Quality of chain
1	A	1522	4% 43% 46% 8% ..
2	B	256	12% 29% 51% 11% 8%
3	C	239	4% 28% 47% 11% 13%
4	D	209	6% 51% 42% 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	135	
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	U	27	
22	X	6	
23	Y	17	

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
25	MG	A	1610	-	-	-	X
25	MG	A	1611	-	-	-	X
25	MG	A	1618	-	-	-	X
25	MG	A	1622	-	-	-	X
25	MG	A	1625	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	MG	A	1630	-	-	-	X
25	MG	A	1653	-	-	-	X
25	MG	A	1667	-	-	-	X
25	MG	A	1669	-	-	-	X
25	MG	A	1671	-	-	-	X
25	MG	A	1673	-	-	-	X
25	MG	A	1700	-	-	-	X
25	MG	A	1711	-	-	-	X
25	MG	A	1716	-	-	-	X
25	MG	A	1739	-	-	-	X
25	MG	A	1742	-	-	-	X
25	MG	A	1758	-	-	-	X
25	MG	A	1773	-	-	-	X
26	K	A	1788	-	-	-	X

2 Entry composition [i](#)

There are 27 unique types of molecules in this entry. The entry contains 52372 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1512	Total	C	N	O	P	0	0	0
			32489	14462	6011	10505	1511			

- Molecule 2 is a protein called 30S RIBOSOMAL PROTEIN S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	235	Total	C	N	O	S	0	0	1
			1901	1213	342	341	5			

- Molecule 3 is a protein called 30S RIBOSOMAL PROTEIN S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	207	Total	C	N	O	S	0	0	1
			1613	1016	315	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	151	Total	C	N	O	S	0	0	1
			1147	724	218	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	S	0	0	0
			1010	639	197	174				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	99	Total	C	N	O	S	0	0	1
			793	498	157	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	125	Total	C	N	O	S	0	0	1
			971	611	196	163	1			

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	P	84	Total	C	N	O	S	0	0	1
			701	443	140	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	160	148	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
			598	381	118	99			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	S	81	Total	C	N	O	S	0	0	1
			648	414	120	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
			763	470	162	129	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	U	25	Total	C	N	O	0	0	1
			209	128	51	30			

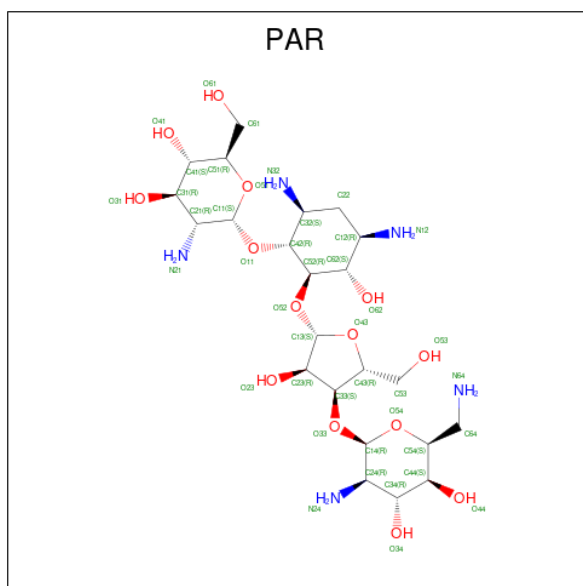
- Molecule 22 is a RNA chain called 5'-R(*GP*UP*AP*AP*AP*AP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	X	4	Total	C	N	O	P	0	0	0
			84	39	17	25	3			

- Molecule 23 is a RNA chain called 5'-R(*CP*CP*UP*CP*CP*CP*UP*CM0P*AP*CP*6MZP*AP*GP*GP*AP*GP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	Y	13	Total	C	N	O	P	0	0	0
			277	126	48	91	12			

- Molecule 24 is PAROMOMYCIN (CCD ID: PAR) (formula: C₂₃H₄₅N₅O₁₄).



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

- Molecule 25 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	A	176	Total	Mg	0	0
			176	176		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	B	1	Total 1	Mg 1	0	0
25	D	1	Total 1	Mg 1	0	0
25	E	1	Total 1	Mg 1	0	0
25	I	1	Total 1	Mg 1	0	0
25	K	1	Total 1	Mg 1	0	0
25	M	1	Total 1	Mg 1	0	0
25	N	1	Total 1	Mg 1	0	0
25	Q	1	Total 1	Mg 1	0	0

- Molecule 26 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
26	A	51	Total 51	K 51	0	0
26	E	3	Total 3	K 3	0	0
26	G	1	Total 1	K 1	0	0
26	Q	1	Total 1	K 1	0	0

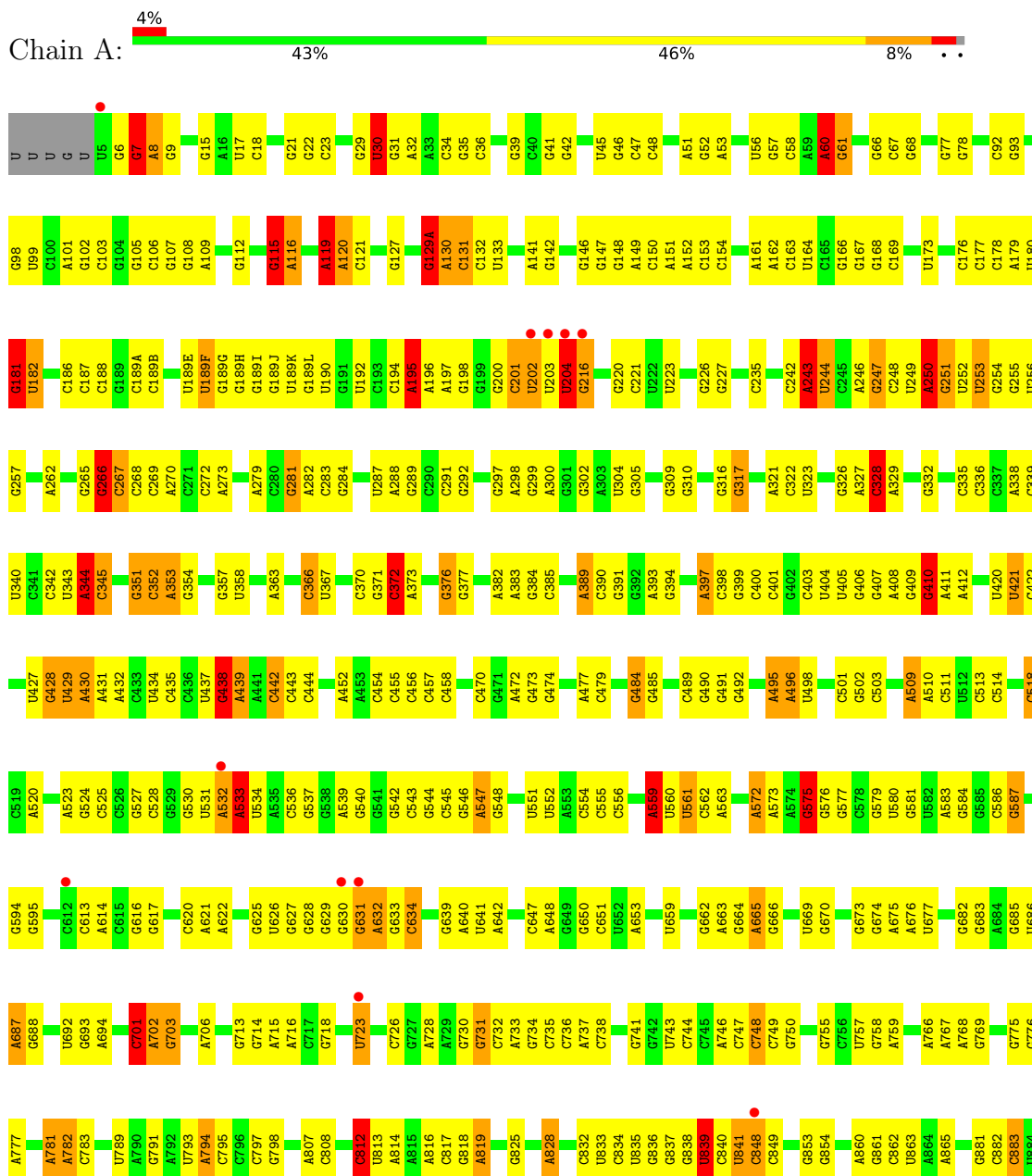
- Molecule 27 is ZINC ION (CCD ID: ZN) (formula: Zn).

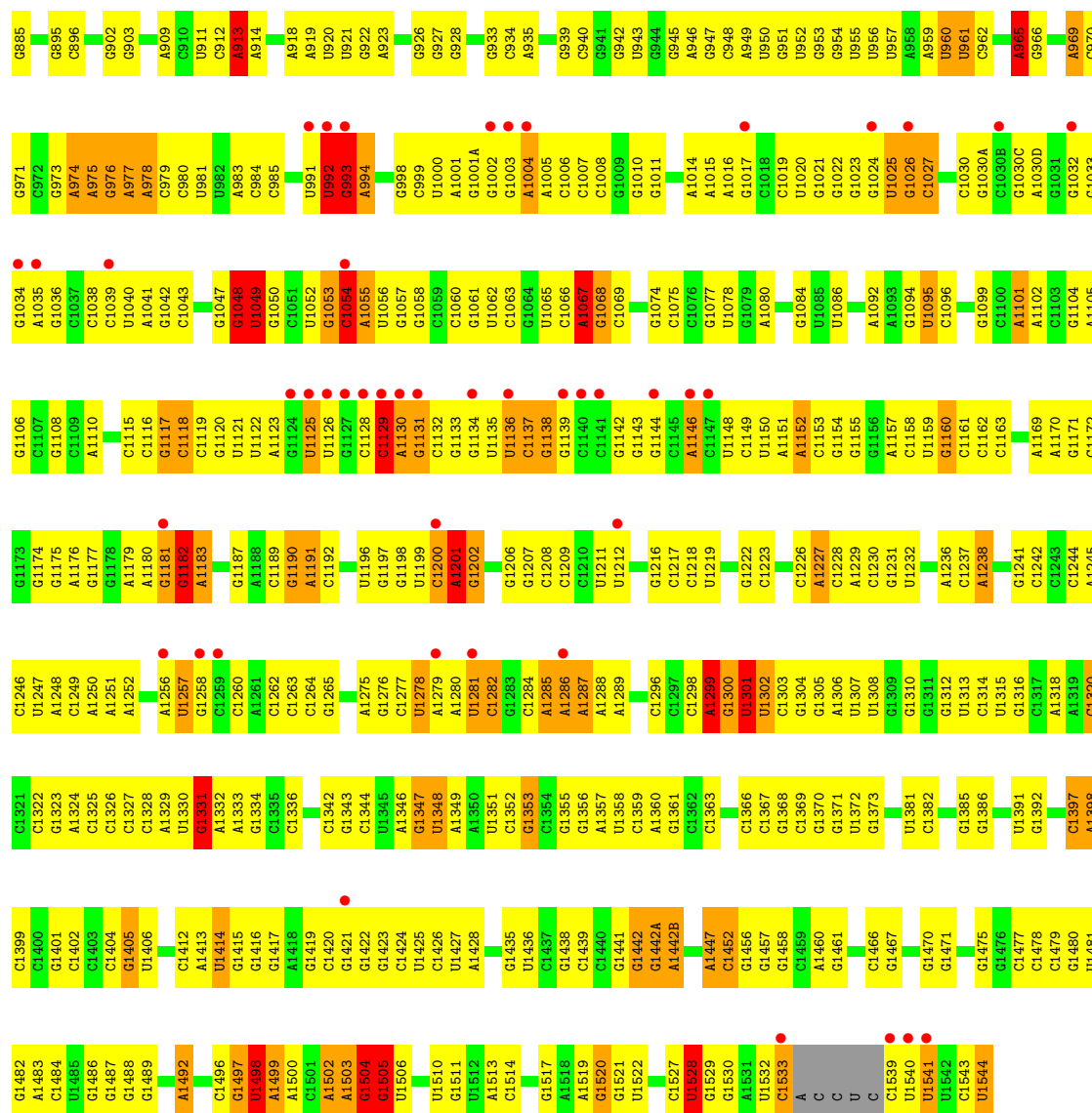
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
27	D	1	Total 1	Zn 1	0	0
27	N	1	Total 1	Zn 1	0	0

3 Residue-property plots

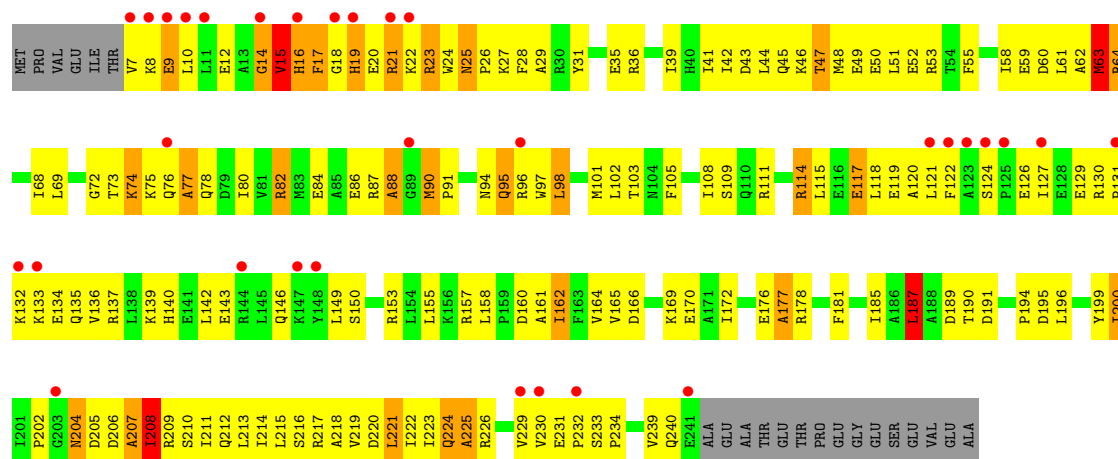
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: 16S Ribosomal RNA

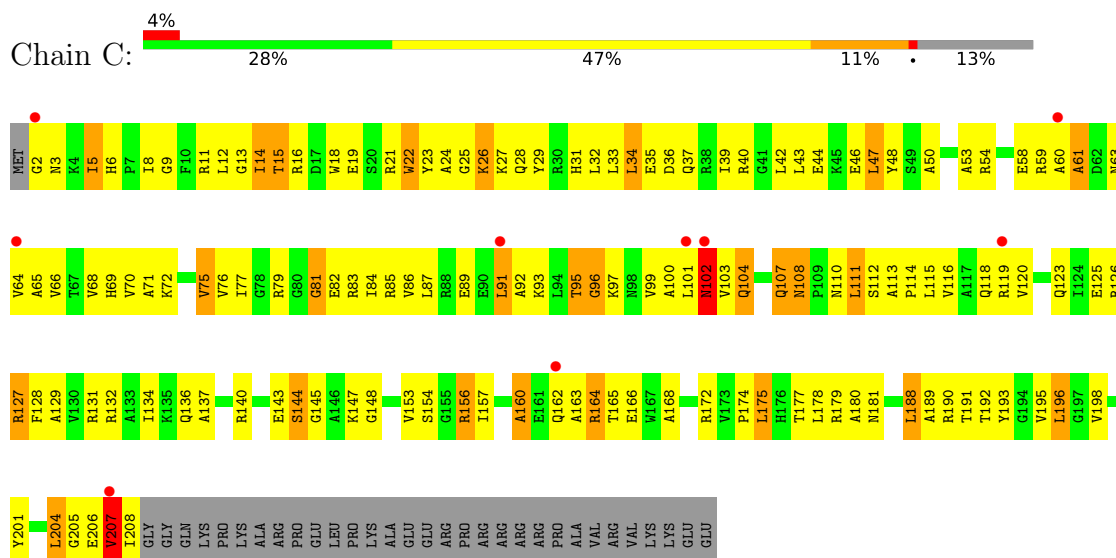




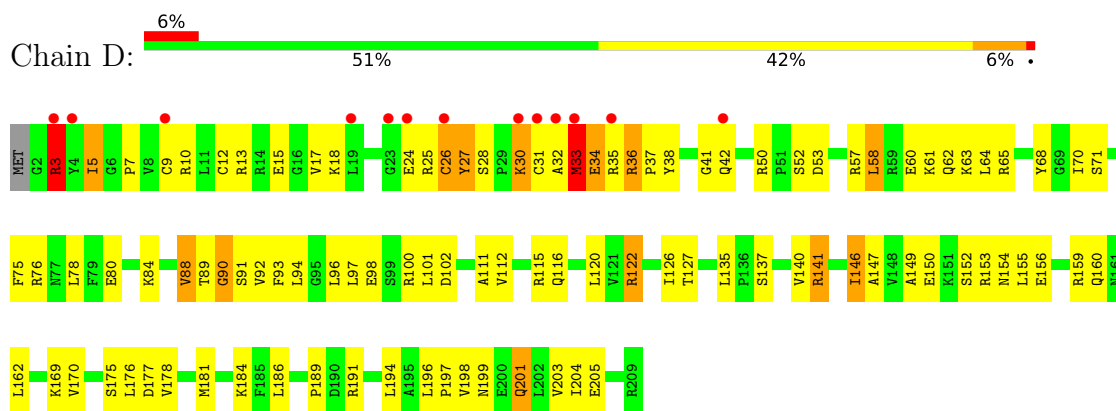
• Molecule 2: 30S RIBOSOMAL PROTEIN S2



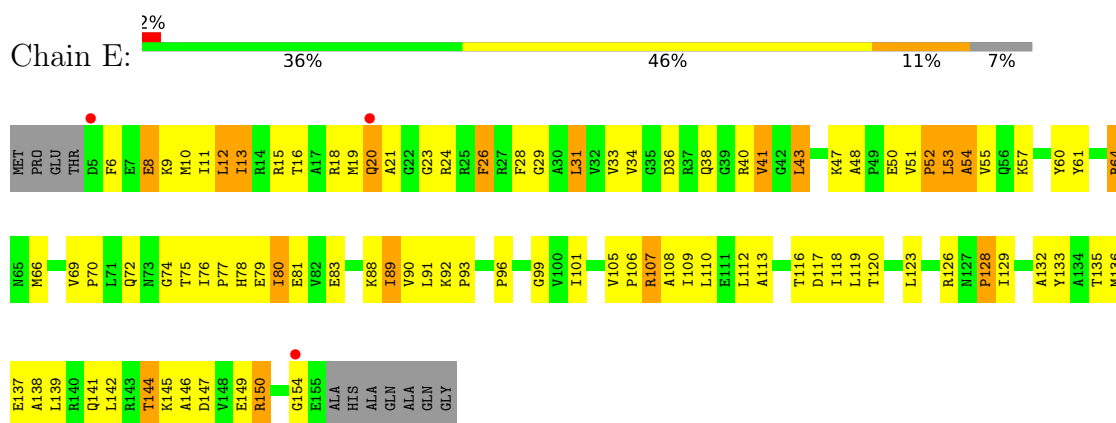
- Molecule 3: 30S RIBOSOMAL PROTEIN S3



- Molecule 4: 30S RIBOSOMAL PROTEIN S4

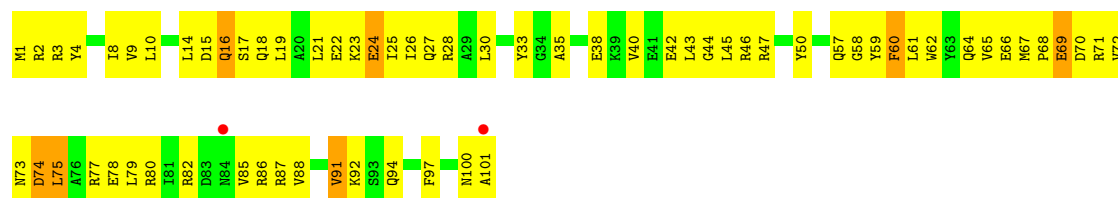


- Molecule 5: 30S RIBOSOMAL PROTEIN S5

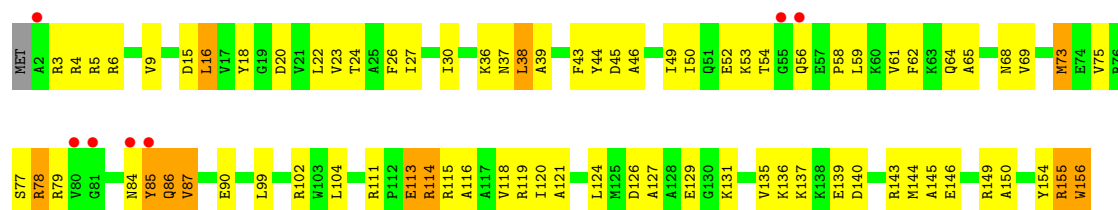


- Molecule 6: 30S RIBOSOMAL PROTEIN S6

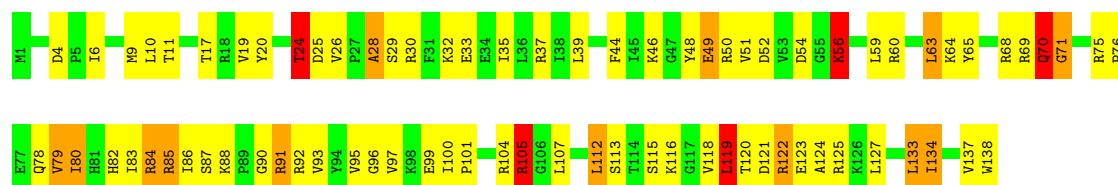




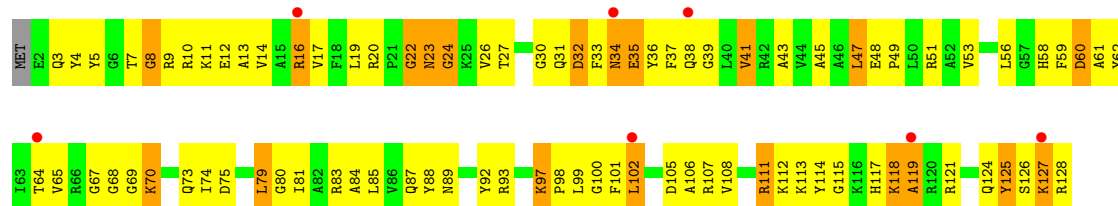
• Molecule 7: 30S RIBOSOMAL PROTEIN S7



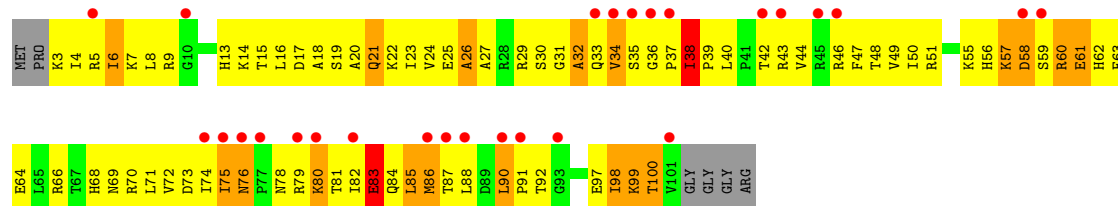
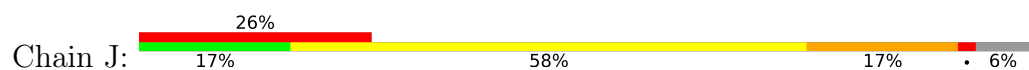
• Molecule 8: 30S RIBOSOMAL PROTEIN S8



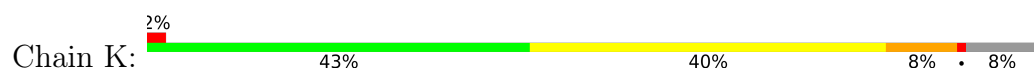
• Molecule 9: 30S RIBOSOMAL PROTEIN S9



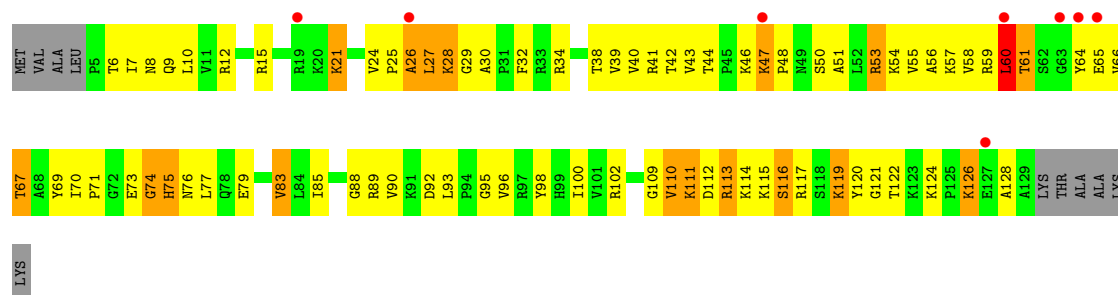
• Molecule 10: 30S RIBOSOMAL PROTEIN S10



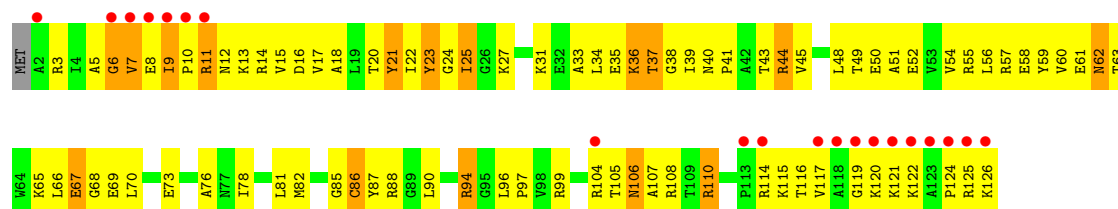
• Molecule 11: 30S RIBOSOMAL PROTEIN S11



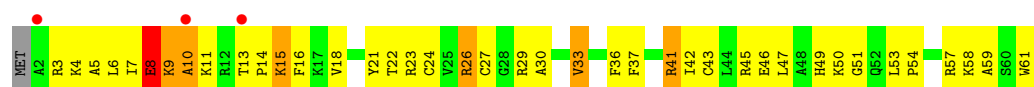
• Molecule 12: 30S RIBOSOMAL PROTEIN S12



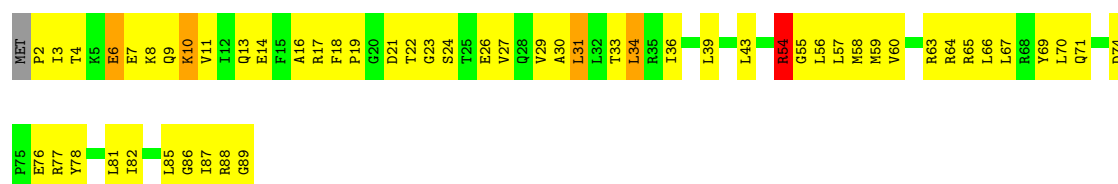
• Molecule 13: 30S RIBOSOMAL PROTEIN S13



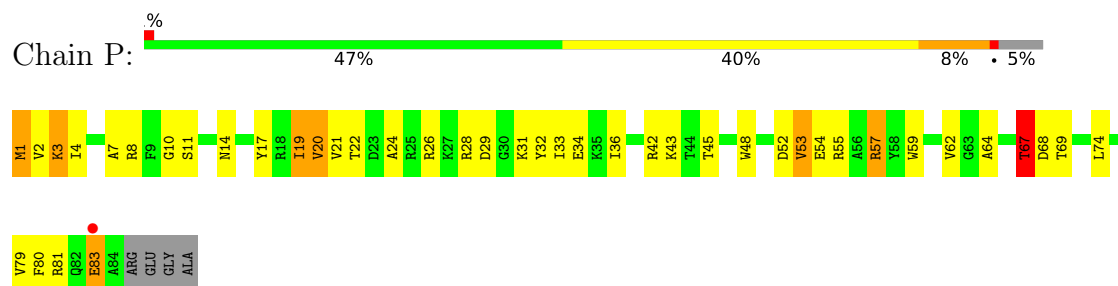
• Molecule 14: 30S RIBOSOMAL PROTEIN S14



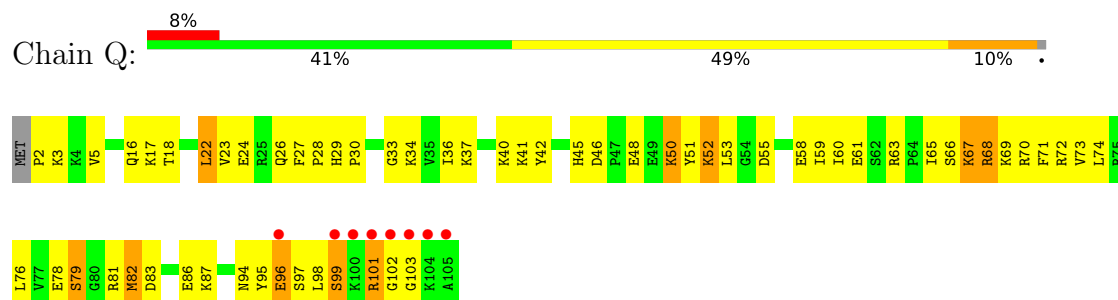
• Molecule 15: 30S RIBOSOMAL PROTEIN S15



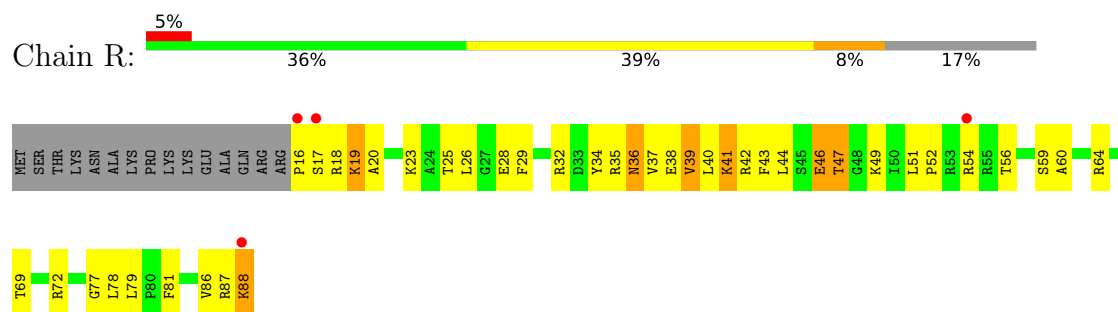
• Molecule 16: 30S RIBOSOMAL PROTEIN S16



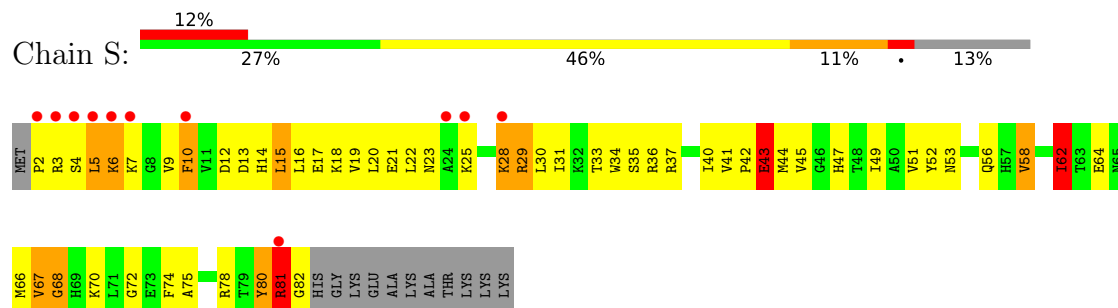
• Molecule 17: 30S RIBOSOMAL PROTEIN S17



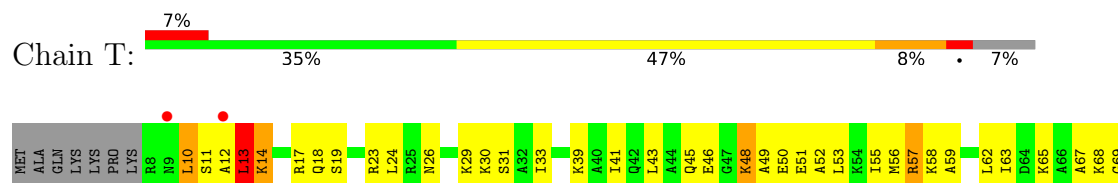
• Molecule 18: 30S RIBOSOMAL PROTEIN S18

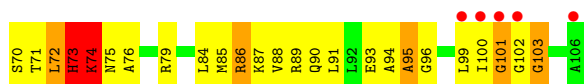


• Molecule 19: 30S RIBOSOMAL PROTEIN S19



• Molecule 20: 30S RIBOSOMAL PROTEIN S20





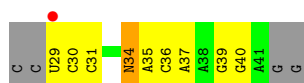
- Molecule 21: 30S RIBOSOMAL PROTEIN THX



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



- Molecule 23: 5'-R(*CP*CP*UP*CP*CP*CP*UP*CM0P*AP*CP*6MZP*AP *GP*GP*AP*GP*G)-3'



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	400.96Å 400.96Å 174.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.89 – 3.10 29.89 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.4 (29.89-3.10) 99.3 (29.89-3.10)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 3.11Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.210 , 0.245 0.202 , 0.235	Depositor DCC
R_{free} test set	12815 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	66.6	Xtriage
Anisotropy	0.306	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 74.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	52372	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.73% 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: K, PAR, ZN, MG, 6MZ, CM0

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.49	0/36365	0.69	67/56754 (0.1%)
2	B	0.48	1/1936 (0.1%)	1.07	12/2611 (0.5%)
3	C	0.50	1/1637 (0.1%)	0.96	2/2207 (0.1%)
4	D	0.50	0/1733	1.02	9/2318 (0.4%)
5	E	0.60	1/1163 (0.1%)	1.11	7/1566 (0.4%)
6	F	0.44	0/856	0.90	2/1154 (0.2%)
7	G	0.46	0/1276	0.95	5/1709 (0.3%)
8	H	0.60	0/1136	1.17	15/1527 (1.0%)
9	I	0.47	0/1029	1.09	5/1379 (0.4%)
10	J	0.54	1/806 (0.1%)	1.02	4/1084 (0.4%)
11	K	0.53	0/900	1.06	6/1213 (0.5%)
12	L	0.63	1/987 (0.1%)	1.29	7/1322 (0.5%)
13	M	0.48	0/1008	1.06	4/1347 (0.3%)
14	N	0.49	0/501	1.01	2/664 (0.3%)
15	O	0.48	0/745	0.88	1/992 (0.1%)
16	P	0.59	1/717 (0.1%)	1.12	4/965 (0.4%)
17	Q	0.58	1/870 (0.1%)	1.14	4/1159 (0.3%)
18	R	0.47	0/604	0.99	3/801 (0.4%)
19	S	0.51	1/662 (0.2%)	1.14	5/892 (0.6%)
20	T	0.57	0/765	1.19	7/1007 (0.7%)
21	U	0.67	1/213 (0.5%)	0.95	0/279
22	X	0.49	0/94	0.78	0/145
23	Y	0.50	0/253	0.71	0/387
All	All	0.50	9/56256 (0.0%)	0.83	171/83482 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	4	21
22	X	0	1
All	All	4	22

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	J	100	THR	C-N	-5.62	1.25	1.33
2	B	240	GLN	C-N	-5.57	1.25	1.33
3	C	207	VAL	C-N	-5.51	1.25	1.33
19	S	81	ARG	C-N	-5.33	1.25	1.33
5	E	154	GLY	C-N	-5.32	1.25	1.33
16	P	83	GLU	C-N	-5.27	1.25	1.33
17	Q	82	MET	SD-CE	5.25	1.92	1.79
21	U	25	LYS	C-N	-5.22	1.26	1.33
12	L	128	ALA	C-N	-5.16	1.26	1.33

All (171) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	L	26	ALA	N-CA-C	-15.59	96.45	112.97
1	A	281	G	C2'-C3'-O3'	14.47	131.21	109.50
1	A	1498	U	C2'-C3'-O3'	14.45	131.17	109.50
1	A	243	A	C2'-C3'-O3'	13.82	130.23	109.50
1	A	1528	U	C2'-C3'-O3'	13.45	129.67	109.50
1	A	181	G	C2'-C3'-O3'	13.36	129.53	109.50
1	A	366	C	C2'-C3'-O3'	13.28	129.41	109.50
1	A	115	G	C2'-C3'-O3'	13.17	129.26	109.50
1	A	328	C	C2'-C3'-O3'	13.13	129.19	109.50
1	A	559	A	C2'-C3'-O3'	12.62	128.44	109.50
1	A	575	G	C2'-C3'-O3'	12.48	128.22	109.50
1	A	687	A	C2'-C3'-O3'	12.23	127.84	109.50
1	A	913	A	C2'-C3'-O3'	11.89	127.34	109.50
1	A	965	A	C2'-C3'-O3'	11.66	126.99	109.50
1	A	812	C	C2'-C3'-O3'	11.50	126.75	109.50
1	A	1503	A	C2'-C3'-O3'	11.24	126.36	109.50
1	A	60	A	C2'-C3'-O3'	10.98	125.96	109.50
1	A	533	A	C2'-C3'-O3'	10.95	125.93	109.50
20	T	75	ASN	N-CA-C	-10.78	100.13	113.18
20	T	13	LEU	N-CA-C	-10.51	97.85	113.61
1	A	484	G	C2'-C3'-O3'	10.32	124.98	109.50
12	L	119	LYS	N-CA-C	-10.28	96.67	110.55
1	A	372	C	C2'-C3'-O3'	9.87	124.31	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	69	VAL	N-CA-C	9.53	116.23	107.56
2	B	90	MET	N-CA-C	9.37	120.37	109.60
1	A	428	G	C2'-C3'-O3'	9.21	123.31	109.50
4	D	26	CYS	N-CA-C	-9.14	102.06	113.02
19	S	80	TYR	N-CA-C	9.11	124.30	109.72
1	A	1528	U	C4'-C3'-O3'	9.07	123.00	109.40
20	T	14	LYS	N-CA-C	-9.05	101.33	111.82
1	A	366	C	C4'-C3'-O3'	9.02	122.92	109.40
9	I	60	ASP	N-CA-C	-8.97	95.38	109.72
18	R	46	GLU	N-CA-C	-8.94	101.53	111.28
17	Q	67	LYS	N-CA-C	-8.85	97.39	110.23
1	A	1067	A	C2'-C3'-O3'	8.82	122.74	109.50
8	H	79	VAL	N-CA-C	-8.82	102.26	110.82
1	A	7	G	C2'-C3'-O3'	8.72	122.58	109.50
1	A	1301	U	C2'-C3'-O3'	8.61	122.42	109.50
1	A	1505	G	C2'-C3'-O3'	8.45	126.37	113.70
1	A	748	C	C2'-C3'-O3'	8.35	122.03	109.50
1	A	281	G	C4'-C3'-O3'	8.20	121.69	109.40
1	A	266	G	C2'-C3'-O3'	8.17	125.96	113.70
1	A	1544	U	C2'-C3'-O3'	-8.13	97.30	109.50
16	P	20	VAL	N-CA-C	8.12	120.47	108.45
1	A	181	G	C4'-C3'-O3'	7.75	121.02	109.40
1	A	687	A	C4'-C3'-O3'	7.73	121.00	109.40
4	D	33	MET	N-CA-C	-7.72	104.00	113.19
3	C	145	GLY	N-CA-C	7.70	126.00	115.30
1	A	243	A	C4'-C3'-O3'	7.69	120.94	109.40
1	A	1285	A	C2'-C3'-O3'	7.66	121.00	109.50
1	A	115	G	C4'-C3'-O3'	7.64	120.86	109.40
11	K	116	HIS	N-CA-C	-7.62	101.88	112.25
12	L	61	THR	N-CA-C	-7.62	102.98	111.82
3	C	111	LEU	N-CA-C	-7.53	102.42	114.09
2	B	64	ARG	N-CA-C	-7.52	103.67	114.12
11	K	91	ARG	N-CA-C	-7.52	102.22	111.40
5	E	26	PHE	N-CA-C	7.42	121.36	110.59
10	J	58	ASP	N-CA-C	7.27	121.86	112.41
1	A	1299	A	N9-C1'-C2'	7.13	122.69	112.00
7	G	114	ARG	N-CA-C	7.08	121.74	113.18
1	A	509	A	C2'-C3'-O3'	6.95	124.13	113.70
12	L	30	ALA	N-CA-C	-6.94	101.07	110.36
1	A	559	A	C4'-C3'-O3'	6.93	119.79	109.40
19	S	62	ILE	N-CA-C	6.91	117.19	107.37
13	M	11	ARG	N-CA-C	6.90	119.03	108.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	47	THR	N-CA-C	-6.83	103.84	111.28
2	B	133	LYS	N-CA-C	-6.83	105.36	113.21
8	H	134	ILE	N-CA-C	6.83	116.97	110.42
13	M	25	ILE	N-CA-C	6.82	117.87	107.77
1	A	533	A	C4'-C3'-O3'	6.78	119.57	109.40
1	A	250	A	C2'-C3'-O3'	6.77	119.66	109.50
7	G	87	VAL	N-CA-C	6.68	114.16	107.55
1	A	1201	A	C2'-C3'-O3'	6.63	119.44	109.50
10	J	60	ARG	N-CA-C	6.54	124.73	110.80
12	L	60	LEU	N-CA-C	6.48	120.08	110.48
2	B	177	ALA	N-CA-C	-6.47	103.92	110.97
4	D	30	LYS	N-CA-C	6.44	120.47	112.03
12	L	58	VAL	N-CA-C	6.41	118.61	108.87
1	A	60	A	C4'-C3'-O3'	6.40	119.00	109.40
9	I	35	GLU	N-CA-C	-6.38	105.51	113.55
7	G	154	TYR	N-CA-C	-6.27	105.27	113.17
16	P	67	THR	N-CA-C	-6.19	102.33	110.43
17	Q	79	SER	N-CA-C	6.19	117.58	108.86
9	I	39	GLY	N-CA-C	-6.17	106.90	114.92
20	T	96	GLY	N-CA-C	6.15	120.98	112.37
2	B	225	ALA	N-CA-C	-6.14	106.11	113.97
5	E	48	ALA	N-CA-C	6.07	113.68	108.22
9	I	22	GLY	N-CA-C	6.06	119.44	110.60
19	S	10	PHE	N-CA-C	6.03	118.45	109.59
1	A	1200	C	N1-C1'-C2'	5.99	120.99	112.00
8	H	69	ARG	N-CA-C	5.99	118.97	109.81
8	H	70	GLN	N-CA-C	5.98	123.53	110.80
5	E	23	GLY	N-CA-C	5.93	118.62	110.56
1	A	993	G	C2'-C3'-O3'	5.89	118.33	109.50
15	O	54	ARG	N-CA-C	-5.87	104.79	111.07
1	A	992	U	C2'-C3'-O3'	5.86	118.29	109.50
1	A	30	U	C2'-C3'-O3'	5.84	118.27	109.50
2	B	14	GLY	N-CA-C	-5.84	106.55	115.66
2	B	77	ALA	N-CA-C	-5.82	106.03	114.12
1	A	129(A)	G	C2'-C3'-O3'	5.78	118.18	109.50
19	S	68	GLY	N-CA-C	5.78	120.96	113.27
17	Q	50	LYS	N-CA-C	5.76	118.02	111.11
8	H	44	PHE	N-CA-C	-5.76	106.39	113.41
8	H	56	LYS	CA-C-N	5.75	127.03	119.84
8	H	56	LYS	C-N-CA	5.75	127.03	119.84
1	A	204	U	C2'-C3'-O3'	5.74	118.11	109.50
8	H	19	VAL	N-CA-C	-5.74	105.80	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1129	C	C2'-C3'-O3'	5.74	118.10	109.50
11	K	28	THR	N-CA-C	-5.73	100.55	109.72
16	P	19	ILE	N-CA-C	-5.71	101.30	108.84
1	A	701	C	C2'-C3'-O3'	5.67	118.00	109.50
11	K	126	ARG	N-CA-C	5.67	118.14	108.90
1	A	438	G	C4'-C3'-O3'	5.60	117.80	109.40
1	A	344	A	C2'-C3'-O3'	5.60	117.90	109.50
1	A	1182	G	C2'-C3'-O3'	5.60	117.90	109.50
12	L	88	GLY	N-CA-C	-5.60	99.91	113.18
20	T	74	LYS	N-CA-C	5.60	122.72	110.80
2	B	187	LEU	N-CA-C	-5.59	100.87	109.76
13	M	106	ASN	CB-CA-C	-5.59	109.14	115.79
20	T	58	LYS	N-CA-C	-5.57	104.90	110.97
2	B	114	ARG	N-CA-C	-5.56	106.17	113.12
18	R	81	PHE	N-CA-C	-5.55	106.64	113.41
1	A	1504	G	O4'-C1'-C2'	5.54	111.34	105.80
14	N	8	GLU	N-CA-C	-5.52	106.39	113.01
8	H	100	ILE	N-CA-C	-5.51	103.55	108.95
1	A	1504	G	C5'-C4'-O4'	-5.50	100.84	109.10
1	A	1049	U	C2'-C3'-O3'	5.49	117.74	109.50
5	E	13	ILE	N-CA-C	-5.48	100.29	108.46
9	I	70	LYS	N-CA-C	5.45	117.93	111.33
1	A	410	G	C2'-C3'-O3'	5.45	121.87	113.70
1	A	1299	A	C4'-C3'-O3'	-5.44	104.84	113.00
2	B	200	ILE	N-CA-C	5.44	116.81	108.71
6	F	91	VAL	N-CA-C	5.42	116.47	108.45
19	S	58	VAL	N-CA-C	5.41	114.43	108.05
6	F	60	PHE	N-CA-C	5.37	118.97	109.96
7	G	85	TYR	N-CA-C	5.36	117.15	108.41
8	H	96	GLY	N-CA-C	-5.36	105.42	112.82
8	H	80	ILE	CB-CA-C	-5.36	107.22	113.22
10	J	38	ILE	CA-C-N	5.34	126.51	119.84
10	J	38	ILE	C-N-CA	5.34	126.51	119.84
16	P	3	LYS	N-CA-C	5.32	118.25	109.85
17	Q	52	LYS	N-CA-C	5.31	118.25	109.85
13	M	37	THR	N-CA-C	-5.30	106.59	114.64
18	R	47	THR	N-CA-C	-5.29	102.69	110.52
4	D	178	VAL	N-CA-C	5.28	115.91	110.36
1	A	839	U	N1-C1'-C2'	5.25	119.88	112.00
8	H	71	GLY	N-CA-C	5.25	123.05	112.34
7	G	24	THR	N-CA-C	-5.24	105.57	111.28
8	H	119	LEU	N-CA-C	5.22	116.73	108.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1331	G	C4'-C3'-O3'	-5.20	105.20	113.00
4	D	12	CYS	N-CA-C	-5.19	104.88	111.11
4	D	50	ARG	CA-C-N	5.17	125.10	119.78
4	D	50	ARG	C-N-CA	5.17	125.10	119.78
1	A	563	A	N9-C1'-C2'	5.15	119.72	112.00
1	A	572	A	N9-C1'-C2'	5.15	119.73	112.00
1	A	1200	C	C2'-C3'-O3'	-5.14	105.98	113.70
11	K	89	ALA	N-CA-C	-5.14	104.08	110.41
1	A	389	A	C5'-C4'-C3'	5.13	123.69	116.00
4	D	191	ARG	N-CA-C	-5.12	105.70	111.28
20	T	86	ARG	N-CA-C	-5.10	103.13	111.04
1	A	397	A	C5'-C4'-C3'	-5.10	108.35	116.00
4	D	27	TYR	N-CA-C	-5.10	107.73	114.31
11	K	101	SER	N-CA-C	5.09	118.32	112.57
5	E	8	GLU	N-CA-C	5.08	117.35	108.76
1	A	389	A	C2'-C3'-O3'	-5.06	106.11	113.70
1	A	119	A	C2'-C3'-O3'	5.05	117.08	109.50
5	E	54	ALA	N-CA-C	-5.04	105.70	111.14
2	B	88	ALA	N-CA-C	-5.04	101.42	109.07
14	N	51	GLY	N-CA-C	-5.03	108.29	115.64
8	H	84	ARG	N-CA-C	5.02	117.08	108.90
8	H	28	ALA	N-CA-C	5.00	118.11	110.20

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	243	A	C3'
1	A	281	G	C3'
1	A	366	C	C3'
1	A	1528	U	C3'

All (22) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1048	G	Sidechain
1	A	1054	C	Sidechain
1	A	1067	A	Sidechain
1	A	1077	G	Sidechain
1	A	1299	A	Sidechain
1	A	1405	G	Sidechain
1	A	1414	U	Sidechain
1	A	195	A	Sidechain

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Mol	Chain	Res	Type	Group
1	A	250	A	Sidechain
1	A	253	U	Sidechain
1	A	297	G	Sidechain
1	A	317	G	Sidechain
1	A	376	G	Sidechain
1	A	410	G	Sidechain
1	A	528	C	Sidechain
1	A	561	U	Sidechain
1	A	575	G	Sidechain
1	A	587	G	Sidechain
1	A	634	C	Sidechain
1	A	733	A	Sidechain
1	A	883	C	Sidechain
22	X	4	A	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	32489	0	16398	790	0
2	B	1901	0	1951	241	0
3	C	1613	0	1677	157	0
4	D	1703	0	1764	115	0
5	E	1147	0	1207	98	0
6	F	843	0	857	77	0
7	G	1257	0	1296	77	0
8	H	1116	0	1177	85	0
9	I	1010	0	1037	109	0
10	J	793	0	835	141	0
11	K	885	0	904	64	0
12	L	971	0	1057	79	0
13	M	997	0	1072	105	0
14	N	492	0	530	58	0
15	O	734	0	771	70	0
16	P	701	0	720	52	0
17	Q	857	0	928	82	0
18	R	598	0	670	54	0
19	S	648	0	673	75	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	T	763	0	861	79	0
21	U	209	0	221	28	0
22	X	84	0	45	3	0
23	Y	277	0	145	9	0
24	A	42	0	45	0	0
25	A	176	0	0	0	0
25	B	1	0	0	0	0
25	D	1	0	0	0	0
25	E	1	0	0	0	0
25	I	1	0	0	0	0
25	K	1	0	0	0	0
25	M	1	0	0	0	0
25	N	1	0	0	0	0
25	Q	1	0	0	0	0
26	A	51	0	0	0	0
26	E	3	0	0	0	0
26	G	1	0	0	0	0
26	Q	1	0	0	0	0
27	D	1	0	0	0	0
27	N	1	0	0	1	0
All	All	52372	0	36841	2444	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 27.

All (2444) 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:243:A:H4'	1:A:244:U:H5'	1.24	1.16
10:J:32:ALA:HB1	10:J:75:ILE:HG13	1.25	1.13
3:C:14:ILE:HG22	3:C:15:THR:H	1.11	1.13
15:O:87:ILE:HG22	15:O:88:ARG:H	1.07	1.11
7:G:73:MET:HE2	7:G:90:GLU:HA	1.33	1.09
3:C:50:ALA:HB1	3:C:70:VAL:HG11	1.31	1.07
7:G:75:VAL:HG21	7:G:86:GLN:HB3	1.36	1.07
20:T:73:HIS:O	20:T:74:LYS:HB2	1.50	1.06
3:C:64:VAL:HB	3:C:99:VAL:HG21	1.40	1.03
2:B:118:LEU:HD22	2:B:142:LEU:HD13	1.39	1.02
1:A:975:A:H4'	1:A:976:G:H5''	1.45	0.99
5:E:80:ILE:CD1	5:E:91:LEU:HB2	1.93	0.97
4:D:30:LYS:HB3	4:D:35:ARG:HH21	1.29	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:38:ILE:HG13	10:J:71:LEU:HB3	1.45	0.96
20:T:50:GLU:HA	20:T:100:ILE:HG22	1.44	0.96
13:M:36:LYS:HB2	13:M:59:TYR:HE2	1.31	0.96
3:C:70:VAL:HG12	3:C:72:LYS:H	1.31	0.95
3:C:91:LEU:HD11	3:C:99:VAL:HG23	1.47	0.95
4:D:7:PRO:HB2	4:D:10:ARG:HD2	1.48	0.95
2:B:84:GLU:HB3	2:B:219:VAL:HG21	1.49	0.95
15:O:55:GLY:HA2	15:O:58:MET:HE3	1.46	0.94
19:S:64:GLU:O	19:S:67:VAL:HG23	1.68	0.93
3:C:64:VAL:HG23	3:C:99:VAL:HG11	1.50	0.93
5:E:79:GLU:HG3	5:E:93:PRO:HD2	1.50	0.93
6:F:2:ARG:NE	6:F:69:GLU:HG2	1.84	0.93
10:J:27:ALA:HA	10:J:81:THR:HG23	1.50	0.93
2:B:60:ASP:HB3	2:B:64:ARG:HH12	1.34	0.92
1:A:1502:A:H2	1:A:1505:G:H1	1.11	0.91
12:L:60:LEU:HD11	12:L:85:ILE:HD12	1.52	0.91
10:J:4:ILE:HD11	10:J:74:ILE:HD12	1.51	0.91
1:A:192:U:H4'	20:T:102:GLY:O	1.71	0.90
1:A:1152:A:H5''	10:J:13:HIS:CD2	2.06	0.90
1:A:1250:A:H4'	9:I:68:GLY:H	1.35	0.90
10:J:30:SER:HB3	10:J:84:GLN:HE21	1.38	0.89
2:B:95:GLN:C	2:B:96:ARG:HD2	1.97	0.89
2:B:87:ARG:HH11	2:B:233:SER:HB2	1.37	0.89
10:J:49:VAL:HG23	14:N:41:ARG:HB2	1.52	0.89
15:O:87:ILE:HG22	15:O:88:ARG:N	1.85	0.89
3:C:91:LEU:HD21	3:C:99:VAL:HG22	1.55	0.89
2:B:16:HIS:NE2	2:B:214:ILE:HD11	1.86	0.89
2:B:77:ALA:HB2	2:B:211:ILE:HD13	1.55	0.89
2:B:178:ARG:HH22	8:H:68:ARG:HH22	1.20	0.88
9:I:128:ARG:O	13:M:126:LYS:HD2	1.73	0.88
9:I:93:ARG:NH1	9:I:93:ARG:HB3	1.89	0.88
1:A:718:G:H5'	11:K:117:ASN:ND2	1.88	0.88
2:B:124:SER:O	2:B:127:ILE:HG13	1.74	0.88
1:A:954:G:H4'	13:M:120:LYS:HB3	1.55	0.87
5:E:74:GLY:HA3	5:E:116:THR:HG22	1.52	0.87
9:I:53:VAL:HG21	9:I:85:LEU:HD21	1.57	0.87
5:E:80:ILE:HD11	5:E:91:LEU:HB2	1.54	0.87
8:H:112:LEU:N	8:H:112:LEU:HD23	1.89	0.87
15:O:3:ILE:HD13	15:O:34:LEU:HD13	1.57	0.86
2:B:84:GLU:OE1	2:B:216:SER:HA	1.75	0.86
1:A:1442(A):G:H4'	1:A:1442(B):A:H5'	1.58	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:17:ARG:HG3	15:O:17:ARG:HH11	1.37	0.86
1:A:1277:C:HO2'	1:A:1279:A:H8	1.24	0.86
10:J:8:LEU:HB2	10:J:70:ARG:HB2	1.57	0.86
1:A:246:A:O2'	17:Q:99:SER:HB3	1.75	0.85
13:M:49:THR:HG22	13:M:51:ALA:H	1.41	0.85
10:J:46:ARG:HG2	10:J:46:ARG:HH11	1.41	0.85
1:A:969:A:H61	13:M:126:LYS:HB2	1.41	0.85
15:O:78:TYR:CZ	15:O:82:ILE:HD11	2.11	0.84
15:O:87:ILE:CG2	15:O:88:ARG:H	1.89	0.84
1:A:1191:A:P	3:C:3:ASN:HD21	2.00	0.84
5:E:51:VAL:HB	5:E:52:PRO:HD3	1.59	0.84
1:A:243:A:C4'	1:A:244:U:H5'	2.07	0.84
1:A:328:C:O2	1:A:328:C:H2'	1.76	0.84
1:A:579:G:H5'	1:A:728:A:H1'	1.58	0.84
5:E:11:ILE:HB	5:E:31:LEU:HB3	1.60	0.84
13:M:3:ARG:HD3	13:M:9:ILE:HG23	1.58	0.84
7:G:46:ALA:O	7:G:50:ILE:HG12	1.78	0.84
15:O:10:LYS:HD3	15:O:10:LYS:C	2.03	0.84
10:J:4:ILE:HA	10:J:100:THR:HA	1.59	0.84
18:R:19:LYS:HG3	18:R:20:ALA:H	1.41	0.84
7:G:146:GLU:HG2	7:G:149:ARG:HH21	1.42	0.84
8:H:82:HIS:HD2	8:H:138:TRP:NE1	1.76	0.84
2:B:223:ILE:HD12	2:B:224:GLN:N	1.93	0.83
6:F:22:GLU:OE2	6:F:82:ARG:HD3	1.78	0.83
8:H:29:SER:OG	8:H:32:LYS:HB2	1.78	0.83
10:J:38:ILE:HD11	10:J:71:LEU:HD12	1.61	0.83
13:M:11:ARG:HG3	13:M:12:ASN:N	1.91	0.83
1:A:1366:C:H2'	1:A:1367:C:H6	1.42	0.83
5:E:50:GLU:HG3	5:E:52:PRO:HD2	1.59	0.83
8:H:24:THR:HG22	8:H:63:LEU:HD21	1.61	0.83
6:F:67:MET:HB2	6:F:68:PRO:HD2	1.61	0.82
12:L:27:LEU:O	12:L:29:GLY:N	2.12	0.82
18:R:87:ARG:O	18:R:88:LYS:HB2	1.78	0.82
1:A:1133:G:H2'	1:A:1134:G:H8	1.44	0.82
19:S:33:THR:HG22	19:S:35:SER:H	1.43	0.82
1:A:129(A):G:O2'	1:A:189(F):U:H2'	1.78	0.82
1:A:1116:C:H2'	1:A:1117:G:H5''	1.59	0.82
7:G:75:VAL:CG2	7:G:86:GLN:HB3	2.09	0.82
9:I:93:ARG:HB3	9:I:93:ARG:HH11	1.41	0.82
11:K:124:LYS:HD2	11:K:125:PHE:CE1	2.14	0.82
10:J:32:ALA:H	10:J:78:ASN:ND2	1.78	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:67:LYS:HA	17:Q:70:ARG:HH12	1.42	0.82
1:A:1532:U:H2'	1:A:1533:C:H3'	1.61	0.81
3:C:14:ILE:O	3:C:16:ARG:N	2.13	0.81
9:I:97:LYS:HG2	9:I:102:LEU:HD21	1.60	0.81
1:A:250:A:H4'	1:A:251:G:O5'	1.81	0.81
9:I:8:GLY:HA2	9:I:79:LEU:HD13	1.60	0.81
2:B:87:ARG:NH1	2:B:233:SER:HB2	1.96	0.81
10:J:99:LYS:HD3	10:J:100:THR:H	1.45	0.81
12:L:74:GLY:O	12:L:75:HIS:HB3	1.80	0.81
10:J:3:LYS:HA	10:J:76:ASN:H	1.45	0.81
20:T:45:GLN:HB2	20:T:91:LEU:HD13	1.63	0.81
12:L:38:THR:HG22	12:L:39:VAL:HG23	1.63	0.81
1:A:975:A:H5'	1:A:975:A:H8	1.46	0.80
1:A:243:A:H4'	1:A:244:U:C5'	2.10	0.80
3:C:8:ILE:HG23	3:C:16:ARG:HG2	1.63	0.80
7:G:23:VAL:O	7:G:27:ILE:HG12	1.80	0.80
7:G:111:ARG:HB3	7:G:113:GLU:OE2	1.82	0.80
2:B:78:GLN:HG3	2:B:94:ASN:OD1	1.80	0.80
13:M:120:LYS:NZ	13:M:122:LYS:HB3	1.97	0.80
1:A:1228:C:H4'	13:M:116:THR:HA	1.61	0.80
3:C:14:ILE:HG22	3:C:15:THR:N	1.94	0.80
1:A:1116:C:C2'	1:A:1117:G:H5''	2.10	0.80
6:F:2:ARG:HE	6:F:69:GLU:HG2	1.45	0.80
10:J:82:ILE:O	10:J:86:MET:HB2	1.82	0.79
12:L:25:PRO:C	12:L:27:LEU:H	1.89	0.79
15:O:54:ARG:HG2	15:O:54:ARG:HH11	1.48	0.79
15:O:64:ARG:NH1	15:O:64:ARG:HB3	1.97	0.79
2:B:17:PHE:HB3	2:B:44:LEU:HD21	1.63	0.79
9:I:65:VAL:HG11	9:I:73:GLN:HB3	1.64	0.79
1:A:1054:C:O2	1:A:1054:C:H3'	1.82	0.79
1:A:1047:G:C2'	1:A:1048:G:H5''	2.13	0.79
3:C:19:GLU:HG2	3:C:54:ARG:HE	1.46	0.79
20:T:56:MET:HE2	20:T:88:VAL:HG11	1.64	0.79
1:A:1366:C:H2'	1:A:1367:C:C6	2.18	0.78
10:J:80:LYS:HA	10:J:83:GLU:OE2	1.83	0.78
1:A:1250:A:H4'	9:I:68:GLY:N	1.98	0.78
2:B:97:TRP:HZ2	2:B:102:LEU:HD13	1.47	0.78
3:C:119:ARG:HG3	3:C:119:ARG:HH11	1.48	0.78
2:B:15:VAL:HG11	2:B:209:ARG:HB2	1.65	0.78
2:B:142:LEU:HG	2:B:146:GLN:HE21	1.49	0.78
6:F:15:ASP:H	6:F:18:GLN:NE2	1.82	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:1:MET:HE3	6:F:66:GLU:HG2	1.64	0.78
10:J:6:ILE:HG22	10:J:98:ILE:HA	1.64	0.78
1:A:664:G:H22	1:A:741:G:H1	1.30	0.78
1:A:1026:G:H2'	1:A:1027:C:H5''	1.66	0.77
10:J:5:ARG:HA	10:J:73:ASP:OD1	1.83	0.77
17:Q:96:GLU:O	17:Q:102:GLY:HA2	1.84	0.77
1:A:351:G:H4'	1:A:352:C:OP1	1.84	0.77
2:B:204:ASN:C	2:B:204:ASN:HD22	1.90	0.77
3:C:123:GLN:O	3:C:128:PHE:HB2	1.84	0.77
17:Q:101:ARG:HA	17:Q:101:ARG:HE	1.49	0.77
12:L:53:ARG:HG2	12:L:69:TYR:HE1	1.50	0.77
18:R:19:LYS:CG	18:R:20:ALA:H	1.98	0.77
10:J:32:ALA:CB	10:J:75:ILE:HG13	2.12	0.76
20:T:73:HIS:O	20:T:74:LYS:CB	2.31	0.76
1:A:377:G:OP1	16:P:3:LYS:HD3	1.85	0.76
6:F:80:ARG:NH1	6:F:88:VAL:HB	2.01	0.76
8:H:60:ARG:HH11	8:H:60:ARG:HG3	1.50	0.76
15:O:6:GLU:H	15:O:6:GLU:CD	1.93	0.76
8:H:51:VAL:HG11	8:H:60:ARG:HH11	1.51	0.76
12:L:47:LYS:HB3	12:L:48:PRO:CD	2.15	0.76
1:A:1048:G:H5'	1:A:1048:G:H8	1.48	0.76
1:A:1132:C:H2'	1:A:1133:G:H8	1.50	0.76
3:C:107:GLN:HE21	3:C:107:GLN:H	1.32	0.76
5:E:12:LEU:HD13	5:E:31:LEU:HB2	1.68	0.76
1:A:371:G:O2'	1:A:372:C:H5'	1.85	0.76
7:G:140:ASP:HA	7:G:143:ARG:NH1	2.01	0.76
1:A:235:C:H5'	17:Q:70:ARG:HG2	1.68	0.76
1:A:1047:G:H2'	1:A:1048:G:H5''	1.65	0.76
6:F:33:TYR:HA	6:F:71:ARG:HH21	1.49	0.76
17:Q:68:ARG:H	17:Q:70:ARG:NH1	1.84	0.76
13:M:10:PRO:HB2	13:M:18:ALA:HB1	1.66	0.75
2:B:19:HIS:HD2	2:B:189:ASP:OD1	1.70	0.75
3:C:91:LEU:HD11	3:C:99:VAL:CG2	2.17	0.75
3:C:107:GLN:H	3:C:107:GLN:NE2	1.84	0.75
17:Q:63:ARG:O	17:Q:65:ILE:HD12	1.86	0.75
12:L:41:ARG:HG2	12:L:42:THR:H	1.50	0.75
13:M:54:VAL:O	13:M:58:GLU:HG2	1.86	0.75
1:A:438:G:H4'	1:A:439:A:OP1	1.87	0.75
5:E:74:GLY:CA	5:E:116:THR:HG22	2.17	0.75
15:O:33:THR:HG23	15:O:63:ARG:HH12	1.51	0.75
19:S:36:ARG:HH21	19:S:53:ASN:HA	1.49	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:51:LEU:HD22	2:B:55:PHE:CE1	2.21	0.75
2:B:80:ILE:HD11	2:B:208:ILE:HG22	1.67	0.75
3:C:60:ALA:HB3	3:C:63:ASN:HD22	1.51	0.75
21:U:14:TRP:HZ3	21:U:15:ARG:HH12	1.35	0.75
2:B:181:PHE:CE2	8:H:70:GLN:HB3	2.20	0.75
10:J:49:VAL:O	10:J:60:ARG:O	2.05	0.75
18:R:46:GLU:H	18:R:46:GLU:CD	1.94	0.75
2:B:18:GLY:O	2:B:19:HIS:HB2	1.85	0.75
8:H:120:THR:OG1	8:H:123:GLU:HG3	1.87	0.75
2:B:178:ARG:HH22	8:H:68:ARG:NH2	1.84	0.75
12:L:27:LEU:HG	12:L:28:LYS:H	1.50	0.75
2:B:134:GLU:HG2	2:B:137:ARG:NH2	2.02	0.74
3:C:148:GLY:HA3	3:C:172:ARG:O	1.87	0.74
5:E:150:ARG:HG3	5:E:150:ARG:HH11	1.51	0.74
15:O:16:ALA:HB1	15:O:21:ASP:HB3	1.67	0.74
20:T:50:GLU:HG3	20:T:100:ILE:HB	1.68	0.74
3:C:14:ILE:CG2	3:C:15:THR:H	1.94	0.74
2:B:215:LEU:O	2:B:219:VAL:HG23	1.88	0.74
1:A:939:G:H5''	7:G:102:ARG:NH2	2.02	0.74
11:K:48:ILE:HG22	11:K:49:GLY:H	1.52	0.74
18:R:88:LYS:HB3	18:R:88:LYS:NZ	2.02	0.74
2:B:7:VAL:HG12	2:B:221:LEU:HD23	1.70	0.74
1:A:1030(C):G:H2'	1:A:1030(D):A:C8	2.23	0.74
2:B:218:ALA:O	2:B:222:ILE:HG13	1.88	0.74
6:F:3:ARG:HH11	6:F:3:ARG:HG3	1.52	0.74
10:J:3:LYS:HA	10:J:74:ILE:O	1.87	0.74
13:M:17:VAL:O	13:M:20:THR:HB	1.87	0.74
2:B:98:LEU:O	2:B:101:MET:HG3	1.88	0.74
9:I:97:LYS:HA	9:I:102:LEU:HD21	1.70	0.74
1:A:1181:G:H4'	1:A:1182:G:OP1	1.86	0.74
1:A:1281:U:H5'	1:A:1282:C:H5	1.53	0.74
13:M:15:VAL:HG23	13:M:43:THR:O	1.87	0.74
1:A:443:C:H2'	1:A:444:C:H6	1.53	0.73
3:C:29:TYR:OH	14:N:54:PRO:HD2	1.88	0.73
11:K:126:ARG:O	11:K:127:LYS:HB2	1.86	0.73
19:S:20:LEU:HD12	19:S:21:GLU:N	2.03	0.73
1:A:1022:G:H2'	1:A:1023:G:H8	1.51	0.73
2:B:178:ARG:HH21	2:B:196:LEU:C	1.97	0.73
1:A:673:G:H2'	1:A:674:G:C8	2.23	0.73
15:O:26:GLU:HG3	15:O:81:LEU:HD12	1.70	0.73
12:L:47:LYS:HB3	12:L:48:PRO:HD3	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:39:LEU:HD11	15:O:56:LEU:HB2	1.70	0.73
3:C:58:GLU:HB2	3:C:65:ALA:HB3	1.70	0.73
3:C:64:VAL:N	3:C:99:VAL:HG11	2.03	0.73
15:O:64:ARG:CB	15:O:64:ARG:HH11	2.02	0.73
1:A:1369:C:H2'	1:A:1370:G:C8	2.24	0.73
6:F:4:TYR:CZ	6:F:72:VAL:HG21	2.24	0.73
19:S:5:LEU:O	19:S:6:LYS:HB2	1.89	0.73
1:A:1047:G:H2'	1:A:1048:G:C5'	2.18	0.73
3:C:108:ASN:HD21	3:C:144:SER:HB3	1.54	0.73
6:F:14:LEU:HA	6:F:18:GLN:NE2	2.03	0.72
7:G:69:VAL:HG21	7:G:104:LEU:HD21	1.71	0.72
7:G:129:GLU:CD	7:G:131:LYS:HE2	2.14	0.72
9:I:118:LYS:O	9:I:119:ALA:HB3	1.89	0.72
16:P:57:ARG:HG2	16:P:57:ARG:HH11	1.52	0.72
17:Q:3:LYS:HB3	17:Q:61:GLU:HB2	1.71	0.72
11:K:126:ARG:O	11:K:127:LYS:HE2	1.89	0.72
13:M:124:PRO:HB3	13:M:126:LYS:HE2	1.70	0.72
12:L:28:LYS:O	12:L:29:GLY:C	2.30	0.72
14:N:14:PRO:O	14:N:15:LYS:HB2	1.87	0.72
17:Q:68:ARG:N	17:Q:70:ARG:NH1	2.37	0.72
1:A:1060:C:C5	3:C:2:GLY:HA3	2.24	0.72
2:B:21:ARG:HH12	2:B:23:ARG:HG2	1.54	0.72
11:K:11:LYS:HD2	11:K:11:LYS:O	1.89	0.72
20:T:56:MET:HG3	20:T:84:LEU:HD22	1.71	0.72
1:A:1492:A:OP1	12:L:47:LYS:N	2.20	0.72
9:I:70:LYS:O	9:I:74:ILE:HG13	1.89	0.72
13:M:90:LEU:HD22	13:M:94:ARG:NH1	2.05	0.72
2:B:60:ASP:C	2:B:64:ARG:HH12	1.98	0.71
5:E:92:LYS:HB3	5:E:119:LEU:HB2	1.70	0.71
1:A:1086:U:H3	1:A:1099:G:H22	1.38	0.71
7:G:54:THR:HG22	7:G:56:GLN:H	1.53	0.71
1:A:1356:G:H2'	1:A:1357:A:C8	2.24	0.71
6:F:26:ILE:O	6:F:30:LEU:HG	1.90	0.71
7:G:64:GLN:HE21	7:G:68:ASN:ND2	1.88	0.71
8:H:51:VAL:HG11	8:H:60:ARG:NH1	2.06	0.71
3:C:102:ASN:N	3:C:102:ASN:HD22	1.86	0.71
7:G:16:LEU:HD22	7:G:16:LEU:N	2.04	0.71
10:J:49:VAL:O	10:J:60:ARG:HA	1.90	0.71
12:L:75:HIS:CD2	12:L:77:LEU:H	2.08	0.71
2:B:97:TRP:CZ2	2:B:102:LEU:HD13	2.25	0.71
3:C:110:ASN:ND2	3:C:140:ARG:HB3	2.06	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1027:C:H42	1:A:1034:G:H1	1.38	0.71
1:A:759:A:H61	17:Q:94:ASN:HD21	1.36	0.71
5:E:88:LYS:HB3	5:E:123:LEU:HB2	1.71	0.71
1:A:818:G:O2'	1:A:819:A:H5''	1.91	0.71
4:D:189:PRO:HB2	4:D:194:LEU:HD21	1.72	0.71
10:J:99:LYS:CD	10:J:100:THR:H	2.03	0.71
10:J:3:LYS:CA	10:J:76:ASN:H	2.03	0.71
10:J:7:LYS:HD3	10:J:9:ARG:HH22	1.55	0.71
13:M:36:LYS:HB2	13:M:59:TYR:CE2	2.22	0.71
15:O:56:LEU:HA	15:O:59:MET:HE2	1.71	0.71
1:A:1054:C:H2'	1:A:1055:A:H5''	1.73	0.70
10:J:61:GLU:OE1	14:N:45:ARG:NH1	2.21	0.70
13:M:11:ARG:HG3	13:M:12:ASN:H	1.55	0.70
17:Q:67:LYS:CA	17:Q:70:ARG:HH12	2.03	0.70
11:K:22:HIS:HB3	11:K:29:ILE:HG23	1.71	0.70
1:A:1125:U:H3	10:J:5:ARG:HH21	1.36	0.70
7:G:140:ASP:HA	7:G:143:ARG:HH11	1.56	0.70
8:H:90:GLY:O	8:H:91:ARG:HB2	1.92	0.70
17:Q:40:LYS:HD2	17:Q:42:TYR:CZ	2.26	0.70
12:L:60:LEU:HD21	12:L:66:VAL:HG22	1.74	0.70
18:R:19:LYS:HG3	18:R:20:ALA:N	2.06	0.70
8:H:119:LEU:HD12	8:H:124:ALA:HA	1.74	0.70
2:B:111:ARG:HB3	2:B:149:LEU:HD11	1.73	0.70
10:J:49:VAL:CG2	14:N:41:ARG:HB2	2.19	0.70
1:A:1117:G:H5'	1:A:1117:G:H8	1.54	0.70
1:A:35:G:H2'	1:A:36:C:C6	2.27	0.70
1:A:1305:G:N2	1:A:1331:G:O2'	2.24	0.70
5:E:74:GLY:HA3	5:E:116:THR:CG2	2.22	0.70
5:E:89:ILE:HD13	5:E:90:VAL:H	1.57	0.70
1:A:620:C:N1	4:D:135:LEU:HD13	2.07	0.70
1:A:1132:C:H2'	1:A:1133:G:C8	2.27	0.69
6:F:21:LEU:O	6:F:24:GLU:HG3	1.92	0.69
1:A:946:A:H2'	1:A:947:G:C8	2.27	0.69
1:A:1142:G:H2'	1:A:1143:G:O4'	1.92	0.69
5:E:80:ILE:HD12	5:E:80:ILE:H	1.57	0.69
15:O:64:ARG:HB3	15:O:64:ARG:HH11	1.57	0.69
4:D:31:CYS:C	4:D:33:MET:H	1.99	0.69
20:T:14:LYS:O	20:T:18:GLN:HG3	1.92	0.69
1:A:1425:U:H2'	1:A:1426:C:C6	2.28	0.69
2:B:80:ILE:HD13	2:B:212:GLN:HB2	1.75	0.69
10:J:64:GLU:HG2	14:N:59:ALA:HB2	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:853:G:O2'	1:A:854:G:H5'	1.93	0.69
1:A:1039:C:H2'	1:A:1040:U:C6	2.26	0.69
2:B:189:ASP:HB2	2:B:205:ASP:OD2	1.91	0.69
4:D:162:LEU:HD13	4:D:181:MET:HG2	1.74	0.69
8:H:10:LEU:HD22	8:H:83:ILE:HD11	1.74	0.69
21:U:6:ARG:HE	21:U:15:ARG:NE	1.90	0.69
1:A:384:G:H2'	1:A:385:C:C6	2.28	0.69
2:B:165:VAL:HG23	2:B:166:ASP:H	1.57	0.69
1:A:1189:C:P	10:J:51:ARG:HH22	2.16	0.69
1:A:1397:C:H4'	1:A:1398:A:OP2	1.91	0.69
4:D:3:ARG:HH11	4:D:115:ARG:HD2	1.58	0.69
9:I:24:GLY:HA2	9:I:59:PHE:O	1.93	0.69
16:P:57:ARG:NH1	16:P:79:VAL:O	2.25	0.69
17:Q:27:PHE:CZ	17:Q:36:ILE:HD11	2.27	0.69
1:A:1038:C:H2'	1:A:1039:C:C6	2.28	0.68
2:B:204:ASN:HD22	2:B:205:ASP:N	1.90	0.68
3:C:70:VAL:HG12	3:C:71:ALA:N	2.07	0.68
1:A:912:C:O2'	1:A:913:A:H5'	1.93	0.68
13:M:49:THR:HG22	13:M:51:ALA:N	2.06	0.68
14:N:57:ARG:HG2	14:N:58:LYS:N	2.08	0.68
15:O:39:LEU:CD1	15:O:56:LEU:HB2	2.23	0.68
14:N:23:ARG:NH1	14:N:30:ALA:HB2	2.08	0.68
2:B:55:PHE:HD2	2:B:58:ILE:HD12	1.57	0.68
2:B:219:VAL:HA	2:B:222:ILE:HD12	1.75	0.68
19:S:22:LEU:HD13	19:S:28:LYS:HB3	1.76	0.68
1:A:1095:U:H2'	1:A:1096:C:C6	2.29	0.68
2:B:88:ALA:HB2	2:B:219:VAL:HG13	1.75	0.68
1:A:1497:G:H2'	1:A:1498:U:H5'	1.75	0.68
7:G:113:GLU:HG2	7:G:119:ARG:HG2	1.75	0.68
16:P:28:ARG:HG3	16:P:29:ASP:OD2	1.94	0.68
3:C:6:HIS:HD2	3:C:8:ILE:H	1.42	0.68
7:G:64:GLN:HE21	7:G:68:ASN:HD21	1.38	0.68
11:K:47:VAL:HG12	11:K:48:ILE:HD13	1.74	0.68
14:N:27:CYS:SG	14:N:29:ARG:HB2	2.34	0.68
12:L:70:ILE:HD13	12:L:77:LEU:HD12	1.76	0.68
1:A:1135:U:H4'	1:A:1136:U:H5	1.59	0.67
2:B:178:ARG:HH21	2:B:196:LEU:HA	1.59	0.67
1:A:299:G:H2'	1:A:300:A:C8	2.29	0.67
1:A:344:A:H4'	1:A:345:C:OP2	1.93	0.67
8:H:63:LEU:HD22	8:H:63:LEU:H	1.58	0.67
6:F:46:ARG:HG2	6:F:47:ARG:N	2.09	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:72:LEU:O	20:T:72:LEU:HG	1.94	0.67
9:I:69:GLY:O	9:I:73:GLN:HG3	1.94	0.67
13:M:34:LEU:HD13	13:M:41:PRO:HA	1.76	0.67
18:R:18:ARG:O	18:R:19:LYS:HB3	1.94	0.67
1:A:1052:U:H2'	1:A:1055:A:OP1	1.94	0.67
1:A:1435:G:H2'	1:A:1436:U:C6	2.30	0.67
1:A:1080:A:H5''	5:E:16:THR:HG21	1.76	0.67
2:B:75:LYS:HA	2:B:78:GLN:HB2	1.76	0.67
4:D:146:ILE:N	4:D:146:ILE:HD12	2.09	0.67
8:H:118:VAL:C	8:H:119:LEU:HD23	2.19	0.67
9:I:93:ARG:HH11	9:I:93:ARG:CB	2.08	0.67
12:L:55:VAL:HG12	12:L:56:ALA:N	2.10	0.67
12:L:126:LYS:HD2	12:L:126:LYS:O	1.94	0.67
19:S:13:ASP:HA	19:S:16:LEU:HB3	1.76	0.67
1:A:1024:G:H2'	1:A:1025:U:O4'	1.95	0.67
2:B:60:ASP:HB3	2:B:64:ARG:NH1	2.09	0.67
3:C:77:ILE:O	3:C:83:ARG:HB3	1.95	0.67
1:A:420:U:H2'	1:A:422:C:C5	2.30	0.67
11:K:69:ALA:O	11:K:73:MET:HG2	1.95	0.67
18:R:36:ASN:HD22	18:R:36:ASN:C	2.03	0.67
10:J:9:ARG:HB3	10:J:9:ARG:NH1	2.10	0.67
1:A:1497:G:C2'	1:A:1498:U:H5'	2.25	0.66
4:D:18:LYS:NZ	4:D:31:CYS:HB3	2.09	0.66
2:B:231:GLU:HB3	2:B:232:PRO:HD2	1.76	0.66
5:E:110:LEU:HD13	5:E:118:ILE:HG21	1.76	0.66
7:G:120:ILE:HG22	7:G:124:LEU:HD11	1.75	0.66
21:U:14:TRP:HZ3	21:U:15:ARG:NH1	1.92	0.66
3:C:82:GLU:O	3:C:86:VAL:HG23	1.94	0.66
6:F:14:LEU:HA	6:F:18:GLN:HE21	1.58	0.66
6:F:47:ARG:N	6:F:47:ARG:HD3	2.11	0.66
8:H:17:THR:HB	8:H:78:GLN:OE1	1.95	0.66
1:A:835:U:OP1	18:R:64:ARG:NH2	2.25	0.66
1:A:975:A:H5'	1:A:975:A:C8	2.30	0.66
3:C:13:GLY:HA3	14:N:57:ARG:HH21	1.61	0.66
18:R:87:ARG:HG2	18:R:88:LYS:H	1.61	0.66
21:U:9:ARG:NH1	21:U:22:ARG:HA	2.11	0.66
1:A:254:G:OP1	17:Q:68:ARG:HB3	1.94	0.66
1:A:1539:C:H2'	1:A:1540:U:H5'	1.76	0.66
16:P:43:LYS:HG3	16:P:48:TRP:CD2	2.31	0.66
16:P:67:THR:HG22	16:P:69:THR:H	1.60	0.66
19:S:80:TYR:O	19:S:82:GLY:N	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:909:A:OP1	12:L:21:LYS:HE2	1.96	0.66
1:A:1026:G:C2'	1:A:1027:C:H5''	2.25	0.66
9:I:10:ARG:HD3	9:I:105:ASP:HB3	1.78	0.66
9:I:5:TYR:O	9:I:84:ALA:HA	1.96	0.65
15:O:29:VAL:HG11	15:O:67:LEU:HD21	1.77	0.65
8:H:122:ARG:HB3	8:H:122:ARG:NH1	2.11	0.65
1:A:112:G:H4'	1:A:389:A:H5''	1.77	0.65
1:A:627:G:O2'	1:A:628:G:H5'	1.95	0.65
1:A:1286:A:C8	1:A:1287:A:H4'	2.31	0.65
1:A:1502:A:H2	1:A:1505:G:N1	1.88	0.65
9:I:8:GLY:HA2	9:I:79:LEU:CD1	2.26	0.65
1:A:1004:A:H8	1:A:1036:G:H22	1.44	0.65
5:E:79:GLU:HG3	5:E:93:PRO:CD	2.25	0.65
6:F:97:PHE:HB2	18:R:32:ARG:NH2	2.11	0.65
9:I:31:GLN:O	9:I:32:ASP:HB3	1.94	0.65
14:N:57:ARG:HG2	14:N:58:LYS:H	1.61	0.65
1:A:1323:G:H2'	1:A:1324:A:C8	2.32	0.65
3:C:77:ILE:C	3:C:83:ARG:HB3	2.22	0.65
13:M:57:ARG:HG2	13:M:61:GLU:HG3	1.78	0.65
21:U:15:ARG:HG2	21:U:15:ARG:HH11	1.62	0.65
23:Y:34:CM0:C8	23:Y:34:CM0:O4	2.45	0.65
1:A:407:G:H2'	1:A:408:A:H8	1.62	0.65
9:I:106:ALA:O	9:I:108:VAL:HG23	1.97	0.65
12:L:27:LEU:C	12:L:29:GLY:N	2.54	0.65
13:M:99:ARG:HG2	13:M:99:ARG:HH11	1.62	0.65
1:A:1026:G:C3'	1:A:1027:C:H5''	2.27	0.65
1:A:1216:G:H5''	14:N:5:ALA:CB	2.27	0.65
11:K:82:VAL:C	11:K:83:ILE:HD12	2.22	0.65
13:M:3:ARG:HA	13:M:8:GLU:O	1.96	0.65
17:Q:27:PHE:CE1	17:Q:36:ILE:HD11	2.32	0.65
1:A:1182:G:O2'	1:A:1183:A:OP2	2.12	0.65
8:H:4:ASP:OD2	8:H:85:ARG:NH1	2.30	0.65
8:H:91:ARG:NH1	17:Q:33:GLY:HA3	2.12	0.65
3:C:64:VAL:H	3:C:99:VAL:CG1	2.09	0.65
9:I:48:GLU:N	9:I:49:PRO:HD2	2.12	0.65
2:B:36:ARG:HB2	2:B:41:ILE:HD11	1.79	0.64
13:M:40:ASN:HD22	13:M:41:PRO:CD	2.09	0.64
3:C:47:LEU:CD2	3:C:68:VAL:HG11	2.27	0.64
4:D:162:LEU:HD13	4:D:181:MET:CG	2.27	0.64
8:H:112:LEU:N	8:H:112:LEU:CD2	2.60	0.64
15:O:39:LEU:HD12	15:O:56:LEU:HD13	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1392:G:N2	1:A:1502:A:H8	1.95	0.64
2:B:126:GLU:HA	2:B:129:GLU:HG3	1.80	0.64
1:A:807:A:H2'	1:A:808:C:C6	2.33	0.64
1:A:1101:A:H4'	1:A:1102:A:O5'	1.95	0.64
2:B:21:ARG:NH1	2:B:23:ARG:HG2	2.12	0.64
2:B:61:LEU:HD21	2:B:160:ASP:CB	2.28	0.64
2:B:161:ALA:HB1	2:B:185:ILE:HD11	1.78	0.64
15:O:17:ARG:HG3	15:O:17:ARG:NH1	2.11	0.64
1:A:370:C:O2'	1:A:371:G:H5'	1.97	0.64
1:A:1241:G:H2'	1:A:1242:C:C6	2.31	0.64
2:B:139:LYS:C	2:B:139:LYS:HD3	2.23	0.64
14:N:9:LYS:HD3	14:N:9:LYS:C	2.22	0.64
15:O:54:ARG:HG2	15:O:54:ARG:NH1	2.13	0.64
2:B:45:GLN:O	2:B:48:MET:HB2	1.98	0.64
5:E:53:LEU:HD23	5:E:53:LEU:H	1.62	0.64
8:H:112:LEU:HD23	8:H:112:LEU:H	1.61	0.64
9:I:3:GLN:HB3	9:I:20:ARG:HG2	1.80	0.64
19:S:44:MET:HE2	19:S:49:ILE:HD11	1.80	0.64
1:A:107:G:C2'	1:A:108:G:H5'	2.28	0.64
1:A:266:G:H5''	1:A:268:C:H41	1.63	0.64
1:A:1201:A:H4'	1:A:1202:G:O5'	1.98	0.64
1:A:248:C:O2'	1:A:249:U:H5'	1.98	0.64
18:R:25:THR:HG22	18:R:42:ARG:HH12	1.61	0.64
1:A:407:G:O2'	4:D:116:GLN:HG3	1.98	0.64
1:A:1039:C:H2'	1:A:1040:U:H6	1.63	0.64
1:A:1330:U:OP1	13:M:23:TYR:O	2.15	0.64
1:A:1499:A:H1'	1:A:1520:G:H5'	1.80	0.64
3:C:110:ASN:O	3:C:111:LEU:HD23	1.97	0.64
4:D:140:VAL:HG11	4:D:146:ILE:HD11	1.80	0.64
5:E:13:ILE:HA	5:E:29:GLY:O	1.97	0.64
13:M:37:THR:HG22	13:M:39:ILE:HG13	1.79	0.64
21:U:9:ARG:HH12	21:U:23:PRO:CD	2.11	0.64
2:B:61:LEU:HD21	2:B:160:ASP:HB3	1.80	0.64
3:C:147:LYS:HE2	3:C:205:GLY:HA2	1.80	0.64
4:D:127:THR:HG23	4:D:147:ALA:HB3	1.80	0.64
1:A:266:G:H5'	1:A:266:G:C8	2.33	0.63
1:A:818:G:C2'	1:A:819:A:H5''	2.28	0.63
8:H:113:SER:HB2	8:H:134:ILE:HD11	1.79	0.63
1:A:390:C:H2'	1:A:391:G:H8	1.63	0.63
1:A:1053:G:C3'	1:A:1054:C:H5'	2.28	0.63
1:A:1054:C:C2'	1:A:1055:A:H5''	2.27	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:204:ASN:C	2:B:204:ASN:ND2	2.54	0.63
3:C:119:ARG:HE	3:C:140:ARG:NE	1.96	0.63
9:I:16:ARG:HB2	9:I:64:THR:HB	1.80	0.63
18:R:88:LYS:HB3	18:R:88:LYS:HZ2	1.63	0.63
23:Y:34:CM0:H2'	23:Y:35:A:C8	2.33	0.63
13:M:11:ARG:CG	13:M:12:ASN:N	2.60	0.63
16:P:43:LYS:HA	16:P:48:TRP:HB3	1.80	0.63
20:T:57:ARG:HH11	20:T:57:ARG:CG	2.12	0.63
20:T:94:ALA:O	20:T:95:ALA:HB2	1.97	0.63
1:A:254:G:OP1	17:Q:67:LYS:O	2.16	0.63
2:B:98:LEU:HD23	2:B:98:LEU:N	2.12	0.63
5:E:8:GLU:HB3	5:E:34:VAL:HG23	1.79	0.63
19:S:15:LEU:HA	19:S:18:LYS:HB3	1.78	0.63
1:A:746:A:O2'	1:A:747:C:H5'	1.97	0.63
10:J:37:PRO:HA	10:J:72:VAL:HG22	1.79	0.63
17:Q:45:HIS:HB3	17:Q:72:ARG:HG2	1.79	0.63
1:A:390:C:H2'	1:A:391:G:C8	2.34	0.63
1:A:457:C:H2'	1:A:458:C:H6	1.62	0.63
2:B:178:ARG:HH21	2:B:196:LEU:CA	2.11	0.63
11:K:41:THR:HG21	11:K:71:LYS:HB3	1.81	0.63
1:A:437:U:H5''	4:D:155:LEU:HD22	1.80	0.63
2:B:181:PHE:CD2	8:H:70:GLN:HB3	2.34	0.63
2:B:206:ASP:O	2:B:207:ALA:HB2	1.99	0.63
13:M:108:ARG:HD3	13:M:114:ARG:NH1	2.14	0.63
16:P:57:ARG:HH11	16:P:57:ARG:CG	2.12	0.63
1:A:1130:A:H3'	1:A:1130:A:OP2	1.99	0.63
3:C:50:ALA:HB1	3:C:70:VAL:CG1	2.20	0.63
1:A:928:G:O2'	1:A:1533:C:OP1	2.17	0.63
2:B:122:PHE:O	2:B:127:ILE:HG12	1.98	0.63
2:B:132:LYS:C	2:B:134:GLU:H	2.03	0.63
1:A:382:A:H2'	1:A:383:A:C8	2.34	0.62
1:A:973:G:H3'	1:A:974:A:H5''	1.81	0.62
1:A:979:C:H2'	1:A:980:C:H5'	1.81	0.62
1:A:1024:G:H3'	1:A:1025:U:H5''	1.79	0.62
2:B:14:GLY:C	2:B:15:VAL:HG22	2.23	0.62
19:S:33:THR:CG2	19:S:35:SER:H	2.12	0.62
1:A:404:U:H2'	1:A:405:U:H6	1.63	0.62
2:B:95:GLN:O	2:B:96:ARG:HD2	1.99	0.62
8:H:60:ARG:HG3	8:H:60:ARG:NH1	2.11	0.62
1:A:677:U:H3	1:A:713:G:H22	1.47	0.62
7:G:120:ILE:H	7:G:120:ILE:HD12	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:115:LYS:C	12:L:117:ARG:H	2.08	0.62
16:P:19:ILE:HG22	16:P:36:ILE:HG13	1.81	0.62
19:S:5:LEU:O	19:S:6:LYS:CB	2.46	0.62
20:T:39:LYS:HD3	20:T:55:ILE:HD13	1.79	0.62
1:A:1068:G:OP2	1:A:1068:G:H8	1.82	0.62
3:C:64:VAL:N	3:C:99:VAL:CG1	2.62	0.62
4:D:58:LEU:CD2	4:D:62:GLN:HG2	2.29	0.62
9:I:84:ALA:O	9:I:87:GLN:HB2	1.99	0.62
20:T:57:ARG:HG2	20:T:57:ARG:NH1	2.13	0.62
1:A:127:G:HO2'	17:Q:2:PRO:N	1.98	0.62
2:B:178:ARG:NH2	8:H:68:ARG:HH22	1.93	0.62
4:D:35:ARG:O	4:D:36:ARG:HB2	1.99	0.62
10:J:26:ALA:O	10:J:85:LEU:HG	1.99	0.62
14:N:43:CYS:SG	27:N:101:ZN:ZN	1.88	0.62
20:T:76:ALA:HA	20:T:79:ARG:NH1	2.15	0.62
1:A:1026:G:H3'	1:A:1027:C:H5''	1.80	0.62
2:B:86:GLU:C	2:B:88:ALA:H	2.08	0.62
2:B:118:LEU:HD23	2:B:118:LEU:C	2.25	0.62
15:O:65:ARG:HH11	15:O:65:ARG:HG2	1.63	0.62
1:A:1412:C:H2'	1:A:1413:A:C8	2.35	0.62
4:D:30:LYS:HB3	4:D:35:ARG:NH2	2.07	0.62
20:T:41:ILE:HD13	20:T:87:LYS:HD2	1.82	0.62
20:T:50:GLU:HA	20:T:100:ILE:CG2	2.26	0.62
1:A:35:G:H2'	1:A:36:C:H6	1.62	0.62
1:A:580:U:H2'	1:A:581:G:O4'	2.00	0.62
10:J:7:LYS:HZ2	10:J:40:LEU:HD11	1.64	0.62
10:J:74:ILE:HD13	10:J:81:THR:HG21	1.82	0.62
13:M:88:ARG:HD2	19:S:3:ARG:HH21	1.64	0.62
1:A:107:G:H2'	1:A:108:G:H5'	1.82	0.62
2:B:60:ASP:CG	2:B:64:ARG:HH22	2.08	0.62
2:B:69:LEU:C	2:B:69:LEU:HD23	2.25	0.62
9:I:11:LYS:O	9:I:11:LYS:HG2	1.99	0.62
20:T:23:ARG:HG2	20:T:23:ARG:HH11	1.65	0.62
2:B:98:LEU:HG	2:B:101:MET:HE3	1.82	0.62
2:B:142:LEU:CG	2:B:146:GLN:HE21	2.12	0.62
3:C:43:LEU:HD12	3:C:68:VAL:HG21	1.82	0.62
5:E:99:GLY:O	5:E:117:ASP:HA	1.99	0.62
5:E:144:THR:HG22	5:E:147:ASP:H	1.64	0.62
18:R:16:PRO:HB2	18:R:18:ARG:HE	1.64	0.62
1:A:1372:U:O2'	1:A:1373:G:H5'	2.00	0.61
6:F:3:ARG:HH11	6:F:3:ARG:CG	2.13	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:44:MET:HA	19:S:47:HIS:HD2	1.64	0.61
20:T:57:ARG:HH11	20:T:57:ARG:HG2	1.64	0.61
1:A:1121:U:H2'	1:A:1122:U:C6	2.34	0.61
3:C:172:ARG:HH12	3:C:174:PRO:HG3	1.64	0.61
4:D:141:ARG:HB2	4:D:141:ARG:HH11	1.65	0.61
10:J:7:LYS:HD3	10:J:9:ARG:NH2	2.15	0.61
10:J:30:SER:HB3	10:J:84:GLN:NE2	2.11	0.61
21:U:12:LYS:HB3	21:U:22:ARG:HD2	1.82	0.61
1:A:15:G:O2'	5:E:24:ARG:HD3	1.99	0.61
1:A:701:C:H5''	1:A:703:G:O4'	2.01	0.61
1:A:1427:U:H2'	1:A:1428:A:C8	2.36	0.61
2:B:114:ARG:NH1	2:B:118:LEU:HD12	2.14	0.61
4:D:32:ALA:C	4:D:34:GLU:H	2.06	0.61
7:G:15:ASP:HB3	7:G:20:ASP:H	1.66	0.61
18:R:86:VAL:HG12	18:R:87:ARG:H	1.65	0.61
20:T:53:LEU:HB2	20:T:100:ILE:CG2	2.30	0.61
1:A:1343:G:H2'	1:A:1344:C:C6	2.34	0.61
2:B:55:PHE:CD2	2:B:58:ILE:HD12	2.34	0.61
3:C:64:VAL:CG2	3:C:99:VAL:HG11	2.27	0.61
5:E:89:ILE:HD13	5:E:90:VAL:N	2.15	0.61
10:J:48:THR:OG1	10:J:62:HIS:CD2	2.53	0.61
11:K:108:ILE:N	11:K:108:ILE:HD12	2.15	0.61
1:A:407:G:H2'	1:A:408:A:C8	2.34	0.61
1:A:984:C:H2'	1:A:985:C:H6	1.65	0.61
1:A:1441:G:H4'	1:A:1442:G:C5	2.35	0.61
2:B:139:LYS:HD3	2:B:139:LYS:O	2.00	0.61
3:C:23:TYR:CD2	3:C:24:ALA:N	2.68	0.61
10:J:31:GLY:HA3	10:J:81:THR:OG1	1.99	0.61
10:J:90:LEU:H	10:J:91:PRO:CD	2.13	0.61
1:A:57:G:H2'	1:A:58:C:C6	2.35	0.61
2:B:60:ASP:C	2:B:64:ARG:NH1	2.58	0.61
12:L:74:GLY:O	12:L:75:HIS:CB	2.49	0.61
1:A:1026:G:H3'	1:A:1027:C:C5'	2.31	0.61
1:A:1121:U:H2'	1:A:1122:U:H6	1.65	0.61
1:A:1342:C:O2'	1:A:1343:G:H5'	2.00	0.61
4:D:24:GLU:OE1	4:D:25:ARG:N	2.26	0.61
4:D:36:ARG:HG2	4:D:38:TYR:OH	2.01	0.61
5:E:6:PHE:CZ	5:E:66:MET:HE2	2.35	0.61
9:I:118:LYS:O	9:I:119:ALA:CB	2.48	0.61
11:K:108:ILE:O	11:K:109:VAL:HG23	2.00	0.61
16:P:34:GLU:OE2	16:P:55:ARG:HD3	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1027:C:N4	1:A:1034:G:H1	1.98	0.61
10:J:4:ILE:O	10:J:73:ASP:HA	2.01	0.61
12:L:27:LEU:HG	12:L:28:LYS:N	2.15	0.61
13:M:81:LEU:HD11	13:M:88:ARG:NH1	2.16	0.61
16:P:67:THR:HG22	16:P:69:THR:N	2.15	0.61
20:T:10:LEU:HD12	20:T:12:ALA:H	1.65	0.61
1:A:1391:U:H2'	1:A:1392:G:C8	2.36	0.61
9:I:125:TYR:CD2	9:I:125:TYR:N	2.69	0.61
10:J:76:ASN:C	10:J:78:ASN:H	2.09	0.61
16:P:74:LEU:O	16:P:79:VAL:HG23	2.01	0.61
19:S:33:THR:HG22	19:S:35:SER:N	2.16	0.61
1:A:1318:A:H5''	19:S:10:PHE:CD1	2.36	0.60
2:B:60:ASP:CB	2:B:64:ARG:HH12	2.12	0.60
5:E:41:VAL:HG13	5:E:113:ALA:HA	1.82	0.60
5:E:81:GLU:HG3	5:E:90:VAL:HG22	1.82	0.60
8:H:119:LEU:HD12	8:H:124:ALA:CA	2.31	0.60
10:J:3:LYS:N	10:J:76:ASN:H	1.99	0.60
20:T:56:MET:CE	20:T:88:VAL:HG11	2.30	0.60
4:D:98:GLU:HG2	4:D:189:PRO:HG3	1.82	0.60
4:D:175:SER:OG	4:D:184:LYS:HB3	2.01	0.60
13:M:15:VAL:HG21	13:M:48:LEU:HD21	1.83	0.60
14:N:26:ARG:O	14:N:26:ARG:HG3	2.00	0.60
1:A:371:G:C2'	1:A:372:C:H5'	2.31	0.60
12:L:90:VAL:HG11	12:L:93:LEU:HG	1.82	0.60
18:R:26:LEU:HD23	18:R:29:PHE:CE2	2.36	0.60
21:U:15:ARG:NH1	21:U:15:ARG:HG2	2.14	0.60
1:A:575:G:OP1	1:A:575:G:H4'	2.01	0.60
1:A:1054:C:O2	1:A:1054:C:C3'	2.49	0.60
1:A:1320:C:O2	19:S:36:ARG:NH1	2.35	0.60
5:E:76:ILE:HG22	5:E:78:HIS:O	2.00	0.60
10:J:34:VAL:HG12	10:J:36:GLY:H	1.66	0.60
10:J:57:LYS:HE2	10:J:60:ARG:NH2	2.16	0.60
13:M:40:ASN:HB3	13:M:43:THR:HG23	1.84	0.60
2:B:8:LYS:O	2:B:9:GLU:HB2	2.02	0.60
9:I:37:PHE:HB3	9:I:43:ALA:HB2	1.84	0.60
14:N:45:ARG:HH11	14:N:45:ARG:HG3	1.66	0.60
15:O:55:GLY:HA2	15:O:58:MET:CE	2.28	0.60
1:A:1022:G:H2'	1:A:1023:G:C8	2.35	0.60
21:U:14:TRP:CZ3	21:U:15:ARG:NH1	2.70	0.60
1:A:353:A:H5'	1:A:353:A:H8	1.67	0.60
1:A:1238:A:H5'	1:A:1336:C:H41	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:3:ARG:NH1	4:D:115:ARG:HB3	2.17	0.60
4:D:30:LYS:C	4:D:32:ALA:H	2.10	0.60
5:E:116:THR:HG23	5:E:117:ASP:OD2	2.01	0.60
12:L:75:HIS:H	12:L:102:ARG:HH22	1.49	0.60
14:N:9:LYS:C	14:N:11:LYS:H	2.10	0.60
1:A:1347:G:N2	1:A:1373:G:H2'	2.17	0.60
2:B:31:TYR:HE1	2:B:200:ILE:HD13	1.67	0.60
2:B:213:LEU:HD22	2:B:214:ILE:HD13	1.83	0.60
5:E:90:VAL:O	5:E:120:THR:HA	2.01	0.60
6:F:44:GLY:O	6:F:60:PHE:N	2.31	0.60
6:F:46:ARG:HG2	6:F:47:ARG:H	1.65	0.60
14:N:29:ARG:HG2	14:N:29:ARG:HH11	1.66	0.60
17:Q:59:ILE:HG23	17:Q:71:PHE:HB3	1.83	0.60
1:A:444:C:H2'	1:A:444:C:O2	2.01	0.60
9:I:113:LYS:H	9:I:119:ALA:HA	1.66	0.60
10:J:90:LEU:N	10:J:91:PRO:CD	2.65	0.60
20:T:23:ARG:HG2	20:T:23:ARG:NH1	2.17	0.60
8:H:63:LEU:HD22	8:H:63:LEU:N	2.17	0.60
9:I:99:LEU:HB3	9:I:101:PHE:CE1	2.37	0.60
1:A:201:C:O2'	1:A:202:U:H3'	2.01	0.59
1:A:1053:G:H3'	1:A:1054:C:H5'	1.83	0.59
4:D:199:ASN:HD21	4:D:201:GLN:HB2	1.67	0.59
14:N:8:GLU:OE1	14:N:8:GLU:C	2.45	0.59
17:Q:40:LYS:HD2	17:Q:42:TYR:CE1	2.36	0.59
20:T:43:LEU:HD11	20:T:55:ILE:HD12	1.84	0.59
1:A:287:U:O2'	1:A:288:A:H5'	2.01	0.59
1:A:1392:G:O2'	1:A:1502:A:H5''	2.01	0.59
8:H:29:SER:OG	8:H:32:LYS:HE3	2.02	0.59
8:H:54:ASP:O	8:H:56:LYS:HD3	2.02	0.59
14:N:9:LYS:HE3	14:N:21:TYR:O	2.02	0.59
1:A:130:A:C8	17:Q:63:ARG:HG3	2.38	0.59
1:A:247:G:OP2	17:Q:99:SER:HB2	2.02	0.59
2:B:23:ARG:HD2	2:B:23:ARG:O	2.02	0.59
5:E:81:GLU:CD	5:E:88:LYS:HE2	2.27	0.59
17:Q:59:ILE:CG2	17:Q:71:PHE:HB3	2.32	0.59
1:A:384:G:H2'	1:A:385:C:H6	1.66	0.59
1:A:1216:G:H5''	14:N:5:ALA:HB2	1.85	0.59
10:J:6:ILE:HG22	10:J:97:GLU:O	2.02	0.59
20:T:13:LEU:H	20:T:13:LEU:HD12	1.66	0.59
1:A:179:A:H2'	1:A:180:U:C6	2.37	0.59
1:A:992:U:H4'	1:A:993:G:O5'	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1032:G:H2'	1:A:1033:G:H8	1.68	0.59
1:A:1287:A:H2'	1:A:1288:A:C8	2.38	0.59
3:C:89:GLU:O	3:C:93:LYS:HG2	2.03	0.59
9:I:26:VAL:HG13	9:I:61:ALA:HB3	1.84	0.59
1:A:105:G:H2'	1:A:106:C:C6	2.38	0.59
1:A:363:A:H62	12:L:28:LYS:HE3	1.68	0.59
1:A:404:U:H2'	1:A:405:U:C6	2.37	0.59
15:O:60:VAL:O	15:O:64:ARG:HG3	2.02	0.59
4:D:3:ARG:HD3	4:D:5:ILE:HD11	1.85	0.59
10:J:99:LYS:HD3	10:J:100:THR:N	2.15	0.59
1:A:1510:U:H2'	1:A:1511:G:C8	2.38	0.59
3:C:111:LEU:HD21	3:C:144:SER:HB2	1.85	0.59
10:J:6:ILE:HD12	10:J:6:ILE:O	2.03	0.59
13:M:73:GLU:O	13:M:76:ALA:HB3	2.03	0.59
1:A:1161:C:H2'	1:A:1162:C:H6	1.68	0.59
4:D:32:ALA:C	4:D:34:GLU:N	2.61	0.59
1:A:1527:C:O2'	1:A:1528:U:H5'	2.03	0.58
2:B:7:VAL:C	2:B:8:LYS:HG3	2.27	0.58
2:B:14:GLY:O	2:B:15:VAL:HG13	2.03	0.58
3:C:188:LEU:CD1	3:C:195:VAL:HG13	2.33	0.58
4:D:189:PRO:HB2	4:D:194:LEU:CD2	2.33	0.58
13:M:124:PRO:CB	13:M:126:LYS:HE2	2.32	0.58
19:S:12:ASP:O	19:S:15:LEU:HD12	2.03	0.58
1:A:56:U:H2'	1:A:57:G:C8	2.38	0.58
1:A:442:C:H42	1:A:492:G:H1	1.49	0.58
1:A:662:G:H2'	1:A:663:A:C8	2.38	0.58
1:A:818:G:C3'	1:A:819:A:H5''	2.32	0.58
1:A:969:A:H61	13:M:126:LYS:CB	2.11	0.58
1:A:1539:C:C2'	1:A:1540:U:H5'	2.34	0.58
5:E:150:ARG:HG3	5:E:150:ARG:NH1	2.18	0.58
7:G:15:ASP:OD2	7:G:16:LEU:N	2.36	0.58
17:Q:5:VAL:HA	17:Q:59:ILE:O	2.03	0.58
19:S:44:MET:HE2	19:S:49:ILE:CD1	2.33	0.58
1:A:539:A:OP1	12:L:114:LYS:HE2	2.03	0.58
1:A:1162:C:H2'	1:A:1163:C:C6	2.39	0.58
5:E:129:ILE:H	5:E:129:ILE:HD12	1.67	0.58
9:I:97:LYS:HB3	9:I:98:PRO:HD3	1.85	0.58
1:A:974:A:OP2	14:N:41:ARG:NH1	2.36	0.58
1:A:1347:G:O2'	1:A:1348:U:P	2.60	0.58
5:E:83:GLU:HG2	5:E:88:LYS:HG3	1.85	0.58
7:G:18:TYR:CD2	7:G:59:LEU:HB2	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:70:GLN:NE2	8:H:70:GLN:HA	2.19	0.58
17:Q:67:LYS:O	17:Q:68:ARG:CB	2.49	0.58
1:A:975:A:H4'	1:A:976:G:C5'	2.29	0.58
13:M:50:GLU:O	13:M:54:VAL:HG23	2.03	0.58
14:N:22:THR:HG23	14:N:33:VAL:CG2	2.33	0.58
1:A:180:U:H2'	1:A:181:G:H5'	1.86	0.58
1:A:1401:G:C2	1:A:1402:C:H1'	2.39	0.58
2:B:87:ARG:HD3	2:B:233:SER:OG	2.02	0.58
8:H:82:HIS:CD2	8:H:138:TRP:NE1	2.66	0.58
2:B:213:LEU:HD23	2:B:213:LEU:C	2.28	0.58
13:M:40:ASN:HD22	13:M:41:PRO:HD2	1.69	0.58
17:Q:69:LYS:C	17:Q:70:ARG:HD2	2.29	0.58
1:A:1128:C:O2'	1:A:1130:A:C8	2.57	0.58
2:B:223:ILE:HD13	2:B:229:VAL:HA	1.86	0.58
3:C:47:LEU:HD23	3:C:68:VAL:HG11	1.86	0.58
10:J:25:GLU:C	10:J:27:ALA:H	2.12	0.58
11:K:57:THR:HG22	11:K:59:TYR:H	1.69	0.58
13:M:33:ALA:O	13:M:37:THR:HB	2.04	0.58
14:N:26:ARG:HH21	14:N:47:LEU:CD2	2.16	0.58
1:A:1392:G:H21	1:A:1502:A:H8	1.50	0.58
10:J:55:LYS:HG3	10:J:56:HIS:N	2.19	0.58
1:A:393:A:O2'	1:A:394:G:H5'	2.04	0.58
1:A:1137:C:H4'	1:A:1138:G:C2	2.38	0.58
7:G:135:VAL:O	7:G:139:GLU:HG3	2.03	0.58
1:A:759:A:H61	17:Q:94:ASN:ND2	2.00	0.57
1:A:977:A:H2'	1:A:978:A:H5'	1.85	0.57
1:A:1277:C:O2'	1:A:1279:A:H8	1.86	0.57
10:J:32:ALA:HB2	10:J:78:ASN:HD21	1.68	0.57
1:A:254:G:O2'	1:A:255:G:H5'	2.05	0.57
1:A:953:G:H5'	1:A:965:A:H61	1.68	0.57
4:D:24:GLU:O	4:D:25:ARG:HB3	2.04	0.57
13:M:37:THR:HG23	13:M:55:ARG:HD2	1.84	0.57
15:O:33:THR:HG23	15:O:63:ARG:NH1	2.17	0.57
16:P:57:ARG:HH12	16:P:79:VAL:HA	1.69	0.57
18:R:34:TYR:CD1	18:R:35:ARG:HG3	2.39	0.57
2:B:21:ARG:HH11	2:B:21:ARG:HG3	1.69	0.57
10:J:46:ARG:HG2	10:J:46:ARG:NH1	2.14	0.57
11:K:21:ILE:HD13	11:K:94:ALA:HB3	1.86	0.57
16:P:10:GLY:HA3	16:P:14:ASN:O	2.04	0.57
1:A:954:G:H4'	13:M:120:LYS:CB	2.33	0.57
1:A:998:G:O2'	1:A:999:C:H5'	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1160:G:O2'	1:A:1161:C:H5'	2.04	0.57
2:B:12:GLU:HA	2:B:12:GLU:OE2	2.04	0.57
2:B:230:VAL:HG12	2:B:231:GLU:N	2.19	0.57
8:H:82:HIS:CE1	8:H:84:ARG:HB2	2.39	0.57
12:L:27:LEU:C	12:L:29:GLY:H	2.12	0.57
1:A:309:G:O2'	1:A:310:G:H5'	2.04	0.57
11:K:120:ARG:HH11	11:K:120:ARG:HG2	1.69	0.57
13:M:14:ARG:HB3	13:M:14:ARG:HH11	1.68	0.57
21:U:6:ARG:HH21	21:U:15:ARG:HE	1.52	0.57
1:A:1262:C:H2'	1:A:1263:C:H6	1.67	0.57
2:B:76:GLN:HB3	2:B:208:ILE:HD13	1.86	0.57
3:C:119:ARG:HG3	3:C:119:ARG:NH1	2.14	0.57
5:E:80:ILE:HD12	5:E:91:LEU:HB2	1.82	0.57
10:J:16:LEU:HD13	10:J:70:ARG:HG2	1.85	0.57
1:A:166:G:O2'	1:A:167:G:H5'	2.04	0.57
2:B:25:ASN:HD22	2:B:25:ASN:C	2.11	0.57
2:B:47:THR:HA	2:B:202:PRO:HG2	1.86	0.57
5:E:60:TYR:CE1	5:E:64:ARG:CZ	2.88	0.57
8:H:20:TYR:CE1	8:H:76:PRO:HG2	2.40	0.57
10:J:32:ALA:H	10:J:78:ASN:HD21	1.52	0.57
13:M:23:TYR:O	13:M:25:ILE:N	2.37	0.57
1:A:176:C:H2'	1:A:177:C:H6	1.69	0.57
1:A:1152:A:H2'	1:A:1153:C:C6	2.39	0.57
1:A:1161:C:H2'	1:A:1162:C:C6	2.40	0.57
1:A:1300:G:O2'	1:A:1301:U:H6	1.88	0.57
3:C:112:SER:O	3:C:116:VAL:HG23	2.03	0.57
4:D:94:LEU:HA	4:D:97:LEU:HD12	1.87	0.57
10:J:4:ILE:HD11	10:J:74:ILE:CD1	2.29	0.57
1:A:539:A:H2'	1:A:540:G:C8	2.40	0.57
1:A:1040:U:H2'	1:A:1041:A:C8	2.40	0.57
1:A:1218:C:H2'	1:A:1219:U:C6	2.40	0.57
6:F:101:ALA:HB1	18:R:28:GLU:OE1	2.04	0.57
8:H:85:ARG:NE	8:H:87:SER:O	2.37	0.57
10:J:44:VAL:HG22	10:J:66:ARG:HE	1.70	0.57
10:J:85:LEU:O	10:J:87:THR:N	2.37	0.57
12:L:41:ARG:HG2	12:L:42:THR:N	2.20	0.57
15:O:24:SER:OG	15:O:27:VAL:HG23	2.05	0.57
1:A:1038:C:H2'	1:A:1039:C:H6	1.70	0.57
1:A:1066:C:C2'	1:A:1067:A:H5'	2.34	0.57
2:B:165:VAL:HG23	2:B:166:ASP:N	2.19	0.57
2:B:212:GLN:NE2	2:B:216:SER:HB3	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:11:ARG:NH1	3:C:177:THR:O	2.38	0.57
4:D:63:LYS:HD2	4:D:198:VAL:HG22	1.86	0.57
8:H:20:TYR:HE2	8:H:75:ARG:HD2	1.69	0.57
1:A:21:G:H2'	1:A:22:G:C8	2.40	0.56
1:A:629:G:H2'	1:A:630:G:O4'	2.05	0.56
1:A:1014:A:C2	1:A:1219:U:H1'	2.39	0.56
2:B:223:ILE:HD12	2:B:224:GLN:H	1.70	0.56
4:D:70:ILE:HG22	4:D:71:SER:O	2.04	0.56
9:I:48:GLU:HA	9:I:51:ARG:HH11	1.70	0.56
15:O:27:VAL:HG12	15:O:31:LEU:HD22	1.87	0.56
1:A:1480:G:H2'	1:A:1481:U:C6	2.40	0.56
3:C:172:ARG:HB3	3:C:172:ARG:HH11	1.70	0.56
10:J:7:LYS:HZ2	10:J:71:LEU:HD23	1.68	0.56
13:M:81:LEU:CD1	13:M:88:ARG:HD3	2.36	0.56
1:A:189(G):G:H4'	1:A:189(H):G:OP2	2.03	0.56
1:A:977:A:C2'	1:A:978:A:H5'	2.35	0.56
1:A:1305:G:H5'	21:U:4:GLY:HA3	1.88	0.56
2:B:72:GLY:HA2	2:B:165:VAL:CG2	2.36	0.56
2:B:74:LYS:O	2:B:74:LYS:HG2	2.04	0.56
6:F:3:ARG:NH1	6:F:38:GLU:OE1	2.38	0.56
7:G:79:ARG:HB3	7:G:84:ASN:OD1	2.06	0.56
7:G:120:ILE:HG22	7:G:124:LEU:CD1	2.36	0.56
9:I:53:VAL:CG2	9:I:85:LEU:HD21	2.30	0.56
13:M:78:ILE:O	13:M:82:MET:HG3	2.05	0.56
1:A:838:G:H2'	1:A:839:U:H5''	1.87	0.56
1:A:1504:G:O2'	1:A:1505:G:OP2	2.20	0.56
2:B:96:ARG:HD2	2:B:96:ARG:N	2.19	0.56
2:B:223:ILE:C	2:B:225:ALA:H	2.13	0.56
10:J:4:ILE:HG12	10:J:74:ILE:HB	1.86	0.56
10:J:6:ILE:CD1	10:J:72:VAL:HB	2.36	0.56
17:Q:95:TYR:C	17:Q:97:SER:H	2.14	0.56
1:A:431:A:O2'	1:A:432:A:H5'	2.06	0.56
8:H:20:TYR:CE2	8:H:75:ARG:HD2	2.40	0.56
1:A:431:A:C2'	1:A:432:A:H5'	2.36	0.56
1:A:523:A:H61	12:L:92:ASP:HB2	1.69	0.56
1:A:797:C:OP1	11:K:124:LYS:HE2	2.06	0.56
2:B:68:ILE:HB	2:B:90:MET:HE3	1.87	0.56
5:E:93:PRO:HG2	8:H:105:ARG:NH2	2.21	0.56
10:J:32:ALA:CB	10:J:75:ILE:O	2.53	0.56
2:B:62:ALA:C	2:B:64:ARG:H	2.14	0.56
3:C:195:VAL:C	3:C:196:LEU:HD22	2.31	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:80:GLU:O	4:D:84:LYS:HG3	2.06	0.56
8:H:25:ASP:OD1	8:H:60:ARG:HG2	2.06	0.56
1:A:714:G:H2'	1:A:715:A:C8	2.41	0.56
13:M:120:LYS:HZ2	13:M:122:LYS:HB3	1.70	0.56
1:A:737:A:H2'	1:A:738:C:C6	2.40	0.56
1:A:1355:G:O2'	1:A:1356:G:H5'	2.06	0.56
5:E:11:ILE:HG23	5:E:105:VAL:HG22	1.88	0.56
18:R:36:ASN:C	18:R:36:ASN:ND2	2.63	0.56
1:A:983:A:H5'	1:A:984:C:OP2	2.06	0.55
1:A:1148:U:H2'	1:A:1149:C:O4'	2.06	0.55
3:C:108:ASN:ND2	3:C:144:SER:HB3	2.20	0.55
17:Q:26:GLN:O	17:Q:27:PHE:HB3	2.05	0.55
1:A:1136:U:H5''	1:A:1137:C:OP2	2.07	0.55
2:B:12:GLU:C	2:B:14:GLY:H	2.14	0.55
5:E:13:ILE:C	5:E:13:ILE:HD12	2.31	0.55
20:T:10:LEU:HD12	20:T:10:LEU:C	2.32	0.55
1:A:865:A:H5'	1:A:1078:U:O4	2.05	0.55
8:H:28:ALA:HB2	8:H:59:LEU:HG	1.88	0.55
18:R:86:VAL:HG12	18:R:87:ARG:N	2.20	0.55
19:S:62:ILE:HA	19:S:66:MET:SD	2.46	0.55
1:A:109:A:H2'	1:A:326:G:N2	2.21	0.55
1:A:1075:C:H5'	2:B:103:THR:HG21	1.87	0.55
10:J:8:LEU:HB3	10:J:16:LEU:HD22	1.87	0.55
11:K:33:THR:HB	11:K:38:ASN:O	2.05	0.55
11:K:84:VAL:HG11	11:K:91:ARG:HD3	1.88	0.55
17:Q:59:ILE:HG22	17:Q:71:PHE:CD1	2.41	0.55
19:S:18:LYS:O	19:S:22:LEU:HG	2.06	0.55
1:A:1032:G:H2'	1:A:1033:G:C8	2.40	0.55
2:B:50:GLU:HB3	2:B:200:ILE:O	2.06	0.55
6:F:21:LEU:O	6:F:25:ILE:HG13	2.07	0.55
16:P:21:VAL:HG21	16:P:59:TRP:CD1	2.41	0.55
18:R:32:ARG:HA	18:R:69:THR:HG21	1.87	0.55
1:A:1423:G:O2'	1:A:1424:C:H5'	2.07	0.55
3:C:193:TYR:HE1	3:C:196:LEU:HD21	1.70	0.55
4:D:62:GLN:HE22	4:D:65:ARG:HH12	1.55	0.55
7:G:149:ARG:HD2	11:K:59:TYR:CE1	2.41	0.55
9:I:7:THR:O	9:I:8:GLY:O	2.25	0.55
12:L:34:ARG:O	12:L:61:THR:HG23	2.06	0.55
1:A:194:C:H2'	1:A:195:A:H5''	1.89	0.55
1:A:1333:A:H2'	1:A:1334:G:O4'	2.07	0.55
4:D:36:ARG:C	4:D:38:TYR:H	2.14	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:126:ARG:HG3	5:E:126:ARG:HH11	1.71	0.55
1:A:757:U:H2'	1:A:758:G:O4'	2.06	0.55
1:A:1325:C:P	21:U:6:ARG:NH2	2.80	0.55
1:A:353:A:H5'	1:A:353:A:C8	2.42	0.55
1:A:551:U:H2'	1:A:552:U:C6	2.41	0.55
1:A:781:A:H2'	1:A:782:A:H5'	1.89	0.55
6:F:23:LYS:NZ	6:F:42:GLU:OE2	2.30	0.55
15:O:82:ILE:O	15:O:86:GLY:N	2.40	0.55
1:A:153:C:O2'	1:A:154:C:H5'	2.06	0.55
1:A:410:G:H2'	1:A:429:U:C5	2.42	0.55
1:A:639:G:O2'	1:A:640:A:H5'	2.07	0.55
2:B:162:ILE:HG23	2:B:164:VAL:HG23	1.89	0.55
3:C:22:TRP:CE3	3:C:22:TRP:O	2.60	0.55
4:D:30:LYS:CB	4:D:35:ARG:HH21	2.10	0.55
10:J:29:ARG:HG3	10:J:84:GLN:HE22	1.71	0.55
12:L:75:HIS:HD2	12:L:77:LEU:H	1.55	0.55
15:O:81:LEU:O	15:O:81:LEU:HD23	2.07	0.55
18:R:43:PHE:C	18:R:51:LEU:HD12	2.32	0.55
1:A:390:C:O3'	16:P:28:ARG:NH2	2.40	0.54
1:A:1040:U:H2'	1:A:1041:A:H8	1.72	0.54
2:B:118:LEU:HD22	2:B:142:LEU:CD1	2.27	0.54
1:A:269:C:H2'	1:A:270:A:C8	2.43	0.54
1:A:338:A:H2	1:A:351:G:H22	1.54	0.54
1:A:1054:C:O2'	1:A:1055:A:H5''	2.07	0.54
2:B:49:GLU:O	2:B:52:GLU:HB3	2.06	0.54
5:E:10:MET:SD	5:E:13:ILE:HG23	2.47	0.54
10:J:60:ARG:O	10:J:61:GLU:O	2.25	0.54
14:N:23:ARG:HH12	14:N:30:ALA:HB2	1.72	0.54
20:T:67:ALA:O	20:T:73:HIS:ND1	2.40	0.54
1:A:45:U:H2'	1:A:46:G:C8	2.42	0.54
1:A:743:U:H2'	1:A:744:C:C6	2.42	0.54
9:I:9:ARG:HG3	9:I:14:VAL:HG12	1.89	0.54
13:M:5:ALA:O	13:M:6:GLY:C	2.50	0.54
1:A:882:C:O2'	1:A:883:C:H5'	2.07	0.54
2:B:137:ARG:CB	2:B:137:ARG:HH11	2.20	0.54
2:B:137:ARG:HH11	2:B:137:ARG:HB3	1.72	0.54
6:F:8:ILE:HD11	6:F:79:LEU:HD13	1.90	0.54
12:L:56:ALA:HB2	12:L:70:ILE:HD11	1.89	0.54
19:S:51:VAL:O	19:S:58:VAL:HG22	2.08	0.54
20:T:43:LEU:HB2	20:T:52:ALA:HB2	1.89	0.54
1:A:807:A:H2'	1:A:808:C:H6	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1001(A):G:H2'	1:A:1002:G:C8	2.42	0.54
1:A:1226:C:N4	13:M:104:ARG:HG3	2.22	0.54
3:C:164:ARG:HB2	3:C:164:ARG:HH11	1.73	0.54
5:E:144:THR:HG22	5:E:147:ASP:OD2	2.08	0.54
6:F:77:ARG:HD2	6:F:77:ARG:C	2.32	0.54
8:H:86:ILE:HD12	8:H:133:LEU:HD22	1.89	0.54
1:A:142:G:N3	1:A:196:A:H2	2.06	0.54
1:A:328:C:O2	1:A:328:C:C2'	2.49	0.54
1:A:923:A:OP1	5:E:21:ALA:HB2	2.08	0.54
1:A:1499:A:O2'	1:A:1500:A:H5'	2.08	0.54
12:L:26:ALA:O	12:L:27:LEU:O	2.26	0.54
17:Q:17:LYS:HA	17:Q:46:ASP:O	2.08	0.54
17:Q:66:SER:O	17:Q:70:ARG:NH1	2.41	0.54
19:S:4:SER:O	19:S:5:LEU:HG	2.08	0.54
1:A:1062:U:H2'	1:A:1063:C:C6	2.43	0.54
1:A:1325:C:OP2	21:U:6:ARG:NH2	2.36	0.54
4:D:184:LYS:HG2	4:D:186:LEU:HD23	1.88	0.54
13:M:36:LYS:HD2	13:M:59:TYR:OH	2.08	0.54
1:A:738:C:OP1	6:F:92:LYS:HD3	2.08	0.54
2:B:82:ARG:O	2:B:86:GLU:HG3	2.07	0.54
3:C:153:VAL:HG22	3:C:198:VAL:HG22	1.90	0.54
4:D:92:VAL:O	4:D:96:LEU:HD13	2.07	0.54
7:G:73:MET:HE1	7:G:90:GLU:HG2	1.90	0.54
10:J:84:GLN:O	10:J:88:LEU:HD12	2.08	0.54
20:T:89:ARG:O	20:T:93:GLU:HG3	2.07	0.54
1:A:1021:G:H2'	1:A:1022:G:C8	2.43	0.54
2:B:15:VAL:CG1	2:B:209:ARG:HB2	2.37	0.54
3:C:188:LEU:HD11	3:C:195:VAL:HG13	1.89	0.54
4:D:100:ARG:HB3	4:D:102:ASP:OD1	2.08	0.54
9:I:89:ASN:O	9:I:92:TYR:HB2	2.08	0.54
10:J:3:LYS:N	10:J:3:LYS:HD3	2.23	0.54
16:P:20:VAL:HG11	16:P:32:TYR:HB3	1.90	0.54
1:A:718:G:C5'	11:K:117:ASN:ND2	2.67	0.54
1:A:731:G:OP1	1:A:766:A:H1'	2.08	0.54
1:A:1181:G:H2'	1:A:1182:G:C5	2.42	0.54
2:B:43:ASP:OD1	2:B:46:LYS:HG3	2.07	0.54
2:B:178:ARG:NH2	2:B:196:LEU:HA	2.22	0.54
3:C:91:LEU:HD23	3:C:92:ALA:N	2.22	0.54
4:D:120:LEU:HB3	4:D:126:ILE:HD11	1.90	0.54
10:J:75:ILE:O	10:J:76:ASN:CB	2.56	0.54
1:A:477:A:O2'	1:A:479:C:H5'	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1191:A:P	3:C:3:ASN:ND2	2.76	0.53
1:A:1303:C:H2'	1:A:1304:G:H5'	1.89	0.53
3:C:89:GLU:OE2	3:C:93:LYS:HE2	2.08	0.53
5:E:107:ARG:HG2	5:E:108:ALA:N	2.22	0.53
13:M:3:ARG:NH1	13:M:7:VAL:HG12	2.23	0.53
1:A:1481:U:O2'	1:A:1482:G:H5'	2.07	0.53
2:B:19:HIS:NE2	2:B:206:ASP:HB3	2.22	0.53
3:C:87:LEU:C	3:C:89:GLU:N	2.65	0.53
6:F:82:ARG:HB2	6:F:85:VAL:CG2	2.37	0.53
7:G:120:ILE:HD12	7:G:120:ILE:N	2.23	0.53
1:A:948:C:O2'	1:A:949:A:H5'	2.08	0.53
3:C:156:ARG:HD2	3:C:160:ALA:O	2.08	0.53
4:D:35:ARG:O	4:D:36:ARG:CB	2.56	0.53
13:M:45:VAL:HA	13:M:48:LEU:HG	1.91	0.53
18:R:34:TYR:CE1	18:R:35:ARG:HG3	2.44	0.53
1:A:501:C:H2'	1:A:502:G:C8	2.43	0.53
2:B:15:VAL:HB	2:B:210:SER:HB2	1.90	0.53
2:B:28:PHE:CD2	2:B:190:THR:HG22	2.44	0.53
12:L:75:HIS:CD2	12:L:75:HIS:C	2.86	0.53
1:A:17:U:H2'	1:A:18:C:C6	2.43	0.53
1:A:242:C:H2'	1:A:243:A:H5'	1.89	0.53
1:A:676:A:H1'	11:K:115:PRO:HB3	1.89	0.53
1:A:839:U:O2	1:A:839:U:H2'	2.07	0.53
18:R:39:VAL:O	18:R:42:ARG:HB2	2.08	0.53
19:S:43:GLU:H	19:S:43:GLU:CD	2.16	0.53
21:U:9:ARG:HH12	21:U:23:PRO:HD3	1.72	0.53
1:A:1016:A:H2'	1:A:1017:G:O4'	2.09	0.53
1:A:1106:G:OP1	3:C:172:ARG:HD3	2.09	0.53
1:A:1262:C:H2'	1:A:1263:C:C6	2.42	0.53
1:A:1326:C:OP1	21:U:12:LYS:NZ	2.40	0.53
2:B:231:GLU:H	2:B:231:GLU:CD	2.16	0.53
4:D:31:CYS:C	4:D:33:MET:N	2.67	0.53
15:O:4:THR:HB	15:O:6:GLU:OE2	2.08	0.53
16:P:8:ARG:HB2	16:P:28:ARG:NH1	2.24	0.53
17:Q:101:ARG:HE	17:Q:101:ARG:CA	2.21	0.53
18:R:16:PRO:HB2	18:R:18:ARG:NE	2.24	0.53
1:A:267:C:P	17:Q:67:LYS:HB2	2.49	0.53
1:A:524:G:H2'	1:A:525:C:C6	2.44	0.53
1:A:961:U:C2'	1:A:962:C:H5'	2.39	0.53
1:A:1152:A:OP1	10:J:68:HIS:ND1	2.41	0.53
2:B:105:PHE:HE1	2:B:155:LEU:HD23	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:137:ARG:NH1	2:B:137:ARG:HB2	2.24	0.53
8:H:116:LYS:HD3	8:H:127:LEU:HD22	1.90	0.53
9:I:7:THR:O	9:I:7:THR:HG22	2.08	0.53
11:K:90:GLY:HA2	11:K:93:GLN:HB2	1.91	0.53
12:L:38:THR:HG22	12:L:39:VAL:CG2	2.38	0.53
14:N:42:ILE:O	14:N:45:ARG:HB3	2.09	0.53
1:A:265:G:H2'	1:A:267:C:H5	1.74	0.53
1:A:443:C:H2'	1:A:444:C:C6	2.40	0.53
1:A:640:A:O2'	1:A:641:U:H5'	2.09	0.53
1:A:954:G:H2'	1:A:955:U:C6	2.44	0.53
10:J:26:ALA:HB3	10:J:85:LEU:HD23	1.91	0.53
1:A:163:C:O2'	1:A:164:U:H5'	2.09	0.53
1:A:269:C:H2'	1:A:270:A:H8	1.74	0.53
3:C:60:ALA:O	3:C:61:ALA:HB2	2.09	0.53
5:E:51:VAL:O	5:E:54:ALA:HB3	2.08	0.53
10:J:30:SER:CB	10:J:84:GLN:HE21	2.17	0.53
10:J:32:ALA:O	10:J:34:VAL:HG23	2.09	0.53
11:K:11:LYS:O	11:K:12:ARG:HB2	2.09	0.53
13:M:35:GLU:C	13:M:37:THR:H	2.17	0.53
1:A:52:G:O2'	1:A:53:A:H5'	2.09	0.53
1:A:457:C:O2'	1:A:458:C:H5'	2.09	0.53
1:A:530:G:O6	22:X:3:A:H1'	2.09	0.53
1:A:1054:C:N3	23:Y:34:CM0:O4'	2.41	0.53
1:A:1373:G:H5''	7:G:36:LYS:HB2	1.91	0.53
2:B:73:THR:O	2:B:73:THR:HG22	2.10	0.53
6:F:62:TRP:CH2	6:F:64:GLN:HB2	2.44	0.53
10:J:26:ALA:HB1	10:J:84:GLN:HB2	1.90	0.53
12:L:24:VAL:HG13	12:L:98:TYR:CE2	2.43	0.53
1:A:537:G:OP1	12:L:113:ARG:NH2	2.43	0.52
2:B:10:LEU:HG	2:B:48:MET:HE2	1.91	0.52
9:I:31:GLN:O	9:I:32:ASP:CB	2.56	0.52
1:A:60:A:H4'	1:A:61:G:O5'	2.10	0.52
1:A:1116:C:H2'	1:A:1117:G:C5'	2.35	0.52
1:A:1151:A:HO2'	1:A:1152:A:H8	1.56	0.52
2:B:42:ILE:H	2:B:42:ILE:HD12	1.74	0.52
4:D:25:ARG:C	4:D:27:TYR:H	2.17	0.52
6:F:101:ALA:HB2	18:R:28:GLU:HG3	1.91	0.52
23:Y:30:C:O2'	23:Y:31:C:H5'	2.09	0.52
1:A:620:C:C2	4:D:135:LEU:HD13	2.44	0.52
1:A:620:C:H2'	1:A:621:A:O4'	2.10	0.52
2:B:181:PHE:HE2	8:H:70:GLN:HB3	1.72	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:10:MET:HG3	5:E:10:MET:O	2.08	0.52
6:F:50:TYR:CE1	18:R:77:GLY:HA2	2.43	0.52
16:P:43:LYS:HA	16:P:48:TRP:CB	2.40	0.52
19:S:20:LEU:HD12	19:S:21:GLU:H	1.72	0.52
20:T:53:LEU:HD13	20:T:101:GLY:N	2.24	0.52
1:A:545:C:O2'	1:A:546:G:H5'	2.09	0.52
1:A:860:A:H2'	1:A:861:G:O4'	2.09	0.52
1:A:895:G:H2'	1:A:896:C:C6	2.44	0.52
1:A:1540:U:H3'	1:A:1540:U:H6	1.73	0.52
2:B:27:LYS:HD3	2:B:195:ASP:OD2	2.09	0.52
3:C:115:LEU:HD23	3:C:118:GLN:OE1	2.08	0.52
12:L:113:ARG:NH1	12:L:116:SER:H	2.08	0.52
13:M:16:ASP:OD1	13:M:17:VAL:N	2.39	0.52
13:M:21:TYR:HD1	13:M:21:TYR:H	1.57	0.52
19:S:15:LEU:O	19:S:19:VAL:N	2.38	0.52
20:T:57:ARG:NH2	20:T:102:GLY:HA3	2.24	0.52
1:A:828:A:H4'	1:A:828:A:OP1	2.10	0.52
1:A:981:U:H5'	14:N:21:TYR:CE1	2.44	0.52
1:A:1424:C:O2'	1:A:1425:U:H5'	2.09	0.52
4:D:17:VAL:HG12	4:D:18:LYS:N	2.22	0.52
6:F:69:GLU:O	6:F:72:VAL:HG23	2.10	0.52
11:K:48:ILE:HG22	11:K:49:GLY:N	2.22	0.52
21:U:9:ARG:HH12	21:U:23:PRO:HD2	1.74	0.52
2:B:16:HIS:O	2:B:204:ASN:HB2	2.10	0.52
2:B:130:ARG:O	2:B:135:GLN:NE2	2.42	0.52
3:C:70:VAL:CG1	3:C:71:ALA:N	2.72	0.52
4:D:76:ARG:HG2	4:D:76:ARG:HH11	1.73	0.52
4:D:78:LEU:HD22	4:D:96:LEU:HB3	1.91	0.52
13:M:67:GLU:O	13:M:69:GLU:N	2.39	0.52
1:A:226:G:O2'	1:A:227:G:H5'	2.09	0.52
1:A:1306:A:N6	1:A:1331:G:H1'	2.24	0.52
1:A:1314:C:C5	19:S:6:LYS:HE2	2.45	0.52
2:B:137:ARG:CB	2:B:137:ARG:NH1	2.73	0.52
4:D:201:GLN:NE2	4:D:204:ILE:HD12	2.24	0.52
5:E:6:PHE:HB3	5:E:34:VAL:HG22	1.90	0.52
7:G:113:GLU:HG3	7:G:118:VAL:HG12	1.92	0.52
15:O:70:LEU:HD12	15:O:78:TYR:HB2	1.91	0.52
1:A:1048:G:H5'	1:A:1048:G:C8	2.36	0.52
1:A:1152:A:H4'	10:J:17:ASP:OD2	2.10	0.52
1:A:1347:G:O2'	1:A:1348:U:OP2	2.26	0.52
2:B:12:GLU:CG	2:B:213:LEU:HD11	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:75:VAL:O	3:C:83:ARG:HG2	2.10	0.52
11:K:33:THR:HB	11:K:38:ASN:C	2.35	0.52
13:M:90:LEU:HD22	13:M:94:ARG:HH12	1.75	0.52
20:T:84:LEU:HD23	20:T:88:VAL:HG23	1.91	0.52
1:A:1442(A):G:C4'	1:A:1442(B):A:H5'	2.35	0.52
2:B:28:PHE:HD1	2:B:194:PRO:HG3	1.75	0.52
2:B:75:LYS:HE2	2:B:96:ARG:HH22	1.75	0.52
2:B:78:GLN:HE22	2:B:96:ARG:HH12	1.58	0.52
2:B:169:LYS:O	2:B:169:LYS:HD3	2.10	0.52
5:E:36:ASP:O	5:E:38:GLN:HG3	2.09	0.52
12:L:27:LEU:O	12:L:28:LYS:C	2.52	0.52
12:L:53:ARG:HG2	12:L:69:TYR:CE1	2.37	0.52
12:L:71:PRO:O	12:L:102:ARG:HD2	2.09	0.52
1:A:1143:G:H2'	1:A:1144:G:C8	2.44	0.52
2:B:42:ILE:HD12	2:B:42:ILE:N	2.25	0.52
5:E:72:GLN:O	5:E:75:THR:HG22	2.10	0.52
7:G:15:ASP:OD2	7:G:44:TYR:OH	2.28	0.52
9:I:115:GLY:HA2	10:J:58:ASP:OD1	2.09	0.52
10:J:3:LYS:HB3	10:J:75:ILE:HA	1.91	0.52
19:S:36:ARG:NH2	19:S:75:ALA:O	2.30	0.52
1:A:457:C:H2'	1:A:458:C:C6	2.44	0.51
1:A:750:G:N3	15:O:23:GLY:HA3	2.24	0.51
1:A:975:A:C4'	1:A:976:G:H5''	2.30	0.51
1:A:1190:G:P	3:C:5:ILE:HG13	2.50	0.51
1:A:1457:G:O2'	1:A:1458:G:H5'	2.10	0.51
2:B:20:GLU:HB2	2:B:190:THR:OG1	2.09	0.51
7:G:5:ARG:HG2	7:G:6:ARG:N	2.25	0.51
7:G:37:ASN:ND2	9:I:41:VAL:HG23	2.25	0.51
8:H:65:TYR:HA	8:H:79:VAL:HG23	1.91	0.51
10:J:23:ILE:O	10:J:23:ILE:HG22	2.09	0.51
13:M:81:LEU:HD11	13:M:88:ARG:HH11	1.74	0.51
20:T:74:LYS:HB3	20:T:76:ALA:H	1.75	0.51
22:X:3:A:N6	22:X:4:A:N6	2.58	0.51
1:A:945:G:H2'	1:A:945:G:N3	2.25	0.51
3:C:63:ASN:HA	3:C:99:VAL:HG12	1.92	0.51
3:C:66:VAL:O	3:C:66:VAL:HG12	2.10	0.51
5:E:76:ILE:HG13	5:E:142:LEU:HD13	1.91	0.51
9:I:126:SER:O	9:I:128:ARG:N	2.43	0.51
10:J:20:ALA:O	10:J:24:VAL:HG23	2.10	0.51
10:J:49:VAL:HG21	14:N:41:ARG:O	2.10	0.51
10:J:76:ASN:O	10:J:78:ASN:N	2.36	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:22:ILE:HD12	13:M:25:ILE:HD12	1.91	0.51
1:A:56:U:H2'	1:A:57:G:H8	1.74	0.51
1:A:342:C:C2'	1:A:343:U:H5'	2.41	0.51
1:A:1133:G:H2'	1:A:1134:G:C8	2.35	0.51
1:A:1312:G:O2'	1:A:1313:U:H5'	2.10	0.51
1:A:1521:G:H2'	1:A:1522:U:C6	2.46	0.51
2:B:132:LYS:HA	2:B:135:GLN:HB2	1.93	0.51
3:C:189:ALA:HB3	3:C:196:LEU:HB2	1.92	0.51
5:E:76:ILE:CG2	5:E:78:HIS:O	2.57	0.51
9:I:111:ARG:HD3	9:I:112:LYS:C	2.35	0.51
19:S:80:TYR:CG	19:S:81:ARG:N	2.78	0.51
1:A:542:G:OP1	4:D:10:ARG:NH2	2.44	0.51
1:A:738:C:H5''	6:F:69:GLU:HB3	1.91	0.51
1:A:920:U:H2'	1:A:921:U:C6	2.45	0.51
1:A:1019:C:O2'	1:A:1020:U:H5'	2.11	0.51
1:A:1056:U:H5'	3:C:163:ALA:CB	2.40	0.51
1:A:1119:C:O2'	1:A:1120:G:H5'	2.10	0.51
1:A:1483:A:H2'	1:A:1484:C:O4'	2.11	0.51
2:B:28:PHE:CD2	2:B:190:THR:HA	2.45	0.51
7:G:20:ASP:OD1	7:G:22:LEU:HB3	2.10	0.51
10:J:75:ILE:O	10:J:76:ASN:HB2	2.11	0.51
14:N:22:THR:HG23	14:N:33:VAL:HG21	1.91	0.51
20:T:56:MET:HE2	20:T:88:VAL:CG1	2.38	0.51
20:T:69:GLY:O	20:T:73:HIS:CD2	2.64	0.51
1:A:918:A:H2'	1:A:919:A:C8	2.45	0.51
8:H:46:LYS:N	8:H:64:LYS:HG3	2.26	0.51
10:J:32:ALA:HB2	10:J:75:ILE:O	2.09	0.51
11:K:21:ILE:HD12	11:K:95:ILE:HD13	1.91	0.51
1:A:442:C:N4	1:A:492:G:H1	2.09	0.51
1:A:794:A:H2'	1:A:795:C:C6	2.45	0.51
1:A:1149:C:H2'	1:A:1150:U:C6	2.46	0.51
11:K:58:PRO:HA	11:K:90:GLY:HA3	1.91	0.51
13:M:20:THR:O	13:M:22:ILE:N	2.43	0.51
19:S:52:TYR:HA	19:S:56:GLN:O	2.10	0.51
21:U:2:GLY:C	21:U:4:GLY:H	2.19	0.51
1:A:1392:G:N2	1:A:1502:A:C8	2.78	0.51
9:I:22:GLY:N	9:I:58:HIS:O	2.43	0.51
9:I:111:ARG:HD2	9:I:113:LYS:HD2	1.92	0.51
10:J:9:ARG:CB	10:J:9:ARG:HH11	2.24	0.51
19:S:16:LEU:O	19:S:19:VAL:HG12	2.11	0.51
19:S:44:MET:C	19:S:62:ILE:HD13	2.36	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1157:A:H4'	1:A:1158:C:O5'	2.11	0.51
4:D:68:TYR:CB	4:D:70:ILE:HD13	2.41	0.51
9:I:10:ARG:HG2	9:I:75:ASP:HB2	1.92	0.51
1:A:189(E):U:O2'	1:A:189(F):U:H5'	2.09	0.51
1:A:1123:A:H4'	10:J:37:PRO:HD2	1.92	0.51
1:A:1208:C:H2'	1:A:1209:C:H6	1.76	0.51
1:A:1299:A:C8	1:A:1301:U:H1'	2.45	0.51
7:G:16:LEU:N	7:G:16:LEU:CD2	2.71	0.51
11:K:12:ARG:O	11:K:12:ARG:HD2	2.11	0.51
12:L:40:VAL:O	12:L:40:VAL:HG12	2.10	0.51
14:N:26:ARG:HE	14:N:47:LEU:HD21	1.76	0.51
17:Q:52:LYS:N	17:Q:55:ASP:OD2	2.39	0.51
19:S:30:LEU:O	19:S:31:ILE:HD13	2.10	0.51
20:T:46:GLU:HB3	20:T:48:LYS:HE2	1.92	0.51
22:X:1:G:O2'	22:X:2:U:H5'	2.11	0.51
1:A:304:U:H2'	1:A:305:G:C8	2.46	0.51
1:A:1004:A:H2'	1:A:1005:A:O4'	2.10	0.51
1:A:1171:G:H2'	1:A:1172:C:C6	2.46	0.51
2:B:7:VAL:HG12	2:B:221:LEU:CD2	2.39	0.51
2:B:96:ARG:O	2:B:98:LEU:HD23	2.11	0.51
2:B:204:ASN:ND2	2:B:206:ASP:H	2.09	0.51
4:D:196:LEU:HD23	4:D:197:PRO:HD2	1.93	0.51
16:P:52:ASP:CG	16:P:55:ARG:HG3	2.35	0.51
1:A:161:A:H2'	1:A:162:A:C8	2.46	0.50
1:A:178:C:O2'	1:A:179:A:H5'	2.11	0.50
1:A:559:A:OP1	5:E:126:ARG:NH2	2.43	0.50
1:A:664:G:OP1	18:R:64:ARG:HD2	2.11	0.50
5:E:96:PRO:HA	5:E:117:ASP:OD2	2.11	0.50
8:H:9:MET:SD	8:H:32:LYS:HG2	2.51	0.50
13:M:20:THR:C	13:M:22:ILE:H	2.20	0.50
13:M:81:LEU:HD13	13:M:88:ARG:HD3	1.93	0.50
15:O:81:LEU:HD21	15:O:85:LEU:HD12	1.93	0.50
2:B:21:ARG:NH1	2:B:21:ARG:HG3	2.26	0.50
2:B:74:LYS:HD3	2:B:206:ASP:HB2	1.92	0.50
4:D:101:LEU:O	4:D:102:ASP:C	2.54	0.50
6:F:44:GLY:HA2	6:F:59:TYR:CE1	2.46	0.50
7:G:126:ASP:CG	7:G:131:LYS:HE3	2.36	0.50
11:K:18:ARG:NH1	11:K:36:ASP:C	2.69	0.50
11:K:111:ASP:CG	11:K:111:ASP:O	2.55	0.50
1:A:438:G:C4'	1:A:439:A:OP1	2.59	0.50
1:A:1425:U:H2'	1:A:1426:C:H6	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1425:U:H3	1:A:1475:G:H1	1.60	0.50
6:F:47:ARG:HA	6:F:57:GLN:HG2	1.93	0.50
8:H:70:GLN:HA	8:H:70:GLN:HE21	1.76	0.50
10:J:7:LYS:NZ	10:J:71:LEU:HD23	2.26	0.50
12:L:55:VAL:CG1	12:L:56:ALA:N	2.75	0.50
15:O:9:GLN:O	15:O:13:GLN:HG3	2.11	0.50
17:Q:40:LYS:HG2	17:Q:41:LYS:N	2.26	0.50
1:A:675:A:H1'	11:K:116:HIS:CD2	2.47	0.50
1:A:1117:G:H5'	1:A:1117:G:C8	2.42	0.50
5:E:24:ARG:HG2	5:E:24:ARG:HH11	1.75	0.50
6:F:82:ARG:HB2	6:F:85:VAL:HG23	1.93	0.50
8:H:82:HIS:HB3	8:H:138:TRP:CD2	2.45	0.50
1:A:22:G:H2'	1:A:23:C:C6	2.47	0.50
1:A:501:C:H2'	1:A:502:G:H8	1.75	0.50
1:A:579:G:H2'	1:A:580:U:C6	2.46	0.50
1:A:959:A:H3'	1:A:960:U:H5''	1.92	0.50
1:A:1236:A:O2'	1:A:1304:G:H4'	2.12	0.50
1:A:1244:C:O2'	1:A:1245:A:H5'	2.11	0.50
1:A:1300:G:HO2'	1:A:1301:U:H6	1.55	0.50
2:B:206:ASP:O	2:B:207:ALA:CB	2.59	0.50
4:D:154:ASN:HA	4:D:159:ARG:CZ	2.41	0.50
7:G:79:ARG:HA	7:G:84:ASN:HA	1.92	0.50
10:J:90:LEU:N	10:J:91:PRO:HD2	2.26	0.50
16:P:74:LEU:HD22	16:P:79:VAL:HG21	1.93	0.50
17:Q:68:ARG:N	17:Q:70:ARG:HH11	2.05	0.50
21:U:5:ASP:O	21:U:11:GLY:HA3	2.12	0.50
21:U:15:ARG:HH11	21:U:15:ARG:CG	2.24	0.50
1:A:662:G:O2'	1:A:836:G:H5'	2.12	0.50
1:A:1381:U:O2'	1:A:1382:C:H5'	2.12	0.50
2:B:35:GLU:HA	2:B:39:ILE:O	2.11	0.50
7:G:65:ALA:HB1	7:G:127:ALA:HB3	1.93	0.50
9:I:56:LEU:O	9:I:56:LEU:HD23	2.12	0.50
13:M:108:ARG:HD3	13:M:114:ARG:HH12	1.74	0.50
1:A:267:C:OP2	17:Q:67:LYS:HD2	2.12	0.50
1:A:1513:A:H2'	1:A:1514:C:C6	2.47	0.50
10:J:20:ALA:C	10:J:22:LYS:H	2.19	0.50
12:L:50:SER:O	12:L:51:ALA:HB2	2.12	0.50
1:A:861:G:O2'	1:A:862:C:H5'	2.12	0.50
1:A:1351:U:O2'	1:A:1352:C:H5'	2.11	0.50
2:B:17:PHE:HB3	2:B:44:LEU:CD2	2.37	0.50
2:B:213:LEU:O	2:B:217:ARG:HG2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:64:GLU:CG	14:N:59:ALA:HB2	2.41	0.50
1:A:1404:C:H2'	1:A:1405:G:C8	2.47	0.50
4:D:100:ARG:HH12	4:D:137:SER:HB3	1.77	0.50
6:F:68:PRO:HG2	6:F:71:ARG:HG3	1.93	0.50
12:L:85:ILE:HG23	12:L:98:TYR:HB3	1.94	0.50
1:A:960:U:O2	1:A:960:U:H2'	2.11	0.49
1:A:1038:C:C6	1:A:1039:C:H5	2.30	0.49
2:B:111:ARG:HB3	2:B:149:LEU:CD1	2.41	0.49
2:B:132:LYS:HB3	2:B:136:VAL:HG23	1.93	0.49
7:G:26:PHE:CE2	7:G:30:ILE:HD11	2.47	0.49
8:H:82:HIS:CD2	8:H:138:TRP:CE2	2.99	0.49
14:N:6:LEU:C	14:N:8:GLU:H	2.17	0.49
19:S:16:LEU:C	19:S:19:VAL:HG12	2.37	0.49
1:A:204:U:O2'	1:A:216:G:OP2	2.26	0.49
1:A:1154:G:H2'	1:A:1155:G:H8	1.77	0.49
1:A:1176:A:H2'	1:A:1177:G:C8	2.47	0.49
1:A:1499:A:C1'	1:A:1520:G:H5'	2.41	0.49
2:B:47:THR:HG23	2:B:202:PRO:O	2.12	0.49
3:C:79:ARG:HG3	3:C:79:ARG:HH11	1.77	0.49
6:F:100:ASN:HB2	18:R:23:LYS:HG3	1.92	0.49
10:J:51:ARG:HG3	10:J:59:SER:HB2	1.95	0.49
20:T:59:ALA:O	20:T:63:ILE:HG13	2.12	0.49
21:U:6:ARG:HG2	21:U:15:ARG:HD2	1.94	0.49
1:A:999:C:H2'	1:A:1000:U:C6	2.47	0.49
1:A:1352:C:H2'	1:A:1353:G:C8	2.47	0.49
3:C:32:LEU:HD22	3:C:59:ARG:NH1	2.28	0.49
13:M:14:ARG:NH1	13:M:16:ASP:OD2	2.42	0.49
19:S:10:PHE:CD2	19:S:10:PHE:N	2.80	0.49
23:Y:34:CM0:H2'	23:Y:35:A:H8	1.77	0.49
1:A:1543:C:O2'	1:A:1544:U:H5'	2.12	0.49
2:B:134:GLU:HG2	2:B:137:ARG:HH21	1.73	0.49
1:A:1314:C:OP2	19:S:6:LYS:HD3	2.13	0.49
4:D:64:LEU:HD12	4:D:75:PHE:CZ	2.47	0.49
6:F:67:MET:HB2	6:F:68:PRO:CD	2.36	0.49
1:A:409:G:OP1	4:D:24:GLU:O	2.31	0.49
1:A:454:C:H2'	1:A:455:C:H5'	1.94	0.49
1:A:1371:G:O3'	9:I:69:GLY:HA3	2.13	0.49
2:B:132:LYS:C	2:B:134:GLU:N	2.71	0.49
2:B:231:GLU:CB	2:B:232:PRO:HD2	2.42	0.49
3:C:110:ASN:HD22	3:C:140:ARG:HB3	1.77	0.49
11:K:108:ILE:HG22	11:K:109:VAL:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:46:LYS:O	12:L:48:PRO:HD2	2.12	0.49
15:O:54:ARG:HG3	15:O:58:MET:HE2	1.95	0.49
20:T:100:ILE:O	20:T:102:GLY:N	2.45	0.49
1:A:1307:U:H2'	1:A:1308:U:C6	2.48	0.49
3:C:23:TYR:CG	3:C:24:ALA:N	2.79	0.49
10:J:34:VAL:HG22	10:J:74:ILE:HG23	1.93	0.49
15:O:22:THR:O	15:O:27:VAL:HG11	2.12	0.49
16:P:11:SER:OG	16:P:14:ASN:HB3	2.13	0.49
1:A:189(I):G:O2'	1:A:189(J):G:H5'	2.13	0.49
1:A:625:G:H2'	1:A:626:U:C6	2.48	0.49
1:A:665:A:N3	1:A:732:C:H2'	2.28	0.49
1:A:818:G:H3'	1:A:819:A:C5'	2.43	0.49
1:A:1019:C:C2'	1:A:1020:U:H5'	2.43	0.49
2:B:115:LEU:HD21	2:B:153:ARG:NH2	2.27	0.49
3:C:58:GLU:OE2	10:J:92:THR:HG21	2.11	0.49
15:O:3:ILE:HD13	15:O:34:LEU:CD1	2.37	0.49
20:T:94:ALA:O	20:T:95:ALA:CB	2.61	0.49
8:H:35:ILE:HG22	8:H:39:LEU:HD21	1.95	0.49
10:J:3:LYS:N	10:J:76:ASN:N	2.60	0.49
12:L:75:HIS:N	12:L:102:ARG:HH22	2.10	0.49
13:M:40:ASN:HD22	13:M:41:PRO:N	2.11	0.49
13:M:96:LEU:C	13:M:110:ARG:HG2	2.37	0.49
16:P:57:ARG:NH1	16:P:57:ARG:CG	2.74	0.49
1:A:951:G:O2'	1:A:952:U:H5'	2.12	0.49
1:A:1532:U:H2'	1:A:1533:C:C3'	2.40	0.49
3:C:23:TYR:CD2	3:C:23:TYR:C	2.90	0.49
7:G:23:VAL:HG13	7:G:43:PHE:CE2	2.48	0.49
7:G:113:GLU:CD	7:G:113:GLU:H	2.21	0.49
17:Q:76:LEU:HD11	17:Q:78:GLU:O	2.13	0.49
1:A:148:G:H2'	1:A:149:A:H8	1.78	0.48
1:A:723:U:O2	1:A:723:U:H2'	2.13	0.48
1:A:939:G:H2'	1:A:940:C:C6	2.48	0.48
1:A:1066:C:H2'	1:A:1067:A:H5'	1.95	0.48
1:A:1125:U:H6	1:A:1125:U:H5''	1.78	0.48
1:A:1447:A:O2'	1:A:1452:C:OP1	2.30	0.48
4:D:68:TYR:HB3	4:D:70:ILE:HD13	1.93	0.48
5:E:126:ARG:HG3	5:E:126:ARG:NH1	2.27	0.48
9:I:97:LYS:CA	9:I:102:LEU:HD21	2.41	0.48
10:J:6:ILE:CG2	10:J:98:ILE:HG22	2.43	0.48
13:M:120:LYS:CE	13:M:122:LYS:HB3	2.43	0.48
1:A:594:G:C2'	1:A:595:G:H5'	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:952:U:O2'	1:A:953:G:H5'	2.14	0.48
1:A:1053:G:C3'	1:A:1054:C:C5'	2.90	0.48
2:B:72:GLY:HA2	2:B:165:VAL:HG22	1.95	0.48
3:C:157:ILE:CD1	3:C:166:GLU:HG3	2.43	0.48
6:F:75:LEU:C	6:F:75:LEU:HD23	2.38	0.48
12:L:60:LEU:HB2	12:L:64:TYR:O	2.14	0.48
13:M:13:LYS:O	13:M:45:VAL:HG23	2.13	0.48
20:T:65:LYS:HA	20:T:68:LYS:HG3	1.93	0.48
1:A:141:A:O2'	1:A:142:G:H5'	2.14	0.48
1:A:1106:G:H5''	3:C:172:ARG:HG2	1.94	0.48
2:B:102:LEU:N	2:B:102:LEU:CD1	2.76	0.48
17:Q:68:ARG:N	17:Q:70:ARG:HH12	2.11	0.48
20:T:45:GLN:NE2	20:T:45:GLN:O	2.46	0.48
20:T:100:ILE:C	20:T:102:GLY:N	2.70	0.48
1:A:682:G:O2'	1:A:683:G:H5'	2.14	0.48
1:A:984:C:H2'	1:A:985:C:C6	2.47	0.48
1:A:1047:G:H2'	1:A:1048:G:H5'	1.92	0.48
2:B:118:LEU:C	2:B:120:ALA:N	2.69	0.48
3:C:47:LEU:N	3:C:47:LEU:HD12	2.28	0.48
4:D:24:GLU:C	4:D:26:CYS:H	2.20	0.48
6:F:9:VAL:HB	6:F:87:ARG:HB2	1.94	0.48
7:G:37:ASN:O	7:G:38:LEU:C	2.56	0.48
7:G:129:GLU:OE1	7:G:131:LYS:HE2	2.14	0.48
10:J:47:PHE:CE2	14:N:37:PHE:HE1	2.32	0.48
17:Q:86:GLU:O	17:Q:87:LYS:C	2.56	0.48
20:T:72:LEU:O	20:T:73:HIS:C	2.55	0.48
1:A:750:G:H1'	15:O:23:GLY:H	1.77	0.48
1:A:1033:G:H2'	1:A:1034:G:H8	1.78	0.48
1:A:1222:G:O2'	1:A:1223:C:H5'	2.14	0.48
2:B:15:VAL:HG21	2:B:210:SER:HA	1.95	0.48
9:I:27:THR:HG23	9:I:62:TYR:HA	1.95	0.48
16:P:54:GLU:CD	16:P:54:GLU:C	2.81	0.48
1:A:942:G:H2'	1:A:943:U:H6	1.78	0.48
1:A:1154:G:O2'	1:A:1155:G:H5'	2.14	0.48
1:A:1249:C:O2'	9:I:73:GLN:NE2	2.47	0.48
1:A:1312:G:N7	19:S:3:ARG:O	2.46	0.48
2:B:28:PHE:HD2	2:B:190:THR:HG22	1.78	0.48
3:C:132:ARG:O	3:C:136:GLN:HG3	2.14	0.48
5:E:15:ARG:HD2	5:E:26:PHE:CD2	2.49	0.48
5:E:144:THR:O	5:E:145:LYS:C	2.56	0.48
6:F:19:LEU:O	6:F:19:LEU:HD23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:18:TYR:CE2	7:G:59:LEU:HB2	2.49	0.48
8:H:9:MET:O	8:H:10:LEU:C	2.55	0.48
12:L:93:LEU:HB2	12:L:96:VAL:HG21	1.95	0.48
1:A:41:G:H2'	1:A:42:G:C8	2.49	0.48
1:A:262:A:H5'	20:T:74:LYS:HG3	1.95	0.48
1:A:1054:C:H42	23:Y:34:CM0:C6	2.26	0.48
1:A:1325:C:P	21:U:6:ARG:HH22	2.34	0.48
2:B:31:TYR:CD1	2:B:202:PRO:HB3	2.48	0.48
4:D:76:ARG:HG2	4:D:76:ARG:NH1	2.29	0.48
4:D:156:GLU:HG2	4:D:160:GLN:HE21	1.79	0.48
9:I:97:LYS:CG	9:I:102:LEU:HD21	2.38	0.48
9:I:111:ARG:HD3	9:I:112:LYS:N	2.28	0.48
14:N:42:ILE:O	14:N:46:GLU:HG3	2.14	0.48
17:Q:3:LYS:HB3	17:Q:61:GLU:CB	2.43	0.48
17:Q:97:SER:HA	17:Q:102:GLY:HA2	1.96	0.48
1:A:1104:G:OP1	2:B:111:ARG:HD2	2.14	0.48
2:B:7:VAL:O	2:B:8:LYS:HG3	2.14	0.48
2:B:157:ARG:O	2:B:158:LEU:C	2.55	0.48
4:D:152:SER:C	4:D:154:ASN:H	2.21	0.48
5:E:12:LEU:CD1	5:E:31:LEU:HB2	2.40	0.48
9:I:17:VAL:HG11	9:I:81:ILE:HA	1.95	0.48
9:I:125:TYR:N	9:I:125:TYR:HD2	2.11	0.48
13:M:14:ARG:HG3	13:M:44:ARG:HH21	1.79	0.48
1:A:922:G:N3	1:A:1398:A:H2	2.12	0.48
1:A:1030:C:H2'	1:A:1030(A):G:H8	1.79	0.48
1:A:1347:G:C2'	1:A:1348:U:OP2	2.62	0.48
3:C:102:ASN:N	3:C:102:ASN:ND2	2.55	0.48
3:C:102:ASN:HD22	3:C:102:ASN:H	1.60	0.48
3:C:193:TYR:CE1	3:C:196:LEU:HD21	2.49	0.48
16:P:20:VAL:HG11	16:P:32:TYR:CB	2.44	0.48
19:S:13:ASP:O	19:S:14:HIS:C	2.56	0.48
20:T:26:ASN:OD1	20:T:71:THR:HA	2.13	0.48
1:A:339:C:H2'	1:A:340:U:C6	2.48	0.48
1:A:1007:C:H2'	1:A:1008:C:H6	1.78	0.48
1:A:1373:G:H5''	7:G:36:LYS:CB	2.43	0.48
2:B:118:LEU:CD2	2:B:142:LEU:HB2	2.43	0.48
7:G:50:ILE:O	7:G:54:THR:HB	2.13	0.48
19:S:80:TYR:CE2	19:S:81:ARG:HB3	2.49	0.48
1:A:200:G:H2'	1:A:201:C:C6	2.49	0.47
1:A:895:G:H2'	1:A:896:C:H6	1.79	0.47
1:A:1060:C:H5	3:C:2:GLY:HA3	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1230:C:O2'	1:A:1231:G:H5'	2.13	0.47
1:A:1327:C:O2'	1:A:1328:C:H5'	2.14	0.47
10:J:4:ILE:CG1	10:J:74:ILE:HB	2.43	0.47
10:J:30:SER:HB2	10:J:80:LYS:O	2.14	0.47
13:M:125:ARG:O	13:M:126:LYS:C	2.56	0.47
14:N:8:GLU:C	14:N:10:ALA:N	2.72	0.47
15:O:26:GLU:HG3	15:O:81:LEU:CD1	2.42	0.47
16:P:20:VAL:HG13	16:P:32:TYR:HB2	1.96	0.47
20:T:43:LEU:HD13	20:T:51:GLU:HG3	1.94	0.47
1:A:322:C:H41	1:A:328:C:H6	1.62	0.47
1:A:1144:G:H21	1:A:1146:A:H62	1.62	0.47
1:A:1223:C:P	19:S:78:ARG:NH1	2.87	0.47
1:A:1241:G:H2'	1:A:1242:C:H6	1.76	0.47
1:A:1368:G:O2'	1:A:1369:C:H5'	2.14	0.47
3:C:164:ARG:HB2	3:C:164:ARG:NH1	2.29	0.47
3:C:172:ARG:HB3	3:C:172:ARG:NH1	2.28	0.47
5:E:145:LYS:O	5:E:149:GLU:HG2	2.14	0.47
11:K:124:LYS:O	11:K:124:LYS:HG2	2.13	0.47
13:M:27:LYS:HB2	13:M:27:LYS:NZ	2.29	0.47
1:A:272:C:O2'	1:A:273:A:H5'	2.14	0.47
1:A:382:A:H2'	1:A:383:A:H8	1.77	0.47
1:A:1054:C:O2'	1:A:1055:A:C5'	2.63	0.47
1:A:1250:A:C4'	9:I:68:GLY:H	2.17	0.47
1:A:1305:G:H22	1:A:1331:G:C2'	2.27	0.47
3:C:188:LEU:HD21	3:C:195:VAL:HG11	1.95	0.47
4:D:64:LEU:HD12	4:D:75:PHE:CE1	2.48	0.47
8:H:9:MET:CE	8:H:32:LYS:HG2	2.44	0.47
9:I:8:GLY:CA	9:I:79:LEU:HB3	2.44	0.47
9:I:36:TYR:HD2	9:I:37:PHE:CE2	2.33	0.47
9:I:100:GLY:C	9:I:102:LEU:N	2.71	0.47
10:J:3:LYS:CB	10:J:75:ILE:HA	2.43	0.47
19:S:42:PRO:C	19:S:44:MET:H	2.22	0.47
20:T:50:GLU:H	20:T:99:LEU:HD12	1.80	0.47
1:A:551:U:H2'	1:A:552:U:H6	1.79	0.47
1:A:555:C:H2'	1:A:556:C:C6	2.50	0.47
1:A:921:U:O2'	5:E:19:MET:O	2.27	0.47
1:A:1226:C:C4	13:M:104:ARG:HG3	2.49	0.47
1:A:1247:U:O2'	1:A:1248:A:H5'	2.14	0.47
1:A:1329:A:O2'	1:A:1330:U:H5'	2.15	0.47
2:B:97:TRP:CZ3	2:B:176:GLU:OE2	2.67	0.47
3:C:70:VAL:HG12	3:C:72:LYS:N	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:28:SER:C	4:D:30:LYS:H	2.22	0.47
4:D:88:VAL:O	4:D:89:THR:C	2.56	0.47
10:J:19:SER:HA	10:J:22:LYS:NZ	2.29	0.47
10:J:39:PRO:HB3	10:J:70:ARG:NH1	2.29	0.47
13:M:65:LYS:O	13:M:66:LEU:HD23	2.14	0.47
16:P:22:THR:HA	16:P:33:ILE:HG13	1.96	0.47
1:A:713:G:H2'	1:A:714:G:C8	2.50	0.47
1:A:759:A:N6	17:Q:94:ASN:HD21	2.08	0.47
1:A:969:A:N6	13:M:126:LYS:HE3	2.30	0.47
1:A:1328:C:O2'	1:A:1329:A:H5'	2.14	0.47
2:B:97:TRP:CZ2	2:B:101:MET:HB2	2.49	0.47
5:E:12:LEU:HD22	5:E:12:LEU:C	2.39	0.47
8:H:6:ILE:HB	8:H:85:ARG:HH12	1.79	0.47
9:I:8:GLY:HA3	9:I:80:GLY:N	2.29	0.47
9:I:33:PHE:CE1	9:I:47:LEU:HD21	2.50	0.47
11:K:46:GLY:O	11:K:48:ILE:O	2.32	0.47
17:Q:68:ARG:HG2	17:Q:68:ARG:HH11	1.79	0.47
1:A:1456:G:H2'	1:A:1457:G:O4'	2.14	0.47
1:A:1479:C:O2'	1:A:1480:G:H5'	2.14	0.47
3:C:79:ARG:C	3:C:81:GLY:H	2.22	0.47
13:M:21:TYR:CD1	13:M:21:TYR:N	2.83	0.47
15:O:18:PHE:HB2	15:O:19:PRO:HD2	1.96	0.47
15:O:36:ILE:HG12	15:O:59:MET:HE3	1.97	0.47
1:A:67:C:H2'	1:A:68:G:C8	2.49	0.47
1:A:189(J):G:O2'	1:A:189(K):U:H5'	2.15	0.47
1:A:265:G:H2'	1:A:267:C:C5	2.49	0.47
1:A:427:U:OP1	4:D:13:ARG:NH2	2.48	0.47
1:A:473:G:H2'	1:A:474:G:H8	1.80	0.47
1:A:812:C:OP1	1:A:903:G:H1'	2.15	0.47
1:A:818:G:C3'	1:A:819:A:C5'	2.92	0.47
1:A:1066:C:O2'	1:A:1067:A:H5'	2.14	0.47
1:A:1069:C:O2'	1:A:1192:C:H1'	2.14	0.47
1:A:1181:G:O2'	1:A:1182:G:O5'	2.32	0.47
1:A:1260:C:O5'	1:A:1284:C:H4'	2.15	0.47
2:B:124:SER:C	2:B:126:GLU:H	2.22	0.47
3:C:18:TRP:O	3:C:54:ARG:NH2	2.47	0.47
3:C:40:ARG:O	3:C:44:GLU:HG3	2.14	0.47
3:C:72:LYS:O	3:C:75:VAL:HG23	2.14	0.47
3:C:181:ASN:ND2	3:C:204:LEU:CD1	2.78	0.47
4:D:150:GLU:HA	4:D:153:ARG:HG3	1.96	0.47
5:E:36:ASP:CG	5:E:40:ARG:HB2	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:85:TYR:O	7:G:87:VAL:HG23	2.15	0.47
10:J:40:LEU:HB2	10:J:69:ASN:CB	2.45	0.47
12:L:8:ASN:O	12:L:12:ARG:HG3	2.15	0.47
12:L:83:VAL:HG11	12:L:100:ILE:HD13	1.95	0.47
12:L:109:GLY:HA3	12:L:121:GLY:O	2.15	0.47
13:M:39:ILE:HD13	13:M:52:GLU:HB3	1.96	0.47
16:P:7:ALA:O	16:P:17:TYR:HA	2.15	0.47
18:R:19:LYS:CD	18:R:20:ALA:H	2.27	0.47
19:S:41:VAL:HB	19:S:42:PRO:HD2	1.96	0.47
1:A:189(L):G:H2'	1:A:190:U:C6	2.49	0.47
1:A:659:U:OP2	15:O:8:LYS:NZ	2.47	0.47
1:A:737:A:H2'	1:A:738:C:H6	1.77	0.47
1:A:1021:G:H2'	1:A:1022:G:H8	1.80	0.47
1:A:1152:A:H5''	10:J:13:HIS:CG	2.48	0.47
1:A:1414:U:H2'	1:A:1415:G:H8	1.80	0.47
2:B:86:GLU:C	2:B:88:ALA:N	2.72	0.47
2:B:189:ASP:HB3	2:B:191:ASP:OD1	2.13	0.47
3:C:34:LEU:HD13	3:C:34:LEU:C	2.39	0.47
3:C:39:ILE:HG22	3:C:40:ARG:N	2.30	0.47
3:C:107:GLN:O	3:C:108:ASN:HB3	2.15	0.47
4:D:111:ALA:HB2	4:D:120:LEU:HD12	1.96	0.47
14:N:7:ILE:O	14:N:7:ILE:HG22	2.15	0.47
16:P:54:GLU:O	16:P:57:ARG:HB2	2.15	0.47
17:Q:82:MET:O	17:Q:86:GLU:HG2	2.14	0.47
19:S:4:SER:OG	19:S:5:LEU:N	2.48	0.47
19:S:5:LEU:HD11	19:S:70:LYS:NZ	2.29	0.47
19:S:15:LEU:O	19:S:16:LEU:C	2.58	0.47
19:S:62:ILE:O	19:S:62:ILE:HG12	2.14	0.47
1:A:978:A:O2'	1:A:1322:C:N3	2.45	0.47
4:D:146:ILE:N	4:D:146:ILE:CD1	2.77	0.47
10:J:19:SER:OG	10:J:91:PRO:HB3	2.14	0.47
12:L:55:VAL:HG12	12:L:56:ALA:H	1.79	0.47
1:A:129(A):G:O2'	1:A:130:A:OP2	2.32	0.47
1:A:1024:G:C3'	1:A:1025:U:H5''	2.44	0.47
1:A:1251:A:H2'	1:A:1252:A:C8	2.49	0.47
4:D:58:LEU:HD22	4:D:62:GLN:HG2	1.96	0.47
5:E:78:HIS:O	5:E:93:PRO:HD3	2.15	0.47
6:F:91:VAL:HG13	18:R:72:ARG:NH2	2.30	0.47
9:I:97:LYS:HG2	9:I:102:LEU:CD2	2.38	0.47
11:K:40:ILE:HD12	11:K:77:MET:HE1	1.97	0.47
18:R:46:GLU:CD	18:R:46:GLU:N	2.68	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:G:H4'	1:A:216:G:OP1	2.15	0.46
1:A:642:A:N7	8:H:115:SER:HA	2.30	0.46
3:C:84:ILE:O	3:C:84:ILE:HG12	2.15	0.46
3:C:111:LEU:CD2	3:C:144:SER:HB2	2.45	0.46
3:C:140:ARG:O	3:C:143:GLU:HB3	2.14	0.46
6:F:75:LEU:HD23	6:F:75:LEU:O	2.16	0.46
18:R:36:ASN:ND2	18:R:39:VAL:H	2.12	0.46
19:S:19:VAL:HG13	19:S:20:LEU:N	2.30	0.46
1:A:187:C:H1'	20:T:85:MET:HE2	1.96	0.46
1:A:235:C:C5'	17:Q:70:ARG:HG2	2.44	0.46
1:A:401:C:H1'	1:A:622:A:H1'	1.96	0.46
1:A:735:C:O2'	1:A:736:C:H5'	2.15	0.46
1:A:836:G:H2'	1:A:837:G:C8	2.50	0.46
1:A:1056:U:H5'	3:C:163:ALA:HB2	1.98	0.46
1:A:1237:C:H4'	1:A:1334:G:N2	2.30	0.46
3:C:5:ILE:O	3:C:5:ILE:HD12	2.15	0.46
3:C:116:VAL:O	3:C:120:VAL:HG23	2.15	0.46
3:C:164:ARG:HH11	3:C:164:ARG:CB	2.27	0.46
5:E:36:ASP:OD2	5:E:40:ARG:HB2	2.16	0.46
6:F:100:ASN:HB2	18:R:23:LYS:HE3	1.97	0.46
7:G:69:VAL:HG12	7:G:69:VAL:O	2.13	0.46
13:M:3:ARG:HD2	13:M:7:VAL:HA	1.97	0.46
19:S:33:THR:HG22	19:S:34:TRP:N	2.30	0.46
20:T:49:ALA:HB3	20:T:99:LEU:HG	1.98	0.46
20:T:53:LEU:HD23	20:T:56:MET:CE	2.45	0.46
1:A:287:U:C2'	1:A:288:A:H5'	2.45	0.46
1:A:832:C:O2'	1:A:833:U:H5'	2.16	0.46
1:A:1300:G:O2'	1:A:1301:U:P	2.72	0.46
3:C:125:GLU:HG2	3:C:190:ARG:O	2.14	0.46
7:G:53:LYS:HE3	7:G:53:LYS:HB2	1.71	0.46
9:I:93:ARG:O	9:I:97:LYS:HB2	2.15	0.46
9:I:127:LYS:HG2	9:I:128:ARG:N	2.30	0.46
10:J:32:ALA:CB	10:J:78:ASN:HD21	2.27	0.46
11:K:108:ILE:N	11:K:108:ILE:CD1	2.79	0.46
13:M:14:ARG:HB3	13:M:14:ARG:NH1	2.30	0.46
15:O:78:TYR:CE1	15:O:82:ILE:HD11	2.51	0.46
1:A:518:C:H2'	1:A:530:G:N3	2.30	0.46
5:E:51:VAL:HB	5:E:52:PRO:CD	2.38	0.46
9:I:112:LYS:C	9:I:112:LYS:HD3	2.40	0.46
10:J:35:SER:HB3	10:J:73:ASP:HB2	1.98	0.46
13:M:85:GLY:O	13:M:86:CYS:C	2.57	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:39:LYS:CD	20:T:55:ILE:HD13	2.42	0.46
1:A:66:G:H4'	1:A:173:U:C5	2.51	0.46
1:A:186:C:H2'	1:A:187:C:C6	2.51	0.46
1:A:642:A:C5	8:H:115:SER:HA	2.51	0.46
1:A:746:A:C2'	1:A:747:C:H5'	2.46	0.46
1:A:1057:G:O2'	1:A:1058:G:H5'	2.16	0.46
1:A:1347:G:H2'	1:A:1373:G:H1	1.80	0.46
1:A:1413:A:H2	1:A:1487:G:H22	1.61	0.46
2:B:9:GLU:CG	2:B:217:ARG:HH22	2.28	0.46
2:B:25:ASN:HD22	2:B:26:PRO:N	2.13	0.46
2:B:75:LYS:HD3	2:B:78:GLN:OE1	2.16	0.46
3:C:33:LEU:HD11	14:N:53:LEU:HD23	1.97	0.46
7:G:50:ILE:HD11	7:G:121:ALA:HA	1.96	0.46
10:J:9:ARG:NH1	10:J:9:ARG:CB	2.78	0.46
11:K:34:ASP:OD2	11:K:38:ASN:HB2	2.16	0.46
11:K:54:ARG:O	11:K:60:ALA:HB2	2.15	0.46
13:M:96:LEU:O	13:M:97:PRO:C	2.59	0.46
16:P:26:ARG:CD	16:P:31:LYS:O	2.64	0.46
17:Q:22:LEU:HD12	17:Q:23:VAL:N	2.31	0.46
19:S:80:TYR:CZ	19:S:81:ARG:HB3	2.50	0.46
1:A:650:G:O2'	1:A:651:C:H5'	2.16	0.46
2:B:9:GLU:HG2	2:B:217:ARG:HH22	1.80	0.46
11:K:24:SER:O	11:K:88:GLY:HA3	2.14	0.46
12:L:10:LEU:HD21	12:L:15:ARG:NE	2.31	0.46
12:L:93:LEU:CB	12:L:96:VAL:HG21	2.46	0.46
16:P:42:ARG:O	16:P:43:LYS:C	2.59	0.46
20:T:43:LEU:HD13	20:T:51:GLU:CG	2.46	0.46
1:A:251:G:H4'	1:A:252:U:O5'	2.15	0.46
1:A:1129:C:O2'	1:A:1130:A:P	2.74	0.46
1:A:1181:G:H2'	1:A:1182:G:C4	2.51	0.46
1:A:1208:C:H2'	1:A:1209:C:C6	2.51	0.46
2:B:221:LEU:O	2:B:221:LEU:HD13	2.15	0.46
4:D:31:CYS:O	4:D:31:CYS:SG	2.73	0.46
4:D:154:ASN:HB3	4:D:159:ARG:NH2	2.31	0.46
6:F:75:LEU:C	6:F:75:LEU:CD2	2.89	0.46
10:J:6:ILE:CG2	10:J:98:ILE:HA	2.39	0.46
10:J:15:THR:O	10:J:18:ALA:HB3	2.16	0.46
12:L:59:ARG:NH1	12:L:65:GLU:OE2	2.49	0.46
17:Q:24:GLU:OE2	17:Q:37:LYS:HD3	2.16	0.46
18:R:47:THR:C	18:R:49:LYS:H	2.24	0.46
1:A:151:A:H2'	1:A:152:A:O4'	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:631:G:H5'	1:A:632:A:OP1	2.16	0.46
1:A:1128:C:O2'	1:A:1130:A:N7	2.45	0.46
1:A:1314:C:OP2	19:S:6:LYS:HG3	2.16	0.46
2:B:97:TRP:CH2	2:B:101:MET:HB2	2.51	0.46
3:C:129:ALA:HB3	3:C:132:ARG:NH1	2.31	0.46
10:J:76:ASN:C	10:J:78:ASN:N	2.73	0.46
12:L:43:VAL:HG12	12:L:44:THR:N	2.31	0.46
14:N:29:ARG:HG2	14:N:29:ARG:NH1	2.29	0.46
19:S:28:LYS:O	19:S:29:ARG:C	2.59	0.46
21:U:6:ARG:NH2	21:U:15:ARG:HE	2.12	0.46
23:Y:29:U:O2'	23:Y:30:C:H5'	2.16	0.46
1:A:542:G:H5'	4:D:41:GLY:HA3	1.98	0.46
1:A:833:U:H2'	1:A:834:C:C6	2.51	0.46
1:A:942:G:H2'	1:A:943:U:C6	2.51	0.46
1:A:1405:G:O2'	1:A:1406:U:H5'	2.15	0.46
1:A:1470:G:O2'	1:A:1471:G:H5'	2.15	0.46
1:A:1487:G:O2'	1:A:1488:G:H5'	2.15	0.46
2:B:140:HIS:HA	2:B:143:GLU:OE1	2.16	0.46
3:C:83:ARG:C	3:C:85:ARG:H	2.24	0.46
4:D:52:SER:O	4:D:53:ASP:C	2.56	0.46
4:D:57:ARG:HD3	4:D:205:GLU:HB2	1.98	0.46
4:D:90:GLY:O	4:D:93:PHE:HB3	2.16	0.46
5:E:28:PHE:O	5:E:47:LYS:HA	2.16	0.46
5:E:36:ASP:OD1	5:E:38:GLN:N	2.46	0.46
5:E:50:GLU:HB3	5:E:53:LEU:HD21	1.98	0.46
7:G:6:ARG:HB3	7:G:6:ARG:HH11	1.81	0.46
11:K:76:GLY:O	11:K:78:GLN:HG3	2.16	0.46
14:N:5:ALA:O	14:N:8:GLU:HG2	2.16	0.46
14:N:22:THR:HG23	14:N:33:VAL:HG23	1.98	0.46
15:O:70:LEU:HD12	15:O:78:TYR:CA	2.46	0.46
15:O:81:LEU:HD23	15:O:81:LEU:C	2.41	0.46
19:S:20:LEU:O	19:S:23:ASN:HB2	2.16	0.46
1:A:956:U:O2'	1:A:957:U:H5'	2.16	0.46
1:A:961:U:O2'	1:A:962:C:H5'	2.16	0.46
1:A:1246:C:O2'	1:A:1247:U:H5'	2.16	0.46
2:B:42:ILE:H	2:B:42:ILE:CD1	2.28	0.46
2:B:109:SER:C	2:B:111:ARG:N	2.74	0.46
2:B:233:SER:OG	2:B:234:PRO:HD2	2.16	0.46
4:D:61:LYS:HA	4:D:203:VAL:HG22	1.98	0.46
12:L:119:LYS:O	12:L:120:TYR:HB2	2.16	0.46
13:M:14:ARG:HH11	13:M:14:ARG:CB	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:45:ARG:O	14:N:49:HIS:CD2	2.69	0.46
17:Q:51:TYR:C	17:Q:52:LYS:HD2	2.41	0.46
20:T:53:LEU:HB2	20:T:100:ILE:HG23	1.96	0.46
1:A:586:C:O2'	1:A:587:G:H5'	2.15	0.45
1:A:666:G:H5'	1:A:726:C:H1'	1.98	0.45
1:A:881:G:P	12:L:12:ARG:HH22	2.39	0.45
1:A:961:U:H2'	1:A:962:C:H5'	1.98	0.45
1:A:1020:U:H2'	1:A:1021:G:H8	1.81	0.45
2:B:72:GLY:HA2	2:B:165:VAL:HG21	1.98	0.45
2:B:74:LYS:C	2:B:76:GLN:H	2.24	0.45
2:B:230:VAL:CG1	2:B:231:GLU:N	2.80	0.45
3:C:34:LEU:O	3:C:34:LEU:HD22	2.15	0.45
4:D:91:SER:O	4:D:94:LEU:N	2.49	0.45
6:F:69:GLU:C	6:F:71:ARG:H	2.24	0.45
6:F:86:ARG:O	6:F:87:ARG:HG2	2.16	0.45
9:I:7:THR:O	9:I:8:GLY:C	2.57	0.45
12:L:111:LYS:O	12:L:112:ASP:HB2	2.16	0.45
13:M:66:LEU:O	13:M:67:GLU:C	2.59	0.45
21:U:23:PRO:C	21:U:25:LYS:H	2.24	0.45
1:A:268:C:O2'	1:A:269:C:H5'	2.16	0.45
1:A:344:A:H5''	1:A:345:C:H5	1.81	0.45
1:A:960:U:H1'	1:A:1223:C:H5'	1.98	0.45
1:A:1144:G:N2	1:A:1146:A:H62	2.15	0.45
1:A:1250:A:H2'	1:A:1251:A:C8	2.51	0.45
2:B:69:LEU:HD12	2:B:155:LEU:HD22	1.99	0.45
6:F:3:ARG:CG	6:F:3:ARG:NH1	2.76	0.45
9:I:79:LEU:HD22	9:I:83:ARG:HG3	1.98	0.45
12:L:109:GLY:O	12:L:110:VAL:C	2.60	0.45
13:M:59:TYR:HE1	13:M:63:THR:HG21	1.81	0.45
14:N:9:LYS:C	14:N:11:LYS:N	2.74	0.45
16:P:57:ARG:HH12	16:P:79:VAL:C	2.22	0.45
18:R:26:LEU:HD21	18:R:39:VAL:HG22	1.98	0.45
1:A:7:G:H5'	1:A:298:A:H5'	1.98	0.45
1:A:775:G:O2'	1:A:776:G:H5'	2.17	0.45
1:A:1229:A:C2	1:A:1230:C:C4	3.04	0.45
1:A:1320:C:OP1	19:S:70:LYS:HE2	2.16	0.45
1:A:1367:C:H4'	10:J:48:THR:HG21	1.99	0.45
1:A:1402:C:O2	1:A:1500:A:N1	2.49	0.45
2:B:9:GLU:HG2	2:B:217:ARG:HH12	1.80	0.45
2:B:102:LEU:N	2:B:102:LEU:HD12	2.31	0.45
4:D:30:LYS:C	4:D:32:ALA:N	2.74	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:127:THR:CG2	4:D:147:ALA:HB3	2.45	0.45
7:G:99:LEU:HD23	7:G:102:ARG:NH1	2.32	0.45
8:H:6:ILE:HB	8:H:85:ARG:NH1	2.31	0.45
12:L:90:VAL:CG1	12:L:93:LEU:HG	2.45	0.45
13:M:114:ARG:HG2	13:M:114:ARG:HH11	1.82	0.45
23:Y:39:G:O2'	23:Y:40:G:H5'	2.17	0.45
1:A:342:C:O2'	1:A:343:U:H5'	2.17	0.45
1:A:1310:G:N7	19:S:2:PRO:HD3	2.31	0.45
1:A:1370:G:O2'	1:A:1371:G:H5'	2.17	0.45
1:A:1399:C:C2	1:A:1502:A:N6	2.85	0.45
1:A:1438:G:H2'	1:A:1439:C:C6	2.51	0.45
2:B:80:ILE:HD11	2:B:208:ILE:CG2	2.41	0.45
3:C:95:THR:OG1	3:C:96:GLY:N	2.46	0.45
3:C:206:GLU:O	3:C:207:VAL:C	2.59	0.45
5:E:81:GLU:HG3	5:E:90:VAL:CG2	2.47	0.45
6:F:15:ASP:N	6:F:18:GLN:NE2	2.60	0.45
7:G:77:SER:HB2	7:G:86:GLN:OE1	2.17	0.45
11:K:18:ARG:NH1	11:K:37:GLY:N	2.64	0.45
16:P:19:ILE:HG22	16:P:36:ILE:CG1	2.45	0.45
16:P:59:TRP:HB3	16:P:64:ALA:HB2	1.99	0.45
18:R:40:LEU:HB3	18:R:79:LEU:HD11	1.99	0.45
1:A:613:C:O2'	1:A:614:A:H5'	2.17	0.45
1:A:1296:C:H5''	13:M:14:ARG:HD2	1.97	0.45
2:B:73:THR:C	2:B:75:LYS:H	2.24	0.45
2:B:111:ARG:CB	2:B:149:LEU:HD11	2.43	0.45
6:F:4:TYR:CE1	6:F:92:LYS:HG2	2.51	0.45
12:L:57:LYS:HE3	12:L:65:GLU:CD	2.42	0.45
14:N:24:CYS:HB2	14:N:29:ARG:HB3	1.98	0.45
21:U:6:ARG:HE	21:U:15:ARG:HE	1.62	0.45
1:A:489:C:H2'	1:A:490:G:H8	1.82	0.45
1:A:736:C:H2'	1:A:737:A:C8	2.50	0.45
1:A:1315:U:H2'	1:A:1316:G:O4'	2.17	0.45
2:B:126:GLU:O	2:B:127:ILE:C	2.60	0.45
3:C:70:VAL:HG12	3:C:71:ALA:H	1.82	0.45
5:E:51:VAL:O	5:E:55:VAL:HG23	2.16	0.45
9:I:36:TYR:CD2	9:I:37:PHE:CE2	3.04	0.45
9:I:100:GLY:C	9:I:102:LEU:H	2.25	0.45
10:J:71:LEU:HD13	10:J:72:VAL:N	2.31	0.45
13:M:31:LYS:O	13:M:35:GLU:HB2	2.16	0.45
15:O:17:ARG:NH1	15:O:17:ARG:CG	2.79	0.45
17:Q:3:LYS:CB	17:Q:61:GLU:HB2	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:43:LEU:HD12	20:T:52:ALA:HA	1.98	0.45
1:A:1003:G:N2	1:A:1038:C:C2	2.84	0.45
1:A:1481:U:C2'	1:A:1482:G:H5'	2.46	0.45
10:J:26:ALA:HB3	10:J:85:LEU:CD2	2.47	0.45
14:N:14:PRO:O	14:N:15:LYS:CB	2.59	0.45
15:O:65:ARG:HG2	15:O:65:ARG:NH1	2.28	0.45
19:S:10:PHE:H	19:S:10:PHE:HD2	1.65	0.45
21:U:2:GLY:C	21:U:4:GLY:N	2.74	0.45
1:A:370:C:C2'	1:A:371:G:H5'	2.47	0.45
1:A:993:G:O2'	1:A:994:A:P	2.75	0.45
1:A:1152:A:H2'	1:A:1153:C:H6	1.78	0.45
5:E:129:ILE:HG23	5:E:133:TYR:HE1	1.81	0.45
5:E:144:THR:HG23	5:E:146:ALA:H	1.80	0.45
6:F:40:VAL:HG23	6:F:62:TRP:O	2.16	0.45
9:I:4:TYR:CE2	9:I:88:TYR:HD1	2.35	0.45
17:Q:95:TYR:N	17:Q:95:TYR:CD1	2.85	0.45
1:A:243:A:C2	1:A:246:A:C8	3.05	0.45
1:A:539:A:H2'	1:A:540:G:H8	1.80	0.45
1:A:825:G:N2	8:H:11:THR:HG21	2.32	0.45
1:A:1047:G:C2'	1:A:1048:G:C5'	2.83	0.45
1:A:1328:C:OP2	21:U:7:ARG:HD3	2.17	0.45
1:A:1427:U:H2'	1:A:1428:A:H8	1.81	0.45
1:A:1488:G:H2'	1:A:1489:G:C8	2.51	0.45
2:B:209:ARG:HG2	2:B:209:ARG:HH11	1.82	0.45
6:F:75:LEU:O	6:F:78:GLU:HB3	2.17	0.45
7:G:156:TRP:CD1	7:G:156:TRP:C	2.94	0.45
8:H:4:ASP:C	8:H:4:ASP:OD1	2.60	0.45
12:L:93:LEU:HB2	12:L:96:VAL:CG2	2.46	0.45
15:O:10:LYS:HE2	15:O:14:GLU:HB2	1.99	0.45
20:T:10:LEU:O	20:T:12:ALA:N	2.50	0.45
1:A:628:G:O2'	1:A:629:G:H5'	2.17	0.45
2:B:27:LYS:C	2:B:29:ALA:H	2.24	0.45
2:B:165:VAL:O	2:B:187:LEU:O	2.35	0.45
3:C:154:SER:HB3	3:C:165:THR:HG23	1.99	0.45
6:F:42:GLU:HG3	6:F:61:LEU:HD23	1.98	0.45
10:J:79:ARG:O	10:J:83:GLU:OE1	2.35	0.45
13:M:125:ARG:HD2	13:M:125:ARG:C	2.41	0.45
17:Q:55:ASP:OD1	17:Q:79:SER:HB3	2.17	0.45
1:A:399:G:H2'	1:A:400:C:C6	2.52	0.44
1:A:408:A:O2'	1:A:409:G:H5'	2.17	0.44
1:A:543:C:O2'	1:A:544:G:H5'	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:951:G:O6	13:M:105:THR:HG21	2.17	0.44
1:A:1227:A:H8	1:A:1227:A:H3'	1.80	0.44
2:B:223:ILE:HA	2:B:226:ARG:NH2	2.32	0.44
3:C:100:ALA:HB1	3:C:102:ASN:HD21	1.82	0.44
4:D:42:GLN:CG	4:D:42:GLN:O	2.65	0.44
5:E:28:PHE:CD2	5:E:51:VAL:HG22	2.52	0.44
10:J:27:ALA:HA	10:J:81:THR:CG2	2.36	0.44
12:L:115:LYS:O	12:L:117:ARG:N	2.47	0.44
1:A:472:A:H4'	16:P:80:PHE:O	2.17	0.44
1:A:536:C:H2'	1:A:537:G:C8	2.52	0.44
1:A:768:A:H2'	1:A:769:G:O4'	2.17	0.44
1:A:814:A:H2'	1:A:816:A:H5''	2.00	0.44
1:A:1074:G:O3'	2:B:103:THR:CG2	2.65	0.44
1:A:1118:C:H1'	1:A:1179:A:C4	2.52	0.44
1:A:1460:A:H2'	1:A:1461:G:O4'	2.17	0.44
2:B:15:VAL:HG21	2:B:210:SER:N	2.32	0.44
2:B:142:LEU:O	2:B:146:GLN:HG3	2.18	0.44
2:B:217:ARG:HA	2:B:220:ASP:OD2	2.17	0.44
9:I:10:ARG:HG2	9:I:75:ASP:CB	2.48	0.44
10:J:48:THR:HG1	10:J:62:HIS:CD2	2.35	0.44
10:J:55:LYS:HG3	10:J:56:HIS:H	1.82	0.44
11:K:16:SER:HA	11:K:79:SER:O	2.16	0.44
14:N:6:LEU:C	14:N:8:GLU:N	2.75	0.44
16:P:57:ARG:HH12	16:P:79:VAL:CA	2.29	0.44
18:R:44:LEU:CD1	18:R:79:LEU:HD22	2.47	0.44
1:A:149:A:H2'	1:A:150:C:C6	2.52	0.44
1:A:168:G:O2'	1:A:169:C:H5'	2.18	0.44
1:A:1305:G:O2'	1:A:1331:G:N2	2.50	0.44
2:B:55:PHE:O	2:B:58:ILE:HB	2.18	0.44
3:C:11:ARG:O	3:C:12:LEU:C	2.60	0.44
3:C:136:GLN:O	3:C:137:ALA:C	2.59	0.44
4:D:201:GLN:O	4:D:205:GLU:HG3	2.17	0.44
9:I:11:LYS:O	9:I:12:GLU:HB3	2.17	0.44
9:I:34:ASN:O	9:I:38:GLN:HB2	2.17	0.44
11:K:116:HIS:O	11:K:117:ASN:HB2	2.18	0.44
17:Q:66:SER:OG	17:Q:69:LYS:HB2	2.18	0.44
18:R:69:THR:O	18:R:72:ARG:HB2	2.18	0.44
1:A:57:G:H2'	1:A:58:C:H6	1.77	0.44
1:A:862:C:O2'	1:A:863:U:H5'	2.17	0.44
1:A:1084:G:H5'	1:A:1102:A:OP2	2.17	0.44
1:A:1318:A:H1'	19:S:37:ARG:HH11	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1347:G:H2'	1:A:1373:G:N1	2.32	0.44
1:A:1349:A:P	9:I:118:LYS:NZ	2.90	0.44
4:D:175:SER:HG	4:D:184:LYS:HB3	1.81	0.44
11:K:40:ILE:HG23	11:K:75:TYR:CE2	2.52	0.44
12:L:57:LYS:HE3	12:L:65:GLU:HG2	1.98	0.44
14:N:50:LYS:HB3	14:N:50:LYS:HE2	1.75	0.44
15:O:26:GLU:HA	15:O:81:LEU:HD11	1.99	0.44
18:R:17:SER:CB	18:R:54:ARG:HB3	2.48	0.44
20:T:70:SER:O	20:T:71:THR:C	2.60	0.44
1:A:403:C:O2'	1:A:404:U:H5'	2.17	0.44
1:A:502:G:O2'	1:A:503:C:H5'	2.18	0.44
1:A:554:C:H2'	1:A:555:C:H6	1.83	0.44
1:A:716:A:N3	11:K:117:ASN:O	2.51	0.44
1:A:1005:A:H2'	1:A:1006:C:H5'	1.99	0.44
1:A:1372:U:C2'	1:A:1373:G:H5'	2.48	0.44
2:B:216:SER:OG	2:B:217:ARG:N	2.51	0.44
5:E:76:ILE:HG23	5:E:77:PRO:HD2	1.99	0.44
8:H:122:ARG:CB	8:H:122:ARG:HH11	2.31	0.44
9:I:8:GLY:HA2	9:I:79:LEU:HB3	1.98	0.44
9:I:47:LEU:C	9:I:49:PRO:HD2	2.41	0.44
13:M:62:ASN:HD22	13:M:62:ASN:HA	1.64	0.44
13:M:119:GLY:O	13:M:121:LYS:HG3	2.17	0.44
16:P:8:ARG:HG2	16:P:17:TYR:CE2	2.53	0.44
18:R:59:SER:O	18:R:60:ALA:C	2.61	0.44
20:T:57:ARG:CZ	20:T:102:GLY:HA3	2.46	0.44
1:A:142:G:N3	1:A:196:A:C2	2.86	0.44
1:A:192:U:H4'	20:T:102:GLY:C	2.40	0.44
1:A:911:U:OP1	12:L:95:GLY:HA2	2.18	0.44
1:A:1251:A:H5''	9:I:12:GLU:OE2	2.17	0.44
2:B:15:VAL:HG21	2:B:210:SER:CA	2.47	0.44
2:B:53:ARG:NH1	2:B:199:TYR:HD2	2.16	0.44
3:C:87:LEU:C	3:C:89:GLU:H	2.25	0.44
4:D:140:VAL:CG1	4:D:146:ILE:HD11	2.47	0.44
6:F:10:LEU:HD23	6:F:85:VAL:HA	2.00	0.44
7:G:115:ARG:HB2	7:G:118:VAL:HG23	2.00	0.44
7:G:126:ASP:OD1	7:G:131:LYS:HE3	2.17	0.44
10:J:20:ALA:C	10:J:22:LYS:N	2.75	0.44
12:L:56:ALA:O	12:L:67:THR:HA	2.17	0.44
13:M:120:LYS:HZ1	13:M:122:LYS:HB3	1.80	0.44
17:Q:22:LEU:HD12	17:Q:23:VAL:H	1.82	0.44
19:S:13:ASP:O	19:S:17:GLU:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:44:MET:HB2	19:S:62:ILE:CD1	2.48	0.44
1:A:187:C:C1'	20:T:85:MET:HE2	2.48	0.44
1:A:730:G:C5	1:A:731:G:H1'	2.52	0.44
1:A:1042:G:O2'	1:A:1043:C:H5'	2.18	0.44
1:A:1130:A:P	1:A:1131:G:OP2	2.75	0.44
3:C:69:HIS:HA	3:C:104:GLN:O	2.17	0.44
3:C:113:ALA:N	3:C:114:PRO:CD	2.80	0.44
4:D:3:ARG:HH12	4:D:115:ARG:HB3	1.81	0.44
5:E:144:THR:HG23	5:E:146:ALA:N	2.33	0.44
6:F:69:GLU:HA	6:F:72:VAL:HG23	2.00	0.44
8:H:85:ARG:C	8:H:85:ARG:HD3	2.43	0.44
8:H:87:SER:CB	8:H:93:VAL:H	2.31	0.44
8:H:105:ARG:H	8:H:105:ARG:HD3	1.83	0.44
9:I:117:HIS:C	9:I:118:LYS:HG3	2.41	0.44
10:J:21:GLN:O	10:J:25:GLU:HG2	2.17	0.44
12:L:54:LYS:N	12:L:54:LYS:HD2	2.33	0.44
13:M:57:ARG:HE	13:M:57:ARG:HB2	1.56	0.44
13:M:87:TYR:O	13:M:90:LEU:HB2	2.18	0.44
15:O:4:THR:OG1	15:O:7:GLU:HG3	2.18	0.44
16:P:28:ARG:HH11	16:P:29:ASP:CG	2.25	0.44
19:S:17:GLU:HA	19:S:20:LEU:HG	1.98	0.44
1:A:22:G:H4'	1:A:885:G:C8	2.52	0.44
1:A:119:A:H4'	1:A:120:A:O5'	2.17	0.44
1:A:186:C:O2	20:T:85:MET:HE1	2.17	0.44
1:A:473:G:H5''	16:P:81:ARG:NH1	2.32	0.44
1:A:1123:A:O2'	10:J:38:ILE:HG23	2.18	0.44
2:B:114:ARG:HH11	2:B:118:LEU:HB2	1.82	0.44
3:C:172:ARG:HH12	3:C:174:PRO:CG	2.27	0.44
4:D:3:ARG:NH1	4:D:115:ARG:HD2	2.28	0.44
4:D:36:ARG:HA	4:D:38:TYR:CE2	2.53	0.44
8:H:121:ASP:OD2	8:H:125:ARG:NH2	2.51	0.44
10:J:42:THR:HG22	10:J:43:ARG:N	2.31	0.44
17:Q:95:TYR:C	17:Q:97:SER:N	2.76	0.44
18:R:26:LEU:HD21	18:R:39:VAL:CG2	2.47	0.44
19:S:66:MET:HE3	19:S:74:PHE:CD2	2.53	0.44
20:T:24:LEU:HD12	20:T:24:LEU:HA	1.74	0.44
1:A:255:G:O6	1:A:266:G:O6	2.35	0.44
1:A:969:A:C2'	1:A:970:C:H5'	2.48	0.44
2:B:55:PHE:CE2	2:B:218:ALA:HA	2.52	0.44
3:C:76:VAL:O	3:C:83:ARG:HG3	2.17	0.44
3:C:162:GLN:O	3:C:164:ARG:HG2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:42:GLU:HG3	6:F:61:LEU:CD2	2.48	0.44
8:H:95:VAL:HB	8:H:99:GLU:HB2	2.00	0.44
9:I:10:ARG:CZ	9:I:105:ASP:OD2	2.65	0.44
9:I:27:THR:OG1	9:I:30:GLY:HA2	2.18	0.44
16:P:81:ARG:HG2	16:P:83:GLU:OE2	2.18	0.44
1:A:376:G:P	16:P:67:THR:HG21	2.57	0.43
1:A:1000:U:O2'	1:A:1001:A:H5'	2.19	0.43
1:A:1020:U:H2'	1:A:1021:G:C8	2.53	0.43
5:E:112:LEU:HD23	5:E:112:LEU:HA	1.85	0.43
10:J:29:ARG:H	10:J:29:ARG:HG2	1.65	0.43
13:M:108:ARG:NH2	13:M:114:ARG:HA	2.33	0.43
14:N:15:LYS:HB3	14:N:16:PHE:CD1	2.53	0.43
1:A:29:G:O2'	1:A:30:U:H5'	2.18	0.43
1:A:490:G:O2'	1:A:491:G:H5'	2.18	0.43
1:A:946:A:H2'	1:A:947:G:H8	1.77	0.43
1:A:983:A:HO2'	1:A:1049:U:HO2'	1.66	0.43
1:A:1010:G:O2'	1:A:1011:G:H5'	2.18	0.43
1:A:1174:G:H2'	1:A:1175:G:H8	1.83	0.43
2:B:90:MET:HA	2:B:91:PRO:HD3	1.72	0.43
4:D:122:ARG:HA	4:D:122:ARG:HE	1.83	0.43
7:G:27:ILE:HD11	7:G:43:PHE:CD2	2.53	0.43
7:G:52:GLU:HG2	7:G:52:GLU:O	2.17	0.43
7:G:115:ARG:O	7:G:116:ALA:C	2.61	0.43
8:H:30:ARG:O	8:H:33:GLU:HB3	2.18	0.43
8:H:60:ARG:NH1	8:H:60:ARG:CG	2.78	0.43
9:I:19:LEU:HB3	9:I:59:PHE:CD2	2.53	0.43
9:I:81:ILE:O	9:I:85:LEU:HB2	2.18	0.43
15:O:88:ARG:HB3	15:O:89:GLY:H	1.66	0.43
1:A:583:A:H2'	1:A:584:G:O4'	2.18	0.43
1:A:633:G:H2'	1:A:634:C:C6	2.52	0.43
1:A:949:A:H2'	1:A:950:U:O4'	2.18	0.43
2:B:78:GLN:O	2:B:94:ASN:ND2	2.51	0.43
4:D:25:ARG:HH11	4:D:25:ARG:CG	2.31	0.43
4:D:61:LYS:O	4:D:62:GLN:C	2.61	0.43
6:F:45:LEU:HA	6:F:58:GLY:O	2.18	0.43
10:J:75:ILE:O	10:J:76:ASN:ND2	2.51	0.43
10:J:81:THR:HG22	10:J:85:LEU:CD1	2.47	0.43
11:K:33:THR:HG22	11:K:39:PRO:HA	2.00	0.43
13:M:25:ILE:HD11	13:M:60:VAL:HG13	2.00	0.43
15:O:64:ARG:HH11	15:O:64:ARG:HB2	1.81	0.43
18:R:37:VAL:O	18:R:41:LYS:CB	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:66:MET:HE3	19:S:74:PHE:CE2	2.54	0.43
20:T:39:LYS:O	20:T:43:LEU:HG	2.18	0.43
1:A:302:G:N3	1:A:556:C:H4'	2.34	0.43
1:A:431:A:H2'	1:A:432:A:O4'	2.19	0.43
1:A:839:U:O2	1:A:839:U:C2'	2.66	0.43
1:A:1264:C:O2'	1:A:1265:G:H5'	2.19	0.43
1:A:1301:U:O2'	1:A:1302:U:OP1	2.34	0.43
2:B:207:ALA:O	2:B:208:ILE:C	2.61	0.43
4:D:25:ARG:HH11	4:D:25:ARG:HG2	1.83	0.43
4:D:91:SER:O	4:D:92:VAL:C	2.60	0.43
4:D:196:LEU:C	4:D:198:VAL:H	2.26	0.43
5:E:89:ILE:CD1	5:E:90:VAL:N	2.80	0.43
5:E:135:THR:O	5:E:138:ALA:HB3	2.18	0.43
10:J:63:PHE:HA	14:N:57:ARG:O	2.18	0.43
10:J:81:THR:HG22	10:J:85:LEU:HD12	2.00	0.43
17:Q:48:GLU:C	17:Q:50:LYS:N	2.76	0.43
18:R:37:VAL:HG22	18:R:78:LEU:HB3	1.99	0.43
20:T:48:LYS:HD3	20:T:48:LYS:N	2.33	0.43
1:A:142:G:O2'	1:A:196:A:N1	2.48	0.43
1:A:342:C:H2'	1:A:343:U:H5'	2.00	0.43
1:A:357:G:O2'	1:A:358:U:H5'	2.18	0.43
1:A:692:U:H2'	1:A:694:A:OP2	2.18	0.43
1:A:797:C:O2'	1:A:798:G:H5'	2.18	0.43
1:A:1329:A:C2'	1:A:1330:U:H5'	2.48	0.43
1:A:1360:A:O2'	1:A:1361:G:H5'	2.18	0.43
1:A:1372:U:H2'	1:A:1373:G:O4'	2.19	0.43
3:C:134:ILE:HD11	3:C:153:VAL:HB	2.00	0.43
6:F:74:ASP:OD1	6:F:77:ARG:NH2	2.52	0.43
9:I:9:ARG:HG3	9:I:14:VAL:HA	2.00	0.43
10:J:7:LYS:NZ	10:J:40:LEU:HD11	2.32	0.43
13:M:8:GLU:HA	13:M:8:GLU:OE2	2.19	0.43
15:O:74:ASP:CG	15:O:77:ARG:HG3	2.43	0.43
16:P:53:VAL:O	16:P:57:ARG:HG3	2.17	0.43
20:T:13:LEU:HD12	20:T:14:LYS:N	2.33	0.43
1:A:34:C:H1'	12:L:32:PHE:CZ	2.53	0.43
1:A:343:U:H2'	1:A:345:C:C4	2.53	0.43
1:A:434:U:H2'	1:A:435:C:C6	2.53	0.43
1:A:954:G:H2'	1:A:955:U:H6	1.83	0.43
1:A:1014:A:H2'	1:A:1015:A:C8	2.53	0.43
2:B:196:LEU:HD12	2:B:196:LEU:N	2.33	0.43
6:F:14:LEU:CA	6:F:18:GLN:HE21	2.28	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:62:TRP:CD1	18:R:35:ARG:CZ	3.02	0.43
9:I:128:ARG:CZ	9:I:128:ARG:HB2	2.49	0.43
10:J:50:ILE:HD11	10:J:57:LYS:HD3	2.00	0.43
16:P:20:VAL:CG1	16:P:32:TYR:HB2	2.49	0.43
1:A:6:G:H4'	1:A:298:A:H4'	2.00	0.43
1:A:148:G:H2'	1:A:149:A:C8	2.53	0.43
1:A:316:G:H2'	1:A:317:G:H8	1.84	0.43
1:A:579:G:C5'	1:A:728:A:H1'	2.39	0.43
1:A:1015:A:H2'	1:A:1016:A:C8	2.54	0.43
1:A:1060:C:H2'	1:A:1061:G:H8	1.83	0.43
1:A:1105:A:H2'	1:A:1106:G:H8	1.83	0.43
1:A:1176:A:H2'	1:A:1177:G:O4'	2.18	0.43
1:A:1227:A:H3'	1:A:1227:A:C8	2.53	0.43
1:A:1278:U:H5''	1:A:1279:A:O4'	2.18	0.43
1:A:1366:C:C2	1:A:1367:C:C5	3.07	0.43
1:A:1419:G:H2'	1:A:1420:C:O4'	2.18	0.43
1:A:1478:C:O2'	1:A:1479:C:H5'	2.19	0.43
2:B:63:MET:O	2:B:63:MET:HE3	2.18	0.43
2:B:114:ARG:HH11	2:B:118:LEU:HD12	1.82	0.43
3:C:28:GLN:HA	3:C:31:HIS:HD2	1.83	0.43
4:D:58:LEU:CD2	4:D:58:LEU:C	2.91	0.43
5:E:76:ILE:HG13	5:E:142:LEU:CD1	2.49	0.43
6:F:94:GLN:CD	18:R:32:ARG:HD3	2.44	0.43
10:J:80:LYS:HB2	10:J:80:LYS:NZ	2.34	0.43
12:L:60:LEU:N	12:L:64:TYR:O	2.36	0.43
14:N:8:GLU:O	14:N:10:ALA:N	2.51	0.43
1:A:335:C:O2'	1:A:336:C:H5'	2.18	0.43
1:A:513:C:H2'	1:A:514:C:H6	1.84	0.43
1:A:1497:G:O2'	1:A:1498:U:H5'	2.18	0.43
4:D:10:ARG:HH11	4:D:10:ARG:HG3	1.84	0.43
4:D:98:GLU:CG	4:D:189:PRO:HG3	2.47	0.43
5:E:20:GLN:O	5:E:21:ALA:C	2.61	0.43
7:G:54:THR:C	7:G:56:GLN:N	2.76	0.43
7:G:84:ASN:O	7:G:85:TYR:HD2	2.01	0.43
14:N:8:GLU:OE1	14:N:9:LYS:N	2.51	0.43
1:A:1226:C:H5'	19:S:80:TYR:CE1	2.54	0.43
1:A:1288:A:H2'	1:A:1289:A:C8	2.54	0.43
2:B:172:ILE:O	2:B:172:ILE:HG22	2.18	0.43
4:D:199:ASN:HD22	4:D:199:ASN:C	2.25	0.43
5:E:31:LEU:HD23	5:E:31:LEU:HA	1.86	0.43
6:F:4:TYR:OH	6:F:72:VAL:HG21	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:83:ILE:HD12	11:K:83:ILE:N	2.33	0.43
12:L:24:VAL:O	12:L:24:VAL:HG12	2.18	0.43
14:N:3:ARG:O	14:N:4:LYS:C	2.61	0.43
17:Q:18:THR:HG23	17:Q:69:LYS:HE3	2.00	0.43
17:Q:29:HIS:CG	17:Q:30:PRO:HD2	2.53	0.43
20:T:53:LEU:O	20:T:57:ARG:HD2	2.19	0.43
1:A:173:U:H6	1:A:198:G:HO2'	1.64	0.43
1:A:335:C:H2'	1:A:336:C:H6	1.83	0.43
1:A:1010:G:H2'	1:A:1011:G:H8	1.83	0.43
1:A:1047:G:O2'	1:A:1048:G:H5''	2.17	0.43
1:A:1349:A:OP2	9:I:118:LYS:NZ	2.52	0.43
3:C:46:GLU:C	3:C:48:TYR:H	2.27	0.43
6:F:3:ARG:HB2	6:F:3:ARG:CZ	2.49	0.43
7:G:150:ALA:O	11:K:57:THR:HG21	2.19	0.43
9:I:87:GLN:O	9:I:88:TYR:C	2.62	0.43
1:A:283:C:C2	1:A:284:G:C8	3.06	0.42
1:A:1198:G:H2'	1:A:1199:U:C6	2.54	0.42
1:A:1232:U:P	9:I:124:GLN:HE21	2.42	0.42
1:A:1422:G:O2'	1:A:1423:G:H5'	2.19	0.42
2:B:14:GLY:O	2:B:15:VAL:HG22	2.18	0.42
2:B:21:ARG:HB2	2:B:22:LYS:H	1.61	0.42
4:D:15:GLU:C	4:D:17:VAL:H	2.27	0.42
5:E:144:THR:O	5:E:147:ASP:N	2.52	0.42
8:H:80:ILE:O	8:H:80:ILE:HG22	2.18	0.42
9:I:11:LYS:O	9:I:12:GLU:CB	2.65	0.42
12:L:73:GLU:O	12:L:74:GLY:O	2.37	0.42
14:N:36:PHE:O	14:N:36:PHE:CD1	2.72	0.42
15:O:76:GLU:C	15:O:78:TYR:N	2.77	0.42
16:P:20:VAL:CG1	16:P:32:TYR:CB	2.97	0.42
16:P:43:LYS:CG	16:P:48:TRP:CD2	3.01	0.42
17:Q:60:ILE:C	17:Q:71:PHE:HD1	2.26	0.42
17:Q:67:LYS:O	17:Q:68:ARG:HB3	2.17	0.42
17:Q:68:ARG:H	17:Q:70:ARG:HH11	1.59	0.42
18:R:51:LEU:HA	18:R:52:PRO:HD3	1.84	0.42
1:A:1001(A):G:H2'	1:A:1002:G:H8	1.84	0.42
1:A:1129:C:OP1	1:A:1130:A:H5''	2.19	0.42
1:A:1250:A:H5'	9:I:68:GLY:O	2.19	0.42
2:B:61:LEU:HD13	2:B:61:LEU:C	2.43	0.42
2:B:73:THR:O	2:B:75:LYS:N	2.52	0.42
2:B:213:LEU:HD23	2:B:213:LEU:O	2.18	0.42
2:B:223:ILE:C	2:B:225:ALA:N	2.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:195:VAL:O	3:C:196:LEU:HD22	2.19	0.42
12:L:110:VAL:O	12:L:122:THR:OG1	2.35	0.42
14:N:11:LYS:C	14:N:13:THR:N	2.74	0.42
16:P:59:TRP:HB3	16:P:64:ALA:CB	2.49	0.42
17:Q:95:TYR:N	17:Q:95:TYR:HD1	2.17	0.42
1:A:102:G:N3	1:A:151:A:H2	2.17	0.42
1:A:327:A:O3'	1:A:328:C:H4'	2.19	0.42
1:A:782:A:H2'	1:A:783:C:O4'	2.19	0.42
1:A:841:U:H3'	1:A:848:C:O4'	2.19	0.42
1:A:1053:G:H3'	1:A:1054:C:C5'	2.48	0.42
1:A:1086:U:H3	1:A:1099:G:N2	2.13	0.42
1:A:1304:G:C6	1:A:1305:G:N1	2.88	0.42
7:G:43:PHE:O	7:G:46:ALA:HB3	2.20	0.42
9:I:79:LEU:HD23	9:I:101:PHE:O	2.19	0.42
9:I:114:TYR:CE1	10:J:59:SER:O	2.73	0.42
11:K:18:ARG:HH11	11:K:37:GLY:N	2.16	0.42
11:K:30:VAL:HG21	11:K:65:ALA:HA	2.02	0.42
13:M:99:ARG:HG2	13:M:99:ARG:NH1	2.31	0.42
17:Q:27:PHE:HD1	17:Q:28:PRO:O	2.03	0.42
1:A:131:C:H2'	1:A:132:C:C6	2.55	0.42
1:A:594:G:H2'	1:A:595:G:H5'	2.00	0.42
1:A:685:G:C2	1:A:686:U:C4	3.08	0.42
1:A:837:G:H1	1:A:849:C:H42	1.67	0.42
3:C:126:ARG:O	3:C:127:ARG:C	2.61	0.42
3:C:188:LEU:HD13	3:C:189:ALA:N	2.33	0.42
5:E:80:ILE:HD11	5:E:91:LEU:CB	2.38	0.42
6:F:33:TYR:HA	6:F:71:ARG:NH2	2.26	0.42
9:I:9:ARG:HD3	9:I:14:VAL:HG12	2.02	0.42
10:J:9:ARG:HG3	10:J:9:ARG:O	2.18	0.42
15:O:81:LEU:CD2	15:O:85:LEU:HD12	2.49	0.42
16:P:67:THR:CG2	16:P:68:ASP:N	2.81	0.42
17:Q:67:LYS:CA	17:Q:70:ARG:NH1	2.78	0.42
20:T:29:LYS:O	20:T:33:ILE:HG13	2.20	0.42
1:A:8:A:N6	4:D:205:GLU:O	2.52	0.42
1:A:107:G:H2'	1:A:108:G:C5'	2.49	0.42
1:A:112:G:H5'	1:A:389:A:H4'	2.00	0.42
1:A:131:C:H2'	1:A:132:C:H6	1.85	0.42
1:A:554:C:H2'	1:A:555:C:C6	2.55	0.42
1:A:693:G:C8	1:A:1539:C:H1'	2.55	0.42
1:A:1179:A:C2'	1:A:1180:A:H5'	2.49	0.42
1:A:1238:A:OP1	1:A:1336:C:H5	2.03	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1357:A:C8	1:A:1358:U:C5	3.07	0.42
1:A:1416:G:C2'	1:A:1417:G:H5'	2.49	0.42
2:B:73:THR:HB	2:B:170:GLU:OE1	2.19	0.42
2:B:204:ASN:ND2	2:B:206:ASP:N	2.66	0.42
3:C:11:ARG:O	3:C:14:ILE:O	2.37	0.42
6:F:3:ARG:HD3	6:F:64:GLN:NE2	2.34	0.42
7:G:136:LYS:O	7:G:137:LYS:C	2.62	0.42
8:H:104:ARG:O	8:H:105:ARG:C	2.61	0.42
9:I:9:ARG:CD	9:I:14:VAL:HG12	2.49	0.42
9:I:17:VAL:HG21	9:I:80:GLY:HA3	2.01	0.42
11:K:58:PRO:O	11:K:61:ALA:HB3	2.18	0.42
16:P:4:ILE:HG13	16:P:64:ALA:HB1	2.02	0.42
17:Q:24:GLU:CD	17:Q:37:LYS:HD3	2.45	0.42
17:Q:51:TYR:CD1	17:Q:51:TYR:N	2.87	0.42
18:R:36:ASN:HD21	18:R:38:GLU:HB2	1.84	0.42
20:T:30:LYS:O	20:T:31:SER:C	2.61	0.42
1:A:115:G:H1'	1:A:116:A:N7	2.35	0.42
1:A:1004:A:H8	1:A:1036:G:N2	2.16	0.42
1:A:1298:C:H4'	1:A:1299:A:O4'	2.20	0.42
1:A:1359:C:OP1	14:N:22:THR:HG22	2.19	0.42
1:A:1435:G:H2'	1:A:1436:U:H6	1.78	0.42
1:A:1496:C:H2'	1:A:1497:G:O4'	2.20	0.42
2:B:120:ALA:C	2:B:122:PHE:N	2.77	0.42
3:C:79:ARG:HG3	3:C:79:ARG:NH1	2.35	0.42
3:C:134:ILE:HG22	3:C:168:ALA:HB3	2.02	0.42
3:C:157:ILE:HD12	3:C:166:GLU:HG3	2.02	0.42
8:H:48:TYR:O	8:H:49:GLU:HB3	2.18	0.42
8:H:50:ARG:O	8:H:51:VAL:HG13	2.20	0.42
10:J:90:LEU:H	10:J:91:PRO:HD3	1.84	0.42
11:K:48:ILE:HD13	11:K:48:ILE:N	2.34	0.42
1:A:706:A:H1'	11:K:29:ILE:HD11	2.02	0.42
1:A:1005:A:H2'	1:A:1006:C:O4'	2.19	0.42
1:A:1360:A:H8	1:A:1360:A:OP1	2.02	0.42
2:B:68:ILE:O	2:B:90:MET:HB3	2.20	0.42
8:H:4:ASP:CG	8:H:85:ARG:NH1	2.78	0.42
8:H:35:ILE:HG22	8:H:39:LEU:CD2	2.49	0.42
10:J:18:ALA:C	10:J:20:ALA:N	2.75	0.42
1:A:268:C:H2'	1:A:269:C:H6	1.84	0.42
1:A:291:C:O2'	1:A:292:G:H5'	2.19	0.42
1:A:620:C:C1'	4:D:135:LEU:HD13	2.49	0.42
1:A:718:G:H5'	11:K:117:ASN:HD22	1.79	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:737:A:H1'	6:F:73:ASN:ND2	2.34	0.42
1:A:1026:G:C3'	1:A:1027:C:C5'	2.94	0.42
1:A:1074:G:O2'	2:B:103:THR:HG22	2.20	0.42
1:A:1108:G:H4'	1:A:1191:A:O4'	2.20	0.42
1:A:1206:G:C6	1:A:1207:G:C5	3.07	0.42
1:A:1251:A:H1'	1:A:1369:C:O2'	2.19	0.42
2:B:24:TRP:N	2:B:24:TRP:CD1	2.86	0.42
2:B:61:LEU:HD21	2:B:160:ASP:HB2	2.01	0.42
2:B:132:LYS:N	2:B:132:LYS:HD2	2.35	0.42
3:C:8:ILE:O	3:C:9:GLY:C	2.63	0.42
3:C:107:GLN:O	3:C:108:ASN:CB	2.68	0.42
4:D:26:CYS:HA	4:D:31:CYS:HB2	2.01	0.42
10:J:81:THR:C	10:J:83:GLU:N	2.77	0.42
13:M:59:TYR:CD1	13:M:59:TYR:C	2.97	0.42
1:A:267:C:OP1	17:Q:67:LYS:HB2	2.19	0.42
1:A:298:A:H2'	1:A:299:G:O4'	2.20	0.42
1:A:669:U:H2'	1:A:670:G:C8	2.55	0.42
1:A:1305:G:H5''	21:U:4:GLY:C	2.45	0.42
1:A:1505:G:C8	1:A:1505:G:H3'	2.55	0.42
2:B:134:GLU:C	2:B:136:VAL:H	2.28	0.42
2:B:213:LEU:C	2:B:213:LEU:CD2	2.92	0.42
3:C:131:ARG:HD3	3:C:166:GLU:OE2	2.19	0.42
5:E:78:HIS:HD2	8:H:107:LEU:HD12	1.85	0.42
7:G:144:MET:O	7:G:145:ALA:C	2.63	0.42
9:I:33:PHE:C	9:I:35:GLU:H	2.28	0.42
10:J:40:LEU:HB2	10:J:69:ASN:HB3	2.01	0.42
11:K:34:ASP:OD1	11:K:34:ASP:C	2.63	0.42
13:M:120:LYS:HE3	13:M:122:LYS:C	2.45	0.42
15:O:29:VAL:HG12	15:O:85:LEU:CD1	2.50	0.42
20:T:53:LEU:HD13	20:T:101:GLY:H	1.85	0.42
1:A:41:G:H2'	1:A:42:G:H8	1.84	0.42
1:A:60:A:N1	1:A:107:G:O2'	2.47	0.42
1:A:179:A:H2'	1:A:180:U:H6	1.81	0.42
1:A:242:C:C2'	1:A:243:A:H5'	2.50	0.42
1:A:495:A:H4'	1:A:496:A:OP1	2.18	0.42
1:A:647:C:O2'	1:A:648:A:H5'	2.19	0.42
1:A:959:A:C2	1:A:1222:G:O4'	2.73	0.42
1:A:1305:G:C5'	21:U:4:GLY:HA3	2.49	0.42
2:B:14:GLY:C	2:B:15:VAL:CG2	2.93	0.42
2:B:88:ALA:HB2	2:B:219:VAL:CG1	2.45	0.42
4:D:199:ASN:C	4:D:199:ASN:ND2	2.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:128:PRO:O	5:E:129:ILE:C	2.62	0.42
7:G:5:ARG:HG2	7:G:6:ARG:H	1.84	0.42
8:H:86:ILE:HD12	8:H:133:LEU:CD2	2.50	0.42
8:H:88:LYS:O	8:H:92:ARG:HD2	2.20	0.42
9:I:99:LEU:CB	9:I:101:PHE:CE1	3.02	0.42
17:Q:78:GLU:OE2	17:Q:81:ARG:HD2	2.20	0.42
19:S:16:LEU:O	19:S:20:LEU:HG	2.20	0.42
1:A:429:U:H1'	1:A:430:A:H5''	2.02	0.41
1:A:1275:A:H2'	1:A:1276:G:O4'	2.20	0.41
1:A:1540:U:C3'	1:A:1540:U:C6	3.03	0.41
2:B:114:ARG:HA	2:B:117:GLU:HG3	2.02	0.41
5:E:43:LEU:HD11	5:E:132:ALA:HB1	2.00	0.41
5:E:144:THR:HG22	5:E:147:ASP:CG	2.45	0.41
7:G:104:LEU:HD23	7:G:104:LEU:HA	1.79	0.41
8:H:6:ILE:O	8:H:10:LEU:HG	2.19	0.41
10:J:57:LYS:CE	10:J:60:ARG:NH2	2.83	0.41
10:J:83:GLU:O	10:J:84:GLN:C	2.63	0.41
11:K:34:ASP:OD1	11:K:36:ASP:N	2.46	0.41
13:M:37:THR:HG22	13:M:37:THR:O	2.19	0.41
13:M:122:LYS:HA	13:M:122:LYS:HD2	1.84	0.41
15:O:8:LYS:O	15:O:11:VAL:CG1	2.68	0.41
17:Q:68:ARG:HA	17:Q:68:ARG:HD2	1.87	0.41
1:A:105:G:H2'	1:A:106:C:H6	1.84	0.41
1:A:162:A:H2'	1:A:163:C:H5'	2.01	0.41
1:A:182:U:O4	1:A:223:U:H1'	2.20	0.41
1:A:818:G:H3'	1:A:819:A:H5''	2.02	0.41
2:B:82:ARG:HB2	2:B:94:ASN:HD22	1.85	0.41
3:C:25:GLY:O	3:C:27:LYS:N	2.54	0.41
3:C:119:ARG:HE	3:C:140:ARG:HE	1.65	0.41
3:C:147:LYS:HE2	3:C:205:GLY:CA	2.46	0.41
4:D:199:ASN:ND2	4:D:201:GLN:HB2	2.35	0.41
8:H:122:ARG:HB3	8:H:122:ARG:HH11	1.80	0.41
1:A:323:U:H5'	20:T:23:ARG:HB2	2.02	0.41
1:A:532:A:O2'	1:A:533:A:P	2.79	0.41
4:D:155:LEU:O	4:D:156:GLU:C	2.63	0.41
5:E:129:ILE:HD12	5:E:129:ILE:N	2.33	0.41
5:E:136:MET:O	5:E:137:GLU:C	2.63	0.41
6:F:30:LEU:O	6:F:35:ALA:HB3	2.21	0.41
8:H:86:ILE:CD1	8:H:133:LEU:HD22	2.50	0.41
9:I:23:ASN:HB3	9:I:60:ASP:OD1	2.21	0.41
13:M:81:LEU:HA	13:M:81:LEU:HD23	1.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:68:ARG:HH11	17:Q:68:ARG:CG	2.33	0.41
1:A:77:G:H2'	1:A:78:G:H8	1.84	0.41
1:A:187:C:H2'	1:A:188:C:C6	2.55	0.41
1:A:1110:A:H8	1:A:1110:A:O5'	2.03	0.41
1:A:1486:G:H2'	1:A:1487:G:O4'	2.20	0.41
2:B:205:ASP:OD1	2:B:206:ASP:N	2.53	0.41
3:C:6:HIS:CD2	3:C:8:ILE:HB	2.55	0.41
3:C:58:GLU:O	3:C:64:VAL:HA	2.20	0.41
6:F:15:ASP:O	6:F:17:SER:N	2.53	0.41
6:F:45:LEU:HD12	6:F:45:LEU:O	2.20	0.41
7:G:54:THR:C	7:G:56:GLN:H	2.28	0.41
8:H:48:TYR:HA	8:H:60:ARG:O	2.21	0.41
9:I:13:ALA:CB	9:I:67:GLY:O	2.69	0.41
11:K:12:ARG:O	11:K:13:GLN:O	2.38	0.41
11:K:60:ALA:O	11:K:61:ALA:C	2.62	0.41
15:O:39:LEU:HD12	15:O:56:LEU:HB2	2.01	0.41
15:O:39:LEU:HD13	15:O:39:LEU:C	2.46	0.41
19:S:40:ILE:HB	19:S:67:VAL:O	2.20	0.41
20:T:23:ARG:HH11	20:T:23:ARG:CG	2.31	0.41
1:A:253:U:H2'	1:A:254:G:C8	2.55	0.41
1:A:1055:A:C6	1:A:1206:G:C5	3.09	0.41
1:A:1056:U:C5'	3:C:163:ALA:HB2	2.50	0.41
1:A:1488:G:H2'	1:A:1489:G:H8	1.85	0.41
2:B:161:ALA:HB1	2:B:185:ILE:CD1	2.47	0.41
3:C:36:ASP:O	3:C:39:ILE:HB	2.20	0.41
3:C:102:ASN:H	3:C:102:ASN:ND2	2.16	0.41
5:E:33:VAL:HG11	5:E:109:ILE:HA	2.02	0.41
6:F:19:LEU:HD23	6:F:19:LEU:C	2.45	0.41
7:G:45:ASP:O	7:G:49:ILE:HG13	2.21	0.41
13:M:40:ASN:HD22	13:M:40:ASN:C	2.27	0.41
19:S:42:PRO:O	19:S:45:VAL:HG23	2.21	0.41
20:T:18:GLN:O	20:T:19:SER:C	2.62	0.41
1:A:98:G:H2'	1:A:99:U:O4'	2.20	0.41
1:A:279:A:C5	17:Q:98:LEU:HD12	2.55	0.41
1:A:473:G:H2'	1:A:474:G:C8	2.56	0.41
1:A:559:A:P	5:E:126:ARG:HH22	2.44	0.41
1:A:1223:C:P	19:S:78:ARG:HH12	2.43	0.41
1:A:1481:U:H2'	1:A:1482:G:O4'	2.21	0.41
2:B:59:GLU:O	2:B:62:ALA:HB3	2.21	0.41
3:C:13:GLY:CA	14:N:57:ARG:HH21	2.31	0.41
4:D:60:GLU:HA	4:D:60:GLU:OE1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:116:LYS:CD	8:H:127:LEU:HD22	2.51	0.41
11:K:21:ILE:HD13	11:K:94:ALA:CB	2.50	0.41
11:K:59:TYR:O	11:K:60:ALA:C	2.63	0.41
13:M:106:ASN:O	13:M:107:ALA:HB3	2.21	0.41
17:Q:59:ILE:HD13	17:Q:73:VAL:HA	2.03	0.41
1:A:103:C:OP2	20:T:17:ARG:NH1	2.54	0.41
1:A:220:G:O2'	1:A:221:C:H5'	2.20	0.41
1:A:421:U:H4'	1:A:422:C:OP2	2.20	0.41
1:A:701:C:O2'	1:A:702:A:P	2.78	0.41
1:A:1249:C:H4'	9:I:36:TYR:OH	2.21	0.41
1:A:1305:G:N2	1:A:1331:G:C2'	2.83	0.41
2:B:64:ARG:NH1	2:B:64:ARG:HB2	2.36	0.41
3:C:207:VAL:HG12	3:C:208:ILE:N	2.35	0.41
4:D:126:ILE:HG22	4:D:127:THR:N	2.35	0.41
7:G:37:ASN:HD21	9:I:41:VAL:HG23	1.86	0.41
7:G:78:ARG:HD3	7:G:79:ARG:N	2.35	0.41
9:I:11:LYS:O	9:I:11:LYS:CG	2.64	0.41
15:O:88:ARG:HD2	15:O:88:ARG:HA	1.93	0.41
17:Q:99:SER:C	17:Q:101:ARG:H	2.29	0.41
18:R:39:VAL:CG1	18:R:40:LEU:N	2.84	0.41
20:T:100:ILE:C	20:T:102:GLY:H	2.29	0.41
1:A:103:C:P	20:T:17:ARG:NH1	2.94	0.41
1:A:146:G:H2'	1:A:147:G:H8	1.85	0.41
1:A:189(A):C:O2'	1:A:189(B):C:H5'	2.20	0.41
1:A:1092:A:H5''	7:G:4:ARG:CZ	2.51	0.41
1:A:1368:G:OP2	9:I:112:LYS:HD2	2.21	0.41
2:B:48:MET:O	2:B:51:LEU:HB2	2.20	0.41
2:B:177:ALA:O	2:B:178:ARG:C	2.64	0.41
3:C:70:VAL:CG1	3:C:71:ALA:H	2.34	0.41
4:D:176:LEU:HD12	4:D:177:ASP:H	1.86	0.41
5:E:9:LYS:HG2	5:E:10:MET:N	2.36	0.41
6:F:45:LEU:HD12	6:F:45:LEU:C	2.46	0.41
7:G:116:ALA:O	7:G:120:ILE:HD12	2.21	0.41
13:M:20:THR:C	13:M:22:ILE:N	2.78	0.41
15:O:18:PHE:CD1	15:O:18:PHE:C	2.98	0.41
15:O:55:GLY:O	15:O:56:LEU:C	2.64	0.41
1:A:421:U:H5'	1:A:422:C:C5	2.56	0.41
1:A:789:U:O2'	1:A:791:G:N7	2.48	0.41
1:A:933:G:OP2	7:G:3:ARG:HB3	2.20	0.41
1:A:1030:C:H2'	1:A:1030(A):G:C8	2.56	0.41
1:A:1034:G:O2'	1:A:1035:A:H5'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1053:G:C4'	1:A:1054:C:H5'	2.51	0.41
1:A:1115:C:H1'	14:N:61:TRP:O	2.20	0.41
1:A:1190:G:H3'	3:C:3:ASN:HD22	1.86	0.41
1:A:1190:G:OP1	3:C:5:ILE:HG13	2.21	0.41
1:A:1202:G:C2	14:N:42:ILE:HG21	2.55	0.41
2:B:12:GLU:C	2:B:14:GLY:N	2.78	0.41
2:B:68:ILE:HG12	2:B:161:ALA:HB3	2.03	0.41
2:B:69:LEU:C	2:B:69:LEU:CD2	2.93	0.41
2:B:114:ARG:O	2:B:117:GLU:HG3	2.20	0.41
3:C:178:LEU:C	3:C:180:ALA:H	2.29	0.41
4:D:120:LEU:HD23	4:D:120:LEU:HA	1.93	0.41
5:E:139:LEU:C	5:E:141:GLN:N	2.79	0.41
7:G:58:PRO:O	7:G:59:LEU:C	2.63	0.41
8:H:101:PRO:HG3	8:H:133:LEU:HD11	2.01	0.41
9:I:43:ALA:C	9:I:45:ALA:N	2.79	0.41
9:I:65:VAL:HG11	9:I:73:GLN:CB	2.45	0.41
10:J:7:LYS:HB2	10:J:97:GLU:HB2	2.03	0.41
10:J:56:HIS:C	10:J:58:ASP:H	2.29	0.41
12:L:75:HIS:HD2	12:L:76:ASN:N	2.19	0.41
13:M:81:LEU:HD11	13:M:88:ARG:HD3	2.02	0.41
15:O:76:GLU:O	15:O:77:ARG:C	2.62	0.41
17:Q:33:GLY:O	17:Q:34:LYS:C	2.63	0.41
17:Q:58:GLU:O	17:Q:59:ILE:HD13	2.20	0.41
17:Q:67:LYS:HA	17:Q:70:ARG:NH1	2.22	0.41
17:Q:69:LYS:O	17:Q:70:ARG:HD2	2.20	0.41
17:Q:98:LEU:O	17:Q:99:SER:O	2.38	0.41
19:S:36:ARG:NH1	19:S:72:GLY:CA	2.84	0.41
20:T:93:GLU:C	20:T:95:ALA:H	2.28	0.41
1:A:92:C:O2'	1:A:93:G:H5'	2.20	0.41
1:A:919:A:O2'	1:A:920:U:H5'	2.21	0.41
1:A:1179:A:O2'	1:A:1180:A:H5'	2.21	0.41
1:A:1310:G:O6	19:S:2:PRO:HB3	2.21	0.41
1:A:1318:A:OP1	19:S:10:PHE:CE1	2.74	0.41
2:B:61:LEU:HD13	2:B:61:LEU:O	2.21	0.41
4:D:194:LEU:HD22	4:D:194:LEU:N	2.36	0.41
5:E:50:GLU:O	5:E:51:VAL:C	2.64	0.41
8:H:87:SER:HB2	8:H:93:VAL:H	1.86	0.41
9:I:43:ALA:HA	9:I:74:ILE:HD13	2.03	0.41
11:K:115:PRO:C	11:K:117:ASN:H	2.27	0.41
15:O:66:LEU:O	15:O:69:TYR:HB3	2.21	0.41
18:R:87:ARG:HG2	18:R:88:LYS:N	2.30	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:40:ILE:HG23	19:S:62:ILE:HD12	2.03	0.41
20:T:41:ILE:CD1	20:T:87:LYS:HD2	2.47	0.41
1:A:132:C:O2'	1:A:133:U:H5'	2.21	0.40
1:A:189(A):C:H2'	1:A:189(B):C:H6	1.86	0.40
1:A:268:C:H2'	1:A:269:C:C6	2.57	0.40
1:A:632:A:O2'	1:A:633:G:H5'	2.20	0.40
1:A:1187:G:OP1	9:I:113:LYS:HE2	2.22	0.40
1:A:1405:G:O4'	1:A:1519:A:H4'	2.21	0.40
2:B:28:PHE:CD1	2:B:194:PRO:HG3	2.56	0.40
2:B:108:ILE:HD13	2:B:108:ILE:HA	1.90	0.40
3:C:156:ARG:CD	3:C:160:ALA:O	2.69	0.40
3:C:175:LEU:HD21	3:C:201:TYR:CE2	2.56	0.40
4:D:33:MET:HE3	4:D:37:PRO:HB2	2.04	0.40
4:D:36:ARG:C	4:D:38:TYR:N	2.79	0.40
7:G:38:LEU:C	7:G:38:LEU:HD12	2.46	0.40
8:H:24:THR:CG2	8:H:63:LEU:HD21	2.43	0.40
10:J:16:LEU:C	10:J:18:ALA:N	2.79	0.40
16:P:48:TRP:CD1	16:P:48:TRP:H	2.39	0.40
18:R:43:PHE:HD2	18:R:56:THR:HG22	1.85	0.40
20:T:84:LEU:C	20:T:86:ARG:H	2.28	0.40
1:A:547:A:H4'	1:A:548:G:O5'	2.20	0.40
1:A:706:A:C1'	11:K:29:ILE:HD11	2.51	0.40
1:A:947:G:H2'	1:A:948:C:O4'	2.22	0.40
1:A:1169:A:H2'	1:A:1170:A:C8	2.56	0.40
1:A:1296:C:H4'	1:A:1302:U:C5	2.56	0.40
1:A:1347:G:C6	9:I:107:ARG:NH2	2.89	0.40
1:A:1385:G:O2'	1:A:1386:G:H5'	2.22	0.40
2:B:84:GLU:HB3	2:B:219:VAL:CG2	2.35	0.40
2:B:119:GLU:O	2:B:122:PHE:HB3	2.20	0.40
3:C:87:LEU:O	3:C:89:GLU:N	2.55	0.40
4:D:100:ARG:NH1	4:D:137:SER:HA	2.37	0.40
6:F:24:GLU:O	6:F:27:GLN:HB2	2.22	0.40
6:F:91:VAL:CG1	18:R:72:ARG:NH2	2.84	0.40
8:H:82:HIS:O	8:H:137:VAL:HA	2.21	0.40
9:I:9:ARG:CG	9:I:14:VAL:HG12	2.52	0.40
10:J:16:LEU:HD23	10:J:16:LEU:HA	1.94	0.40
10:J:33:GLN:O	10:J:34:VAL:HB	2.21	0.40
12:L:7:ILE:O	12:L:8:ASN:C	2.64	0.40
15:O:2:PRO:HB2	15:O:3:ILE:H	1.74	0.40
15:O:10:LYS:HD3	15:O:11:VAL:N	2.35	0.40
16:P:26:ARG:HD2	16:P:31:LYS:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:28:ARG:NH1	16:P:29:ASP:OD1	2.54	0.40
17:Q:48:GLU:C	17:Q:50:LYS:H	2.28	0.40
17:Q:82:MET:O	17:Q:83:ASP:C	2.64	0.40
19:S:17:GLU:HG3	19:S:18:LYS:N	2.36	0.40
23:Y:35:A:H2'	23:Y:36:C:O4'	2.21	0.40
1:A:256:U:O2'	1:A:257:G:H5'	2.21	0.40
1:A:327:A:H3'	1:A:328:C:H5''	2.03	0.40
1:A:520:A:O2'	12:L:73:GLU:HG2	2.22	0.40
1:A:616:G:O2'	1:A:617:G:H5'	2.21	0.40
1:A:769:G:H4'	1:A:1513:A:H4'	2.03	0.40
1:A:969:A:O2'	1:A:970:C:H5'	2.21	0.40
1:A:1367:C:H5'	10:J:60:ARG:NH1	2.36	0.40
1:A:1540:U:H2'	1:A:1541:U:O5'	2.22	0.40
2:B:62:ALA:C	2:B:64:ARG:N	2.79	0.40
3:C:8:ILE:O	3:C:11:ARG:N	2.49	0.40
3:C:35:GLU:OE2	3:C:59:ARG:NH2	2.50	0.40
4:D:36:ARG:HG2	4:D:38:TYR:CZ	2.56	0.40
4:D:149:ALA:O	4:D:150:GLU:C	2.63	0.40
5:E:57:LYS:HG2	5:E:61:TYR:CE2	2.56	0.40
6:F:15:ASP:H	6:F:18:GLN:HE21	1.65	0.40
12:L:117:ARG:NH2	12:L:124:LYS:HB2	2.36	0.40
14:N:11:LYS:HE2	14:N:11:LYS:HB2	1.89	0.40
16:P:1:MET:O	16:P:24:ALA:HB2	2.21	0.40
18:R:25:THR:O	18:R:26:LEU:HB2	2.20	0.40
19:S:44:MET:O	19:S:45:VAL:C	2.64	0.40
20:T:56:MET:HG3	20:T:84:LEU:CD2	2.46	0.40
20:T:101:GLY:C	20:T:103:GLY:H	2.29	0.40
1:A:455:C:O2'	1:A:456:C:H5'	2.22	0.40
1:A:640:A:C2'	1:A:641:U:H5'	2.51	0.40
1:A:1217:C:H2'	1:A:1218:C:O4'	2.21	0.40
1:A:1257:U:O2	1:A:1257:U:C2'	2.68	0.40
1:A:1296:C:C5'	13:M:14:ARG:HD2	2.52	0.40
1:A:1466:C:H2'	1:A:1467:G:O4'	2.21	0.40
1:A:1477:C:H2'	1:A:1478:C:C6	2.57	0.40
4:D:17:VAL:CG1	4:D:18:LYS:N	2.84	0.40
5:E:106:PRO:O	5:E:110:LEU:HG	2.22	0.40
8:H:54:ASP:O	8:H:54:ASP:CG	2.62	0.40
9:I:48:GLU:OE2	9:I:51:ARG:HD2	2.21	0.40
11:K:101:SER:C	11:K:103:LEU:H	2.30	0.40
12:L:6:THR:OG1	12:L:9:GLN:HG3	2.22	0.40
13:M:59:TYR:C	13:M:59:TYR:HD1	2.29	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:30:ALA:HA	15:O:85:LEU:HD11	2.03	0.40
1:A:767:A:H2'	1:A:768:A:O4'	2.22	0.40
1:A:836:G:H2'	1:A:837:G:H8	1.86	0.40
5:E:34:VAL:O	5:E:34:VAL:HG13	2.22	0.40
6:F:15:ASP:O	6:F:16:GLN:C	2.63	0.40
6:F:28:ARG:HG3	6:F:28:ARG:HH11	1.86	0.40
7:G:61:VAL:O	7:G:62:PHE:C	2.64	0.40
15:O:43:LEU:HD12	15:O:56:LEU:HD22	2.03	0.40
18:R:34:TYR:CD1	18:R:34:TYR:C	2.99	0.40
19:S:6:LYS:HB3	19:S:7:LYS:H	1.73	0.40
19:S:33:THR:CG2	19:S:34:TRP:N	2.84	0.40
19:S:67:VAL:HG12	19:S:68:GLY:N	2.37	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	233/256 (91%)	158 (68%)	61 (26%)	14 (6%)	1	7
3	C	205/239 (86%)	151 (74%)	36 (18%)	18 (9%)	0	3
4	D	206/209 (99%)	168 (82%)	33 (16%)	5 (2%)	4	22
5	E	149/162 (92%)	130 (87%)	16 (11%)	3 (2%)	6	25
6	F	99/101 (98%)	84 (85%)	13 (13%)	2 (2%)	6	25
7	G	153/156 (98%)	123 (80%)	27 (18%)	3 (2%)	6	25
8	H	136/138 (99%)	118 (87%)	12 (9%)	6 (4%)	2	12
9	I	125/128 (98%)	99 (79%)	18 (14%)	8 (6%)	1	6
10	J	97/105 (92%)	69 (71%)	17 (18%)	11 (11%)	0	2
11	K	117/129 (91%)	92 (79%)	21 (18%)	4 (3%)	3	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	L	123/135 (91%)	99 (80%)	16 (13%)	8 (6%)	1	6
13	M	123/126 (98%)	90 (73%)	22 (18%)	11 (9%)	0	3
14	N	58/61 (95%)	46 (79%)	9 (16%)	3 (5%)	1	10
15	O	86/89 (97%)	71 (83%)	15 (17%)	0	100	100
16	P	82/88 (93%)	69 (84%)	12 (15%)	1 (1%)	10	37
17	Q	102/105 (97%)	86 (84%)	13 (13%)	3 (3%)	3	19
18	R	71/88 (81%)	60 (84%)	9 (13%)	2 (3%)	4	20
19	S	79/93 (85%)	65 (82%)	5 (6%)	9 (11%)	0	1
20	T	97/106 (92%)	71 (73%)	20 (21%)	6 (6%)	1	7
21	U	23/27 (85%)	16 (70%)	6 (26%)	1 (4%)	2	12
All	All	2364/2541 (93%)	1865 (79%)	381 (16%)	118 (5%)	1	11

All (118) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	15	VAL
2	B	74	LYS
2	B	207	ALA
3	C	15	THR
3	C	61	ALA
3	C	95	THR
3	C	207	VAL
4	D	3	ARG
8	H	70	GLN
8	H	71	GLY
8	H	91	ARG
9	I	8	GLY
9	I	23	ASN
10	J	61	GLU
10	J	76	ASN
10	J	83	GLU
10	J	85	LEU
10	J	86	MET
11	K	12	ARG
11	K	13	GLN
11	K	127	LYS
12	L	27	LEU
12	L	28	LYS

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Mol	Chain	Res	Type
12	L	47	LYS
13	M	23	TYR
13	M	67	GLU
13	M	86	CYS
17	Q	99	SER
19	S	6	LYS
19	S	9	VAL
19	S	29	ARG
19	S	67	VAL
19	S	81	ARG
20	T	11	SER
20	T	74	LYS
20	T	95	ALA
2	B	19	HIS
3	C	160	ALA
4	D	88	VAL
7	G	155	ARG
8	H	105	ARG
9	I	121	ARG
10	J	34	VAL
10	J	57	LYS
10	J	75	ILE
12	L	74	GLY
12	L	75	HIS
12	L	79	GLU
13	M	6	GLY
13	M	21	TYR
13	M	24	GLY
13	M	68	GLY
14	N	9	LYS
14	N	15	LYS
19	S	5	LEU
19	S	28	LYS
19	S	43	GLU
2	B	16	HIS
2	B	95	GLN
3	C	26	LYS
3	C	47	LEU
3	C	53	ALA
3	C	102	ASN
7	G	39	ALA
7	G	86	GLN

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Mol	Chain	Res	Type
8	H	24	THR
9	I	32	ASP
9	I	34	ASN
9	I	119	ALA
9	I	127	LYS
12	L	116	SER
14	N	10	ALA
20	T	101	GLY
20	T	103	GLY
2	B	63	MET
2	B	131	PRO
2	B	150	SER
2	B	224	GLN
6	F	16	GLN
9	I	24	GLY
10	J	32	ALA
13	M	36	LYS
16	P	53	VAL
18	R	19	LYS
18	R	41	LYS
19	S	25	LYS
2	B	9	GLU
2	B	17	PHE
2	B	208	ILE
3	C	91	LEU
3	C	108	ASN
3	C	144	SER
4	D	36	ARG
6	F	70	ASP
8	H	49	GLU
10	J	26	ALA
10	J	90	LEU
20	T	73	HIS
21	U	3	LYS
3	C	22	TRP
3	C	81	GLY
3	C	127	ARG
5	E	52	PRO
17	Q	96	GLU
17	Q	103	GLY
4	D	5	ILE
13	M	117	VAL

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Mol	Chain	Res	Type
3	C	96	GLY
3	C	103	VAL
4	D	90	GLY
5	E	128	PRO
13	M	38	GLY
2	B	239	VAL
12	L	110	VAL
3	C	14	ILE
5	E	70	PRO
11	K	109	VAL
13	M	7	VAL

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%)	188 (93%)	14 (7%)	14	41
3	C	160/188 (85%)	139 (87%)	21 (13%)	4	17
4	D	180/181 (99%)	168 (93%)	12 (7%)	15	43
5	E	115/123 (94%)	101 (88%)	14 (12%)	5	20
6	F	90/90 (100%)	84 (93%)	6 (7%)	15	43
7	G	126/127 (99%)	117 (93%)	9 (7%)	13	41
8	H	119/119 (100%)	106 (89%)	13 (11%)	6	24
9	I	98/99 (99%)	89 (91%)	9 (9%)	8	31
10	J	87/92 (95%)	79 (91%)	8 (9%)	8	31
11	K	90/99 (91%)	84 (93%)	6 (7%)	15	43
12	L	104/111 (94%)	95 (91%)	9 (9%)	9	34
13	M	100/101 (99%)	92 (92%)	8 (8%)	11	37
14	N	49/50 (98%)	44 (90%)	5 (10%)	7	28
15	O	79/80 (99%)	72 (91%)	7 (9%)	9	33
16	P	72/74 (97%)	66 (92%)	6 (8%)	10	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	Q	96/97 (99%)	90 (94%)	6 (6%)	16	45
18	R	64/77 (83%)	61 (95%)	3 (5%)	23	55
19	S	71/80 (89%)	68 (96%)	3 (4%)	26	58
20	T	76/82 (93%)	68 (90%)	8 (10%)	6	26
21	U	19/22 (86%)	19 (100%)	0	100	100
All	All	1997/2112 (95%)	1830 (92%)	167 (8%)	10	35

All (167) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	15	VAL
2	B	21	ARG
2	B	23	ARG
2	B	25	ASN
2	B	63	MET
2	B	82	ARG
2	B	98	LEU
2	B	117	GLU
2	B	121	LEU
2	B	162	ILE
2	B	187	LEU
2	B	204	ASN
2	B	208	ILE
2	B	221	LEU
3	C	5	ILE
3	C	21	ARG
3	C	26	LYS
3	C	34	LEU
3	C	37	GLN
3	C	42	LEU
3	C	75	VAL
3	C	97	LYS
3	C	101	LEU
3	C	102	ASN
3	C	104	GLN
3	C	107	GLN
3	C	156	ARG
3	C	164	ARG
3	C	175	LEU
3	C	179	ARG

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Mol	Chain	Res	Type
3	C	188	LEU
3	C	191	THR
3	C	192	THR
3	C	196	LEU
3	C	204	LEU
4	D	3	ARG
4	D	9	CYS
4	D	33	MET
4	D	34	GLU
4	D	58	LEU
4	D	112	VAL
4	D	122	ARG
4	D	141	ARG
4	D	146	ILE
4	D	169	LYS
4	D	170	VAL
4	D	201	GLN
5	E	12	LEU
5	E	18	ARG
5	E	20	GLN
5	E	31	LEU
5	E	41	VAL
5	E	43	LEU
5	E	53	LEU
5	E	64	ARG
5	E	80	ILE
5	E	89	ILE
5	E	101	ILE
5	E	107	ARG
5	E	144	THR
5	E	150	ARG
6	F	24	GLU
6	F	43	LEU
6	F	65	VAL
6	F	69	GLU
6	F	74	ASP
6	F	75	LEU
7	G	9	VAL
7	G	16	LEU
7	G	38	LEU
7	G	73	MET
7	G	78	ARG

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Mol	Chain	Res	Type
7	G	113	GLU
7	G	114	ARG
7	G	155	ARG
7	G	156	TRP
8	H	24	THR
8	H	26	VAL
8	H	37	ARG
8	H	52	ASP
8	H	56	LYS
8	H	63	LEU
8	H	85	ARG
8	H	97	VAL
8	H	105	ARG
8	H	112	LEU
8	H	119	LEU
8	H	122	ARG
8	H	133	LEU
9	I	16	ARG
9	I	41	VAL
9	I	47	LEU
9	I	79	LEU
9	I	97	LYS
9	I	102	LEU
9	I	111	ARG
9	I	118	LYS
9	I	125	TYR
10	J	6	ILE
10	J	14	LYS
10	J	21	GLN
10	J	38	ILE
10	J	80	LYS
10	J	83	GLU
10	J	98	ILE
10	J	99	LYS
11	K	12	ARG
11	K	18	ARG
11	K	29	ILE
11	K	47	VAL
11	K	96	ARG
11	K	114	VAL
12	L	21	LYS
12	L	53	ARG

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Mol	Chain	Res	Type
12	L	60	LEU
12	L	67	THR
12	L	83	VAL
12	L	89	ARG
12	L	111	LYS
12	L	113	ARG
12	L	126	LYS
13	M	9	ILE
13	M	44	ARG
13	M	56	LEU
13	M	62	ASN
13	M	70	LEU
13	M	94	ARG
13	M	110	ARG
13	M	115	LYS
14	N	8	GLU
14	N	18	VAL
14	N	26	ARG
14	N	33	VAL
14	N	41	ARG
15	O	6	GLU
15	O	10	LYS
15	O	31	LEU
15	O	34	LEU
15	O	54	ARG
15	O	57	LEU
15	O	71	GLN
16	P	1	MET
16	P	2	VAL
16	P	45	THR
16	P	57	ARG
16	P	62	VAL
16	P	67	THR
17	Q	16	GLN
17	Q	22	LEU
17	Q	53	LEU
17	Q	68	ARG
17	Q	74	LEU
17	Q	101	ARG
18	R	36	ASN
18	R	39	VAL
18	R	88	LYS

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Mol	Chain	Res	Type
19	S	15	LEU
19	S	43	GLU
19	S	62	ILE
20	T	10	LEU
20	T	13	LEU
20	T	48	LYS
20	T	57	ARG
20	T	62	LEU
20	T	72	LEU
20	T	73	HIS
20	T	90	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (72) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	19	HIS
2	B	25	ASN
2	B	78	GLN
2	B	146	GLN
2	B	204	ASN
2	B	212	GLN
3	C	3	ASN
3	C	6	HIS
3	C	28	GLN
3	C	31	HIS
3	C	37	GLN
3	C	63	ASN
3	C	102	ASN
3	C	107	GLN
3	C	110	ASN
3	C	162	GLN
3	C	176	HIS
3	C	181	ASN
4	D	42	GLN
4	D	62	GLN
4	D	123	HIS
4	D	154	ASN
4	D	160	GLN
4	D	199	ASN
4	D	201	GLN
5	E	20	GLN
5	E	73	ASN

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Mol	Chain	Res	Type
6	F	18	GLN
6	F	27	GLN
6	F	32	ASN
6	F	64	GLN
6	F	73	ASN
7	G	37	ASN
7	G	56	GLN
7	G	68	ASN
7	G	96	GLN
7	G	106	GLN
8	H	70	GLN
8	H	82	HIS
9	I	3	GLN
9	I	23	ASN
9	I	31	GLN
9	I	73	GLN
9	I	124	GLN
10	J	21	GLN
10	J	76	ASN
10	J	78	ASN
10	J	84	GLN
11	K	116	HIS
11	K	117	ASN
12	L	49	ASN
12	L	75	HIS
12	L	78	GLN
12	L	80	HIS
13	M	12	ASN
13	M	40	ASN
13	M	62	ASN
14	N	49	HIS
15	O	13	GLN
15	O	37	ASN
15	O	46	HIS
15	O	53	HIS
16	P	16	HIS
16	P	65	GLN
16	P	76	GLN
17	Q	26	GLN
17	Q	94	ASN
18	R	36	ASN
19	S	14	HIS

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Mol	Chain	Res	Type
19	S	47	HIS
19	S	56	GLN
20	T	45	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1510/1522 (99%)	203 (13%)	62 (4%)
22	X	3/6 (50%)	1 (33%)	0
23	Y	12/17 (70%)	0	0
All	All	1525/1545 (98%)	204 (13%)	62 (4%)

All (204) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	8	A
1	A	9	G
1	A	31	G
1	A	32	A
1	A	39	G
1	A	47	C
1	A	48	C
1	A	51	A
1	A	61	G
1	A	101	A
1	A	116	A
1	A	120	A
1	A	121	C
1	A	130	A
1	A	131	C
1	A	182	U
1	A	189(F)	U
1	A	195	A
1	A	197	A
1	A	202	U
1	A	203	U
1	A	204	U
1	A	216	G
1	A	244	U
1	A	247	G
1	A	251	G

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Mol	Chain	Res	Type
1	A	266	G
1	A	267	C
1	A	282	A
1	A	289	G
1	A	321	A
1	A	328	C
1	A	329	A
1	A	332	G
1	A	345	C
1	A	352	C
1	A	353	A
1	A	354	G
1	A	367	U
1	A	373	A
1	A	397	A
1	A	398	C
1	A	406	G
1	A	411	A
1	A	412	A
1	A	421	U
1	A	429	U
1	A	430	A
1	A	439	A
1	A	442	C
1	A	452	A
1	A	470	C
1	A	484	G
1	A	485	G
1	A	496	A
1	A	498	U
1	A	509	A
1	A	510	A
1	A	511	C
1	A	518	C
1	A	527	G
1	A	531	U
1	A	532	A
1	A	533	A
1	A	534	U
1	A	547	A
1	A	559	A
1	A	560	U

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Mol	Chain	Res	Type
1	A	561	U
1	A	562	C
1	A	572	A
1	A	573	A
1	A	575	G
1	A	576	G
1	A	577	G
1	A	631	G
1	A	632	A
1	A	653	A
1	A	665	A
1	A	688	G
1	A	701	C
1	A	702	A
1	A	703	G
1	A	723	U
1	A	731	G
1	A	734	G
1	A	749	C
1	A	755	G
1	A	777	A
1	A	781	A
1	A	782	A
1	A	794	A
1	A	812	C
1	A	813	U
1	A	817	C
1	A	819	A
1	A	828	A
1	A	839	U
1	A	840	C
1	A	841	U
1	A	848	C
1	A	902	G
1	A	913	A
1	A	914	A
1	A	926	G
1	A	927	G
1	A	934	C
1	A	935	A
1	A	960	U
1	A	961	U

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Mol	Chain	Res	Type
1	A	965	A
1	A	966	G
1	A	969	A
1	A	971	G
1	A	974	A
1	A	975	A
1	A	976	G
1	A	977	A
1	A	978	A
1	A	991	U
1	A	992	U
1	A	993	G
1	A	994	A
1	A	1004	A
1	A	1025	U
1	A	1026	G
1	A	1027	C
1	A	1048	G
1	A	1050	G
1	A	1053	G
1	A	1054	C
1	A	1055	A
1	A	1065	U
1	A	1068	G
1	A	1094	G
1	A	1095	U
1	A	1101	A
1	A	1117	G
1	A	1118	C
1	A	1125	U
1	A	1126	U
1	A	1129	C
1	A	1130	A
1	A	1131	G
1	A	1136	U
1	A	1137	C
1	A	1138	G
1	A	1139	G
1	A	1146	A
1	A	1152	A
1	A	1159	U
1	A	1160	G

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Mol	Chain	Res	Type
1	A	1182	G
1	A	1183	A
1	A	1191	A
1	A	1196	U
1	A	1197	G
1	A	1200	C
1	A	1201	A
1	A	1202	G
1	A	1211	U
1	A	1212	U
1	A	1227	A
1	A	1238	A
1	A	1256	A
1	A	1257	U
1	A	1258	G
1	A	1278	U
1	A	1280	A
1	A	1281	U
1	A	1282	C
1	A	1285	A
1	A	1286	A
1	A	1287	A
1	A	1300	G
1	A	1301	U
1	A	1302	U
1	A	1320	C
1	A	1332	A
1	A	1346	A
1	A	1348	U
1	A	1353	G
1	A	1363	C
1	A	1398	A
1	A	1421	G
1	A	1442	G
1	A	1442(A)	G
1	A	1442(B)	A
1	A	1452	C
1	A	1492	A
1	A	1497	G
1	A	1499	A
1	A	1502	A
1	A	1503	A

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Mol	Chain	Res	Type
1	A	1504	G
1	A	1505	G
1	A	1506	U
1	A	1517	G
1	A	1520	G
1	A	1529	G
1	A	1530	G
1	A	1533	C
1	A	1541	U
22	X	4	A

All (62) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	7	G
1	A	30	U
1	A	60	A
1	A	115	G
1	A	119	A
1	A	129(A)	G
1	A	181	G
1	A	201	C
1	A	204	U
1	A	243	A
1	A	250	A
1	A	266	G
1	A	281	G
1	A	328	C
1	A	344	A
1	A	351	G
1	A	353	A
1	A	366	C
1	A	372	C
1	A	410	G
1	A	428	G
1	A	429	U
1	A	438	G
1	A	484	G
1	A	495	A
1	A	509	A
1	A	532	A
1	A	533	A

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Mol	Chain	Res	Type
1	A	559	A
1	A	560	U
1	A	575	G
1	A	687	A
1	A	701	C
1	A	748	C
1	A	793	U
1	A	812	C
1	A	913	A
1	A	960	U
1	A	965	A
1	A	992	U
1	A	993	G
1	A	1049	U
1	A	1067	A
1	A	1117	G
1	A	1129	C
1	A	1181	G
1	A	1182	G
1	A	1190	G
1	A	1201	A
1	A	1281	U
1	A	1285	A
1	A	1300	G
1	A	1301	U
1	A	1331	G
1	A	1347	G
1	A	1397	C
1	A	1447	A
1	A	1498	U
1	A	1503	A
1	A	1504	G
1	A	1505	G
1	A	1528	U

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CM0	Y	34	23	22,26,27	1.51	3 (13%)	28,37,40	3.06	3 (10%)
23	6MZ	Y	37	23	22,25,26	0.55	0	30,36,39	0.60	1 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CM0	Y	34	23	-	5/12/30/31	0/2/2/2
23	6MZ	Y	37	23	-	0/9/27/28	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	Y	34	CM0	O9-C8	4.42	1.36	1.22
23	Y	34	CM0	O5-C7	4.10	1.54	1.44
23	Y	34	CM0	O8-C8	-2.16	1.23	1.30

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	Y	34	CM0	C7-O5-C5	14.58	136.67	117.58
23	Y	34	CM0	O5-C7-C8	5.59	123.01	110.88
23	Y	37	6MZ	C9-N6-C6	2.14	124.72	122.87
23	Y	34	CM0	O4-C4-N3	-2.07	116.15	120.12

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	Y	34	CM0	C4-C5-O5-C7
23	Y	34	CM0	C6-C5-O5-C7
23	Y	34	CM0	C8-C7-O5-C5
23	Y	34	CM0	O5-C7-C8-O8
23	Y	34	CM0	O5-C7-C8-O9

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	Y	34	CM0	5	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 243 ligands modelled in this entry, 242 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	$\# Z > 2$
24	PAR	A	1601	-	45,45,45	1.56	6 (13%)	64,67,67	1.26	8 (12%)

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
24	PAR	A	1601	-	-	5/18/94/94	0/4/4/4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	1601	PAR	C64-C54	4.67	1.58	1.52
24	A	1601	PAR	O54-C14	3.29	1.50	1.41
24	A	1601	PAR	C52-C42	3.01	1.58	1.52
24	A	1601	PAR	C11-C21	2.75	1.57	1.52
24	A	1601	PAR	C31-C21	2.39	1.56	1.53
24	A	1601	PAR	O54-C54	2.01	1.49	1.44

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	1601	PAR	O33-C14-C24	4.04	115.17	108.22
24	A	1601	PAR	O54-C54-C64	3.62	112.76	106.01
24	A	1601	PAR	C14-O54-C54	3.33	120.22	113.69
24	A	1601	PAR	O11-C11-C21	2.83	113.09	108.22
24	A	1601	PAR	O52-C13-C23	2.76	113.69	107.96
24	A	1601	PAR	O52-C13-O43	-2.68	108.53	111.43
24	A	1601	PAR	C22-C32-C42	2.36	115.48	109.53
24	A	1601	PAR	C11-O51-C51	2.21	118.03	113.69

There are no chirality outliers.

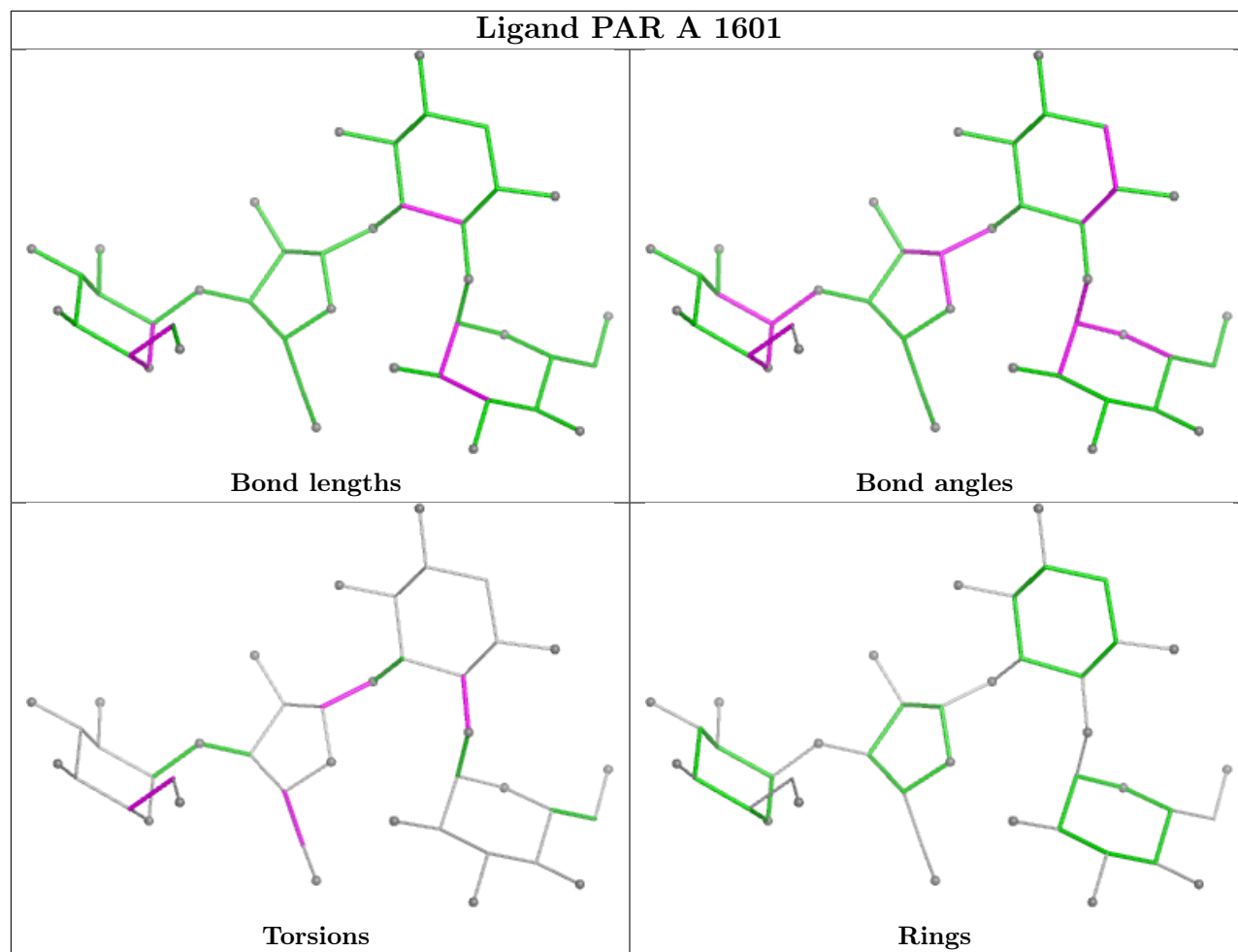
All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	A	1601	PAR	C44-C54-C64-N64
24	A	1601	PAR	O54-C54-C64-N64
24	A	1601	PAR	C52-C42-O11-C11
24	A	1601	PAR	C33-C43-C53-O53
24	A	1601	PAR	C23-C13-O52-C52

There are no ring outliers.

No monomer is involved in short contacts.

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	1512/1522 (99%)	0.10	56 (3%) 45 25	32, 58, 130, 183	0
2	B	235/256 (91%)	0.73	31 (13%) 7 4	50, 84, 126, 147	0
3	C	207/239 (86%)	0.57	9 (4%) 40 22	48, 74, 109, 117	0
4	D	208/209 (99%)	0.26	13 (6%) 26 14	45, 63, 83, 94	0
5	E	151/162 (93%)	-0.18	3 (1%) 65 44	35, 50, 68, 86	0
6	F	101/101 (100%)	0.29	2 (1%) 65 44	62, 81, 93, 98	0
7	G	155/156 (99%)	0.25	7 (4%) 38 20	50, 70, 104, 120	0
8	H	138/138 (100%)	-0.25	0 100 100	33, 50, 65, 70	0
9	I	127/128 (99%)	0.61	7 (5%) 30 16	45, 81, 99, 113	0
10	J	99/105 (94%)	1.43	27 (27%) 1 1	46, 102, 141, 147	0
11	K	119/129 (92%)	0.10	3 (2%) 58 37	39, 58, 81, 96	0
12	L	125/135 (92%)	0.27	8 (6%) 25 14	23, 54, 71, 104	0
13	M	125/126 (99%)	0.78	20 (16%) 5 2	52, 70, 131, 162	0
14	N	60/61 (98%)	0.57	3 (5%) 34 18	50, 65, 88, 100	0
15	O	88/89 (98%)	-0.04	0 100 100	46, 64, 82, 102	0
16	P	84/88 (95%)	-0.13	1 (1%) 76 58	39, 50, 62, 89	0
17	Q	104/105 (99%)	0.34	8 (7%) 19 10	40, 56, 100, 133	0
18	R	73/88 (82%)	0.18	4 (5%) 30 16	52, 67, 107, 137	0
19	S	81/93 (87%)	0.92	11 (13%) 7 4	52, 83, 105, 117	0
20	T	99/106 (93%)	0.29	7 (7%) 22 12	39, 55, 77, 84	0
21	U	25/27 (92%)	0.69	1 (4%) 42 23	47, 59, 82, 87	0
22	X	4/6 (66%)	0.11	0 100 100	55, 57, 60, 81	0
23	Y	11/17 (64%)	0.49	1 (9%) 15 8	54, 85, 110, 114	0
All	All	3931/4086 (96%)	0.27	222 (5%) 30 16	23, 63, 115, 183	0

All (222) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
17	Q	105	ALA	11.6
19	S	3	ARG	8.3
13	M	124	PRO	8.0
13	M	125	ARG	7.6
2	B	16	HIS	7.5
1	A	1129	C	7.5
13	M	126	LYS	7.1
13	M	123	ALA	6.5
13	M	119	GLY	6.0
1	A	1003	G	5.9
13	M	121	LYS	5.7
1	A	1539	C	5.4
4	D	31	CYS	5.1
10	J	75	ILE	5.0
17	Q	99	SER	5.0
1	A	1541	U	4.9
2	B	7	VAL	4.7
4	D	26	CYS	4.6
1	A	723	U	4.5
1	A	1130	A	4.5
10	J	76	ASN	4.4
13	M	8	GLU	4.3
10	J	90	LEU	4.1
16	P	83	GLU	4.1
20	T	12	ALA	4.1
13	M	122	LYS	4.1
2	B	131	PRO	4.1
13	M	7	VAL	4.0
19	S	5	LEU	4.0
1	A	204	U	4.0
17	Q	100	LYS	4.0
17	Q	104	LYS	4.0
1	A	631	G	4.0
3	C	207	VAL	3.9
11	K	128	ALA	3.9
4	D	9	CYS	3.8
1	A	1127	G	3.8
13	M	9	ILE	3.7
2	B	229	VAL	3.7
1	A	1125	U	3.7
12	L	64	TYR	3.6
2	B	10	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	993	G	3.6
3	C	2	GLY	3.6
1	A	1131	G	3.5
13	M	118	ALA	3.5
20	T	100	ILE	3.5
2	B	133	LYS	3.5
7	G	80	VAL	3.5
13	M	120	LYS	3.5
10	J	82	ILE	3.5
1	A	1281	U	3.5
17	Q	103	GLY	3.4
10	J	77	PRO	3.4
9	I	16	ARG	3.3
13	M	10	PRO	3.3
4	D	23	GLY	3.3
1	A	1126	U	3.3
19	S	4	SER	3.3
1	A	1533	C	3.3
7	G	55	GLY	3.1
20	T	102	GLY	3.1
17	Q	101	ARG	3.1
2	B	122	PHE	3.1
10	J	35	SER	3.1
2	B	18	GLY	3.1
10	J	43	ARG	3.1
1	A	532	A	3.1
1	A	1124	G	3.0
18	R	16	PRO	3.0
1	A	1017	G	3.0
2	B	96	ARG	3.0
13	M	117	VAL	3.0
18	R	17	SER	3.0
7	G	56	GLN	3.0
2	B	144	ARG	2.9
1	A	1146	A	2.9
10	J	101	VAL	2.9
10	J	88	LEU	2.9
1	A	1421	G	2.9
1	A	1141	C	2.9
1	A	992	U	2.9
7	G	81	GLY	2.9
2	B	127	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	1026	G	2.9
1	A	1034	G	2.9
1	A	1212	U	2.8
17	Q	102	GLY	2.8
1	A	630	G	2.8
17	Q	96	GLU	2.8
12	L	26	ALA	2.8
7	G	85	TYR	2.7
1	A	1140	C	2.7
3	C	162	GLN	2.7
10	J	86	MET	2.7
3	C	91	LEU	2.7
1	A	1139	G	2.7
19	S	2	PRO	2.7
5	E	154	GLY	2.7
9	I	38	GLN	2.7
12	L	19	ARG	2.7
1	A	1004	A	2.6
19	S	81	ARG	2.6
2	B	14	GLY	2.6
12	L	60	LEU	2.6
2	B	19	HIS	2.6
1	A	1181	G	2.6
2	B	132	LYS	2.6
12	L	47	LYS	2.6
2	B	121	LEU	2.6
10	J	91	PRO	2.6
2	B	230	VAL	2.6
13	M	2	ALA	2.6
1	A	1039	C	2.6
1	A	1128	C	2.6
12	L	63	GLY	2.6
2	B	241	GLU	2.6
10	J	34	VAL	2.6
1	A	991	U	2.6
20	T	101	GLY	2.6
12	L	65	GLU	2.6
18	R	54	ARG	2.6
10	J	37	PRO	2.5
10	J	93	GLY	2.5
13	M	114	ARG	2.5
4	D	42	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
19	S	6	LYS	2.5
4	D	32	ALA	2.5
2	B	232	PRO	2.5
2	B	89	GLY	2.5
20	T	9	ASN	2.5
9	I	64	THR	2.5
2	B	22	LYS	2.5
9	I	102	LEU	2.5
1	A	1032	G	2.5
4	D	24	GLU	2.5
4	D	19	LEU	2.5
3	C	102	ASN	2.4
10	J	58	ASP	2.4
1	A	216	G	2.4
10	J	74	ILE	2.4
21	U	25	LYS	2.4
2	B	11	LEU	2.4
1	A	1147	C	2.4
9	I	119	ALA	2.4
19	S	7	LYS	2.4
5	E	5	ASP	2.4
7	G	2	ALA	2.4
1	A	1256	A	2.4
1	A	1286	A	2.4
23	Y	29	U	2.4
4	D	4	TYR	2.4
4	D	35	ARG	2.4
10	J	79	ARG	2.4
5	E	20	GLN	2.4
1	A	202	U	2.4
1	A	1540	U	2.4
2	B	125	PRO	2.4
19	S	24	ALA	2.3
1	A	1035	A	2.3
10	J	59	SER	2.3
10	J	87	THR	2.3
1	A	1002	G	2.3
1	A	1134	G	2.3
14	N	2	ALA	2.3
19	S	10	PHE	2.3
4	D	30	LYS	2.3
10	J	80	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
11	K	129	SER	2.3
14	N	13	THR	2.3
2	B	8	LYS	2.3
3	C	119	ARG	2.3
3	C	60	ALA	2.3
1	A	1030(B)	C	2.3
12	L	127	GLU	2.2
2	B	203	GLY	2.2
10	J	36	GLY	2.2
1	A	1279	A	2.2
2	B	124	SER	2.2
10	J	46	ARG	2.2
3	C	64	VAL	2.2
6	F	101	ALA	2.2
10	J	10	GLY	2.2
11	K	11	LYS	2.2
1	A	5	U	2.2
2	B	76	GLN	2.2
1	A	1054	C	2.2
20	T	106	ALA	2.2
4	D	3	ARG	2.2
1	A	1136	U	2.2
2	B	123	ALA	2.2
9	I	127	LYS	2.2
1	A	612	C	2.2
10	J	42	THR	2.2
3	C	101	LEU	2.2
19	S	28	LYS	2.2
10	J	5	ARG	2.2
1	A	1144	G	2.2
1	A	1258	G	2.2
1	A	848	C	2.1
2	B	9	GLU	2.1
14	N	10	ALA	2.1
10	J	45	ARG	2.1
13	M	104	ARG	2.1
2	B	148	TYR	2.1
19	S	25	LYS	2.1
4	D	33	MET	2.1
1	A	203	U	2.1
13	M	113	PRO	2.1
18	R	88	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
20	T	99	LEU	2.1
1	A	1200	C	2.1
10	J	33	GLN	2.1
2	B	21	ARG	2.0
7	G	84	ASN	2.0
13	M	6	GLY	2.0
1	A	1259	C	2.0
2	B	147	LYS	2.0
1	A	1024	G	2.0
13	M	11	ARG	2.0
6	F	84	ASN	2.0
9	I	34	ASN	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	CM0	Y	34	25/26	0.92	0.10	60,65,68,69	0
23	6MZ	Y	37	23/24	0.94	0.11	56,60,63,66	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
25	MG	A	1673	1/1	0.36	0.44	89,89,89,89	0
25	MG	A	1622	1/1	0.41	0.63	116,116,116,116	0
25	MG	A	1610	1/1	0.45	0.83	106,106,106,106	0
25	MG	A	1758	1/1	0.47	0.53	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	MG	A	1763	1/1	0.55	0.29	96,96,96,96	0
25	MG	A	1630	1/1	0.59	0.55	87,87,87,87	0
25	MG	A	1667	1/1	0.62	0.67	89,89,89,89	0
26	K	A	1820	1/1	0.62	0.22	108,108,108,108	0
25	MG	A	1672	1/1	0.63	0.35	86,86,86,86	0
25	MG	A	1669	1/1	0.64	0.59	91,91,91,91	0
25	MG	A	1625	1/1	0.64	0.43	74,74,74,74	0
25	MG	A	1612	1/1	0.67	0.26	83,83,83,83	0
25	MG	A	1603	1/1	0.71	0.28	89,89,89,89	0
26	K	A	1806	1/1	0.72	0.38	129,129,129,129	0
25	MG	A	1618	1/1	0.73	0.50	85,85,85,85	0
26	K	A	1788	1/1	0.73	0.47	117,117,117,117	0
25	MG	A	1690	1/1	0.74	0.35	64,64,64,64	0
25	MG	A	1746	1/1	0.75	0.26	62,62,62,62	0
25	MG	A	1671	1/1	0.75	0.41	70,70,70,70	0
25	MG	A	1739	1/1	0.75	0.44	74,74,74,74	0
25	MG	A	1742	1/1	0.76	0.79	88,88,88,88	0
25	MG	A	1653	1/1	0.77	0.53	78,78,78,78	0
26	K	A	1792	1/1	0.77	0.25	111,111,111,111	0
25	MG	A	1611	1/1	0.77	0.44	65,65,65,65	0
25	MG	A	1773	1/1	0.77	0.82	86,86,86,86	0
26	K	A	1821	1/1	0.77	0.26	90,90,90,90	0
25	MG	N	102	1/1	0.78	0.14	48,48,48,48	0
25	MG	A	1688	1/1	0.78	0.24	50,50,50,50	0
25	MG	A	1716	1/1	0.79	0.50	68,68,68,68	0
25	MG	A	1759	1/1	0.79	0.20	50,50,50,50	0
25	MG	A	1700	1/1	0.79	0.49	62,62,62,62	0
25	MG	A	1752	1/1	0.79	0.13	45,45,45,45	0
25	MG	A	1754	1/1	0.79	0.15	42,42,42,42	0
25	MG	A	1703	1/1	0.80	0.33	44,44,44,44	0
25	MG	A	1711	1/1	0.80	0.51	89,89,89,89	0
25	MG	A	1627	1/1	0.80	0.20	45,45,45,45	0
25	MG	A	1753	1/1	0.81	0.32	56,56,56,56	0
26	K	A	1825	1/1	0.81	0.18	100,100,100,100	0
26	K	A	1809	1/1	0.82	0.11	93,93,93,93	0
26	K	A	1818	1/1	0.82	0.38	131,131,131,131	0
25	MG	A	1771	1/1	0.82	0.22	45,45,45,45	0
25	MG	Q	201	1/1	0.82	0.13	56,56,56,56	0
26	K	A	1787	1/1	0.82	0.15	83,83,83,83	0
26	K	E	203	1/1	0.82	0.39	115,115,115,115	0
25	MG	A	1681	1/1	0.83	0.28	57,57,57,57	0
25	MG	A	1738	1/1	0.83	0.27	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	MG	A	1613	1/1	0.83	0.48	68,68,68,68	0
25	MG	A	1741	1/1	0.83	0.12	79,79,79,79	0
26	K	A	1780	1/1	0.83	0.11	88,88,88,88	0
25	MG	A	1768	1/1	0.84	0.31	37,37,37,37	0
25	MG	A	1602	1/1	0.84	0.07	44,44,44,44	0
26	K	A	1811	1/1	0.84	0.15	99,99,99,99	0
25	MG	A	1620	1/1	0.84	0.46	105,105,105,105	0
25	MG	A	1709	1/1	0.85	0.44	48,48,48,48	0
25	MG	A	1692	1/1	0.85	0.24	47,47,47,47	0
25	MG	A	1650	1/1	0.85	0.23	36,36,36,36	0
25	MG	A	1731	1/1	0.85	0.31	33,33,33,33	0
25	MG	A	1749	1/1	0.85	0.39	85,85,85,85	0
26	K	A	1824	1/1	0.85	0.16	115,115,115,115	0
25	MG	A	1735	1/1	0.85	0.42	77,77,77,77	0
25	MG	A	1657	1/1	0.85	0.31	50,50,50,50	0
25	MG	A	1621	1/1	0.86	0.23	76,76,76,76	0
25	MG	A	1631	1/1	0.86	0.24	51,51,51,51	0
25	MG	A	1658	1/1	0.86	0.38	47,47,47,47	0
26	K	A	1807	1/1	0.86	0.12	86,86,86,86	0
25	MG	A	1633	1/1	0.86	0.32	29,29,29,29	0
25	MG	A	1699	1/1	0.86	0.24	50,50,50,50	0
25	MG	A	1636	1/1	0.86	0.45	80,80,80,80	0
25	MG	A	1702	1/1	0.86	0.43	58,58,58,58	0
25	MG	A	1642	1/1	0.86	0.36	65,65,65,65	0
25	MG	A	1707	1/1	0.86	0.30	33,33,33,33	0
25	MG	A	1644	1/1	0.86	0.12	36,36,36,36	0
26	K	A	1828	1/1	0.86	0.12	98,98,98,98	0
25	MG	A	1615	1/1	0.86	0.12	57,57,57,57	0
25	MG	A	1674	1/1	0.87	0.45	51,51,51,51	0
25	MG	A	1704	1/1	0.87	0.20	52,52,52,52	0
25	MG	A	1680	1/1	0.87	0.47	62,62,62,62	0
25	MG	A	1774	1/1	0.87	0.29	56,56,56,56	0
26	K	A	1795	1/1	0.87	0.16	86,86,86,86	0
26	K	A	1799	1/1	0.87	0.17	94,94,94,94	0
26	K	A	1805	1/1	0.87	0.16	96,96,96,96	0
25	MG	A	1762	1/1	0.87	0.19	29,29,29,29	0
25	MG	A	1694	1/1	0.87	0.12	28,28,28,28	0
25	MG	A	1733	1/1	0.88	0.30	35,35,35,35	0
25	MG	A	1670	1/1	0.88	0.33	67,67,67,67	0
26	K	A	1789	1/1	0.88	0.20	103,103,103,103	0
26	K	A	1812	1/1	0.88	0.19	104,104,104,104	0
25	MG	A	1678	1/1	0.88	0.40	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	MG	A	1765	1/1	0.88	0.27	47,47,47,47	0
26	K	A	1798	1/1	0.88	0.13	93,93,93,93	0
25	MG	A	1659	1/1	0.88	0.41	60,60,60,60	0
26	K	A	1800	1/1	0.88	0.10	97,97,97,97	0
25	MG	A	1769	1/1	0.88	0.17	35,35,35,35	0
26	K	A	1786	1/1	0.88	0.20	94,94,94,94	0
25	MG	A	1705	1/1	0.89	0.18	39,39,39,39	0
26	K	A	1801	1/1	0.89	0.09	82,82,82,82	0
25	MG	A	1776	1/1	0.89	0.15	52,52,52,52	0
25	MG	A	1757	1/1	0.89	0.24	82,82,82,82	0
25	MG	A	1632	1/1	0.89	0.66	74,74,74,74	0
25	MG	A	1701	1/1	0.89	0.49	71,71,71,71	0
25	MG	A	1760	1/1	0.89	0.14	50,50,50,50	0
25	MG	A	1682	1/1	0.89	0.24	43,43,43,43	0
26	K	A	1816	1/1	0.89	0.17	88,88,88,88	0
25	MG	A	1684	1/1	0.89	0.17	41,41,41,41	0
25	MG	A	1717	1/1	0.89	0.20	73,73,73,73	0
26	K	A	1790	1/1	0.89	0.15	85,85,85,85	0
26	K	A	1823	1/1	0.89	0.17	109,109,109,109	0
25	MG	A	1718	1/1	0.89	0.17	55,55,55,55	0
25	MG	A	1724	1/1	0.89	0.19	35,35,35,35	0
25	MG	A	1729	1/1	0.89	0.34	33,33,33,33	0
25	MG	A	1676	1/1	0.89	0.11	37,37,37,37	0
25	MG	A	1687	1/1	0.90	0.25	35,35,35,35	0
26	K	A	1794	1/1	0.90	0.45	96,96,96,96	0
24	PAR	A	1601	42/42	0.90	0.19	48,50,71,74	0
25	MG	A	1719	1/1	0.90	0.40	58,58,58,58	0
25	MG	A	1767	1/1	0.90	0.11	36,36,36,36	0
26	K	A	1783	1/1	0.90	0.10	82,82,82,82	0
25	MG	A	1722	1/1	0.90	0.34	34,34,34,34	0
25	MG	A	1614	1/1	0.90	0.08	48,48,48,48	0
25	MG	A	1713	1/1	0.90	0.26	27,27,27,27	0
25	MG	A	1646	1/1	0.90	0.18	51,51,51,51	0
25	MG	A	1748	1/1	0.90	0.13	43,43,43,43	0
25	MG	A	1677	1/1	0.91	0.21	21,21,21,21	0
26	K	A	1802	1/1	0.91	0.16	95,95,95,95	0
25	MG	A	1737	1/1	0.91	0.34	58,58,58,58	0
26	K	A	1782	1/1	0.91	0.27	92,92,92,92	0
25	MG	A	1712	1/1	0.91	0.57	68,68,68,68	0
25	MG	A	1604	1/1	0.91	0.49	59,59,59,59	0
25	MG	A	1679	1/1	0.91	0.20	48,48,48,48	0
25	MG	A	1640	1/1	0.91	0.32	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	MG	A	1626	1/1	0.91	0.67	88,88,88,88	0
25	MG	A	1617	1/1	0.91	0.48	62,62,62,62	0
25	MG	A	1629	1/1	0.91	0.51	85,85,85,85	0
25	MG	A	1685	1/1	0.91	0.41	64,64,64,64	0
25	MG	A	1666	1/1	0.91	0.35	59,59,59,59	0
26	K	A	1797	1/1	0.91	0.18	94,94,94,94	0
25	MG	A	1675	1/1	0.91	0.17	91,91,91,91	0
25	MG	A	1756	1/1	0.91	0.09	43,43,43,43	0
25	MG	A	1647	1/1	0.91	0.19	38,38,38,38	0
25	MG	A	1740	1/1	0.92	0.09	28,28,28,28	0
26	K	A	1815	1/1	0.92	0.20	88,88,88,88	0
25	MG	A	1641	1/1	0.92	0.38	49,49,49,49	0
26	K	A	1817	1/1	0.92	0.16	97,97,97,97	0
25	MG	K	201	1/1	0.92	0.13	49,49,49,49	0
25	MG	A	1714	1/1	0.92	0.38	57,57,57,57	0
26	K	A	1804	1/1	0.92	0.09	85,85,85,85	0
25	MG	A	1744	1/1	0.92	0.28	90,90,90,90	0
25	MG	A	1616	1/1	0.92	0.14	31,31,31,31	0
25	MG	A	1638	1/1	0.92	0.32	30,30,30,30	0
26	K	A	1826	1/1	0.92	0.56	152,152,152,152	0
25	MG	A	1635	1/1	0.92	0.74	81,81,81,81	0
25	MG	A	1750	1/1	0.92	0.15	36,36,36,36	0
26	K	A	1803	1/1	0.93	0.11	76,76,76,76	0
25	MG	A	1668	1/1	0.93	0.41	38,38,38,38	0
25	MG	A	1732	1/1	0.93	0.13	45,45,45,45	0
26	K	A	1785	1/1	0.93	0.08	92,92,92,92	0
25	MG	A	1743	1/1	0.93	0.16	51,51,51,51	0
26	K	A	1808	1/1	0.93	0.14	120,120,120,120	0
25	MG	A	1772	1/1	0.93	0.12	47,47,47,47	0
26	K	A	1810	1/1	0.93	0.40	100,100,100,100	0
25	MG	A	1686	1/1	0.93	0.16	28,28,28,28	0
25	MG	A	1734	1/1	0.93	0.21	29,29,29,29	0
26	K	A	1814	1/1	0.93	0.16	110,110,110,110	0
25	MG	A	1623	1/1	0.93	0.25	98,98,98,98	0
25	MG	B	301	1/1	0.93	0.13	43,43,43,43	0
26	K	A	1793	1/1	0.93	0.10	90,90,90,90	0
25	MG	D	302	1/1	0.93	0.14	41,41,41,41	0
25	MG	E	201	1/1	0.93	0.32	44,44,44,44	0
26	K	A	1796	1/1	0.93	0.20	101,101,101,101	0
26	K	A	1822	1/1	0.93	0.09	87,87,87,87	0
25	MG	A	1643	1/1	0.93	0.19	34,34,34,34	0
25	MG	M	201	1/1	0.93	0.10	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	MG	A	1605	1/1	0.93	0.19	18,18,18,18	0
25	MG	A	1728	1/1	0.93	0.21	40,40,40,40	0
26	K	A	1779	1/1	0.93	0.07	78,78,78,78	0
25	MG	A	1708	1/1	0.93	0.15	33,33,33,33	0
26	K	E	204	1/1	0.93	0.13	96,96,96,96	0
26	K	Q	202	1/1	0.93	0.09	95,95,95,95	0
25	MG	A	1624	1/1	0.94	0.38	48,48,48,48	0
25	MG	I	201	1/1	0.94	0.31	78,78,78,78	0
26	K	A	1813	1/1	0.94	0.07	127,127,127,127	0
25	MG	A	1652	1/1	0.94	0.29	55,55,55,55	0
25	MG	A	1696	1/1	0.94	0.44	50,50,50,50	0
25	MG	A	1608	1/1	0.94	0.09	54,54,54,54	0
25	MG	A	1656	1/1	0.94	0.29	31,31,31,31	0
26	K	A	1778	1/1	0.94	0.05	68,68,68,68	0
25	MG	A	1619	1/1	0.94	0.21	80,80,80,80	0
25	MG	A	1751	1/1	0.94	0.11	41,41,41,41	0
25	MG	A	1770	1/1	0.94	0.23	58,58,58,58	0
25	MG	A	1736	1/1	0.94	0.20	44,44,44,44	0
25	MG	A	1609	1/1	0.94	0.24	1,1,1,1	0
25	MG	A	1628	1/1	0.94	0.36	39,39,39,39	0
25	MG	A	1662	1/1	0.94	0.36	43,43,43,43	0
25	MG	A	1775	1/1	0.94	0.18	48,48,48,48	0
25	MG	A	1663	1/1	0.94	0.42	47,47,47,47	0
25	MG	A	1665	1/1	0.94	0.61	67,67,67,67	0
26	K	G	201	1/1	0.94	0.07	87,87,87,87	0
25	MG	A	1648	1/1	0.94	0.42	73,73,73,73	0
25	MG	A	1645	1/1	0.95	0.35	45,45,45,45	0
25	MG	A	1683	1/1	0.95	0.52	56,56,56,56	0
25	MG	A	1726	1/1	0.95	0.22	28,28,28,28	0
25	MG	A	1727	1/1	0.95	0.13	27,27,27,27	0
25	MG	A	1654	1/1	0.95	0.12	24,24,24,24	0
25	MG	A	1715	1/1	0.95	0.08	24,24,24,24	0
25	MG	A	1730	1/1	0.95	0.31	48,48,48,48	0
25	MG	A	1664	1/1	0.95	0.14	18,18,18,18	0
26	K	A	1781	1/1	0.95	0.15	94,94,94,94	0
25	MG	A	1693	1/1	0.95	0.49	65,65,65,65	0
26	K	E	202	1/1	0.95	0.09	83,83,83,83	0
25	MG	A	1745	1/1	0.95	0.10	25,25,25,25	0
25	MG	A	1710	1/1	0.95	0.46	61,61,61,61	0
25	MG	A	1660	1/1	0.95	0.25	28,28,28,28	0
25	MG	A	1720	1/1	0.95	0.39	45,45,45,45	0
27	ZN	D	301	1/1	0.95	0.23	69,69,69,69	0

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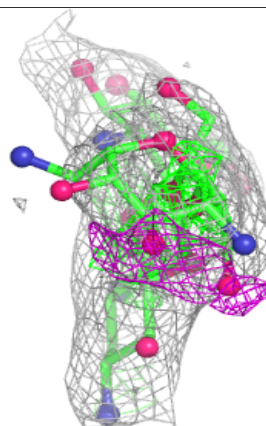
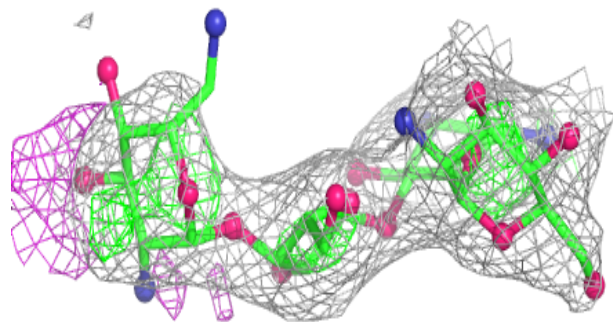
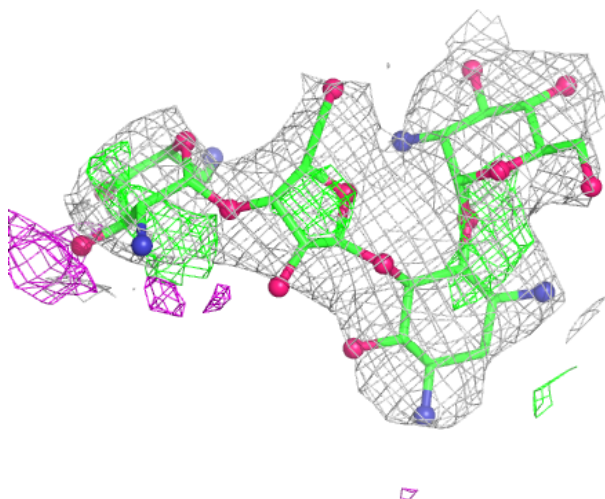
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	MG	A	1697	1/1	0.96	0.31	48,48,48,48	0
25	MG	A	1691	1/1	0.96	0.12	48,48,48,48	0
26	K	A	1784	1/1	0.96	0.09	76,76,76,76	0
25	MG	A	1649	1/1	0.96	0.30	1,1,1,1	0
25	MG	A	1606	1/1	0.96	0.47	40,40,40,40	0
25	MG	A	1766	1/1	0.96	0.08	28,28,28,28	0
25	MG	A	1721	1/1	0.96	0.12	26,26,26,26	0
25	MG	A	1655	1/1	0.96	0.44	46,46,46,46	0
25	MG	A	1607	1/1	0.96	0.35	39,39,39,39	0
25	MG	A	1725	1/1	0.96	0.15	36,36,36,36	0
25	MG	A	1764	1/1	0.97	0.08	26,26,26,26	0
25	MG	A	1695	1/1	0.97	0.23	47,47,47,47	0
25	MG	A	1661	1/1	0.97	0.41	54,54,54,54	0
25	MG	A	1706	1/1	0.97	0.39	36,36,36,36	0
26	K	A	1791	1/1	0.97	0.14	98,98,98,98	0
26	K	A	1819	1/1	0.97	0.17	130,130,130,130	0
25	MG	A	1651	1/1	0.97	0.33	39,39,39,39	0
25	MG	A	1755	1/1	0.97	0.11	42,42,42,42	0
25	MG	A	1777	1/1	0.97	0.04	38,38,38,38	0
25	MG	A	1637	1/1	0.97	0.31	44,44,44,44	0
25	MG	A	1689	1/1	0.98	0.38	46,46,46,46	0
25	MG	A	1639	1/1	0.98	0.34	32,32,32,32	0
25	MG	A	1634	1/1	0.98	0.38	36,36,36,36	0
25	MG	A	1747	1/1	0.98	0.05	28,28,28,28	0
25	MG	A	1698	1/1	0.98	0.07	12,12,12,12	0
25	MG	A	1723	1/1	0.98	0.05	29,29,29,29	0
26	K	A	1827	1/1	0.98	0.07	72,72,72,72	0
27	ZN	N	101	1/1	0.99	0.02	64,64,64,64	0
25	MG	A	1761	1/1	1.00	0.03	11,11,11,11	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 1601:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.