



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:45 AM UTC

PDB ID : 4B3T / pdb_00004b3t
Title : Crystal structure of the 30S ribosome in complex with compound 39
Authors : Ng, C.L.; Lang, K.; Shcherbakov, D.; Matt, T.; Perez-Fernandez, D.; Patak, R.; Meyer, M.; Duscha, S.; Akbergenov, R.; Boukari, H.; Freihofer, P.; Kudyba, I.; Reddy, M.S.K.; Nandurikar, R.S.; Ramakrishnan, V.; Vasella, A.; Bottger, E.C.
Deposited on : 2012-07-26
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

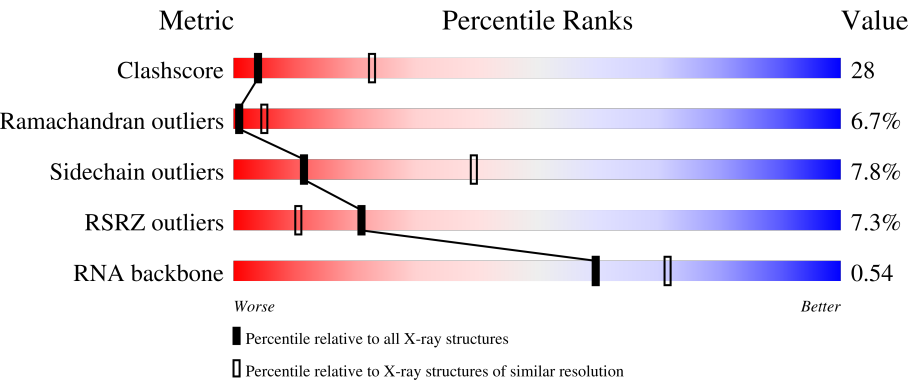
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtrriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 3.00 Å.

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



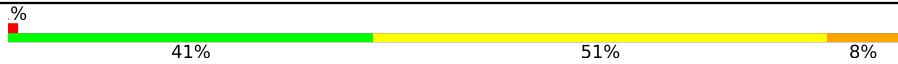
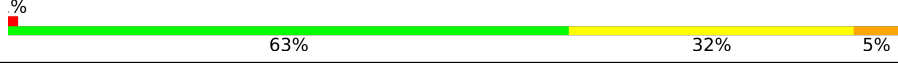
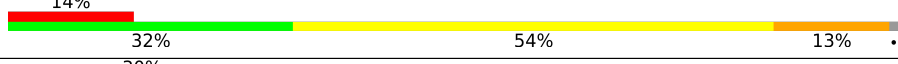
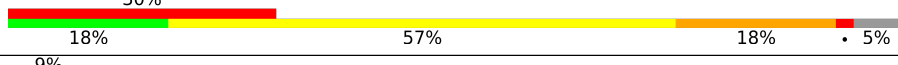
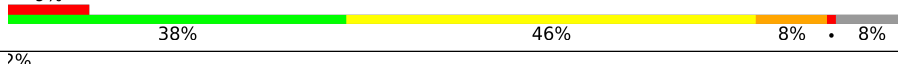
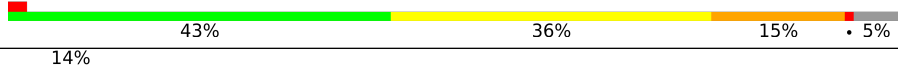
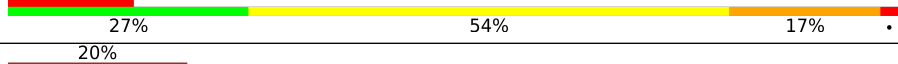
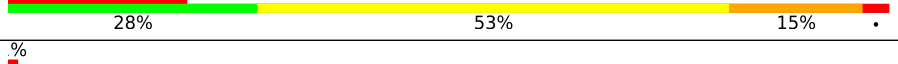
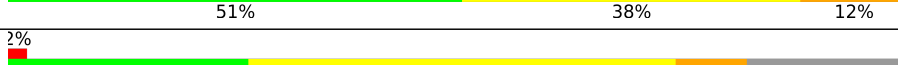
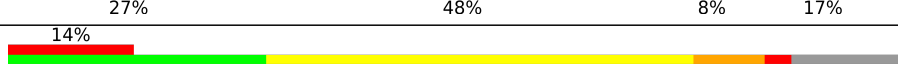
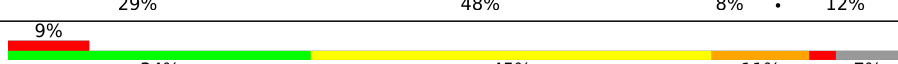
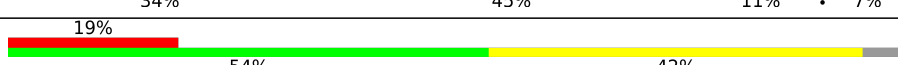
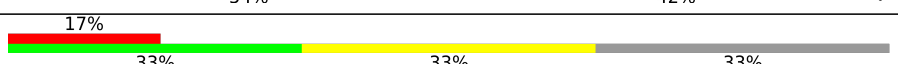
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)
RNA backbone	3983	1109 (3.20-2.80)

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	1521	4% 38% 48% 11%
2	B	256	11% 23% 52% 16% 8%
3	C	239	7% 28% 48% 10% 13%
4	D	208	9% 49% 42% 7%
5	E	161	3% 48% 37% 8% 6%

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Mol	Chain	Length	Quality of chain
6	F	101	
7	G	155	
8	H	138	
9	I	128	
10	J	104	
11	K	129	
12	L	132	
13	M	126	
14	N	60	
15	O	88	
16	P	88	
17	Q	104	
18	R	88	
19	S	92	
20	T	106	
21	V	26	
22	W	6	
23	Z	16	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	MG	A	2546	-	-	-	X
24	MG	A	2562	-	-	-	X
24	MG	A	2571	-	-	-	X
24	MG	A	2593	-	-	-	X
24	MG	A	2609	-	-	-	X
24	MG	A	2637	-	-	-	X
24	MG	A	2713	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	MG	A	2714	-	-	-	X
24	MG	A	2718	-	-	-	X
24	MG	A	2722	-	-	-	X
24	MG	A	3743	-	-	-	X
24	MG	A	3822	-	-	-	X
24	MG	A	3910	-	-	-	X
24	MG	A	3911	-	-	-	X
24	MG	A	3923	-	-	-	X
24	MG	A	3941	-	-	-	X
24	MG	A	3963	-	-	-	X

2 Entry composition

There are 28 unique types of molecules in this entry. The entry contains 52411 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
			32486	14462	6011	10503	1510			

- 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
			1011	639	198	174				

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	57	ARG	HIS	conflict	UNP P80374

- 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
			795	499	157	138	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	125	Total	C	N	O	S	0	0	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 TYPE Z.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	O	88	Total	C	N	O	S	0	0	0
			733	458	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	161	147	2			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	95	GLN	GLU	conflict	UNP Q5SHP7

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

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	45	GLY	ALA	conflict	UNP Q5SLQ0

- 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
			762	469	162	129	2			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	34	VAL	ILE	conflict	UNP P80380

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	W	4	Total	C	N	O	P	0	0	0
			79	37	12	27	3			

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	A	204	Total	Mg	0	0
			204	204		
24	C	1	Total	Mg	0	0
			1	1		

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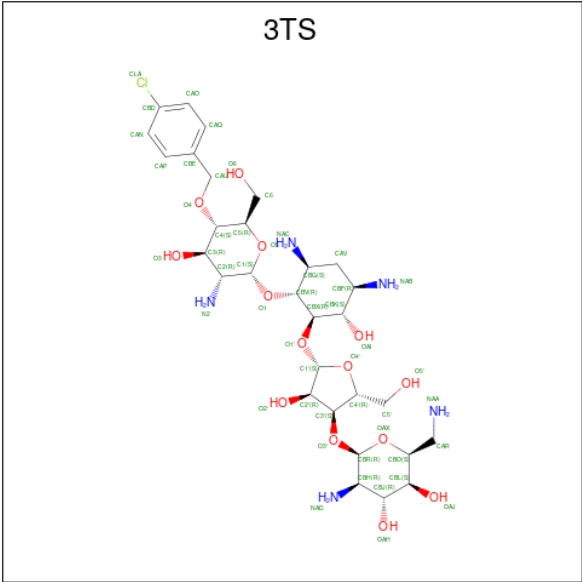
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	D	1	Total Mg 1 1	0	0
24	E	2	Total Mg 2 2	0	0
24	G	1	Total Mg 1 1	0	0
24	H	1	Total Mg 1 1	0	0
24	L	3	Total Mg 3 3	0	0
24	M	1	Total Mg 1 1	0	0
24	N	1	Total Mg 1 1	0	0
24	P	1	Total Mg 1 1	0	0
24	Q	1	Total Mg 1 1	0	0
24	T	2	Total Mg 2 2	0	0

- Molecule 25 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	16	Total K 16 16	0	0
25	E	1	Total K 1 1	0	0

- Molecule 26 is (2S,3S,4R,5R,6R)-2-(aminomethyl)-5-azanyl-6-[(2R,3S,4R,5S)-5-[(1R,2R,3S,5R,6S)-3,5-bis(azanyl)-2-[(2S,3R,4R,5S,6R)-3-azanyl-5-[(4-chlorophenyl)methoxy]-6-(hydroxymethyl)-4-oxidanyl-oxan-2-yl]oxy-6-oxidanyl-cyclohexyl]oxy-2-(hydroxymethyl)-4-oxidanyl-oxolan-3-yl]oxy-oxane-3,4-diol (CCD ID: 3TS) (formula: C₃₀H₅₀ClN₅O₁₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	A	1	Total	C	Cl	N	O	0
			50	30	1	5	14	

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

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

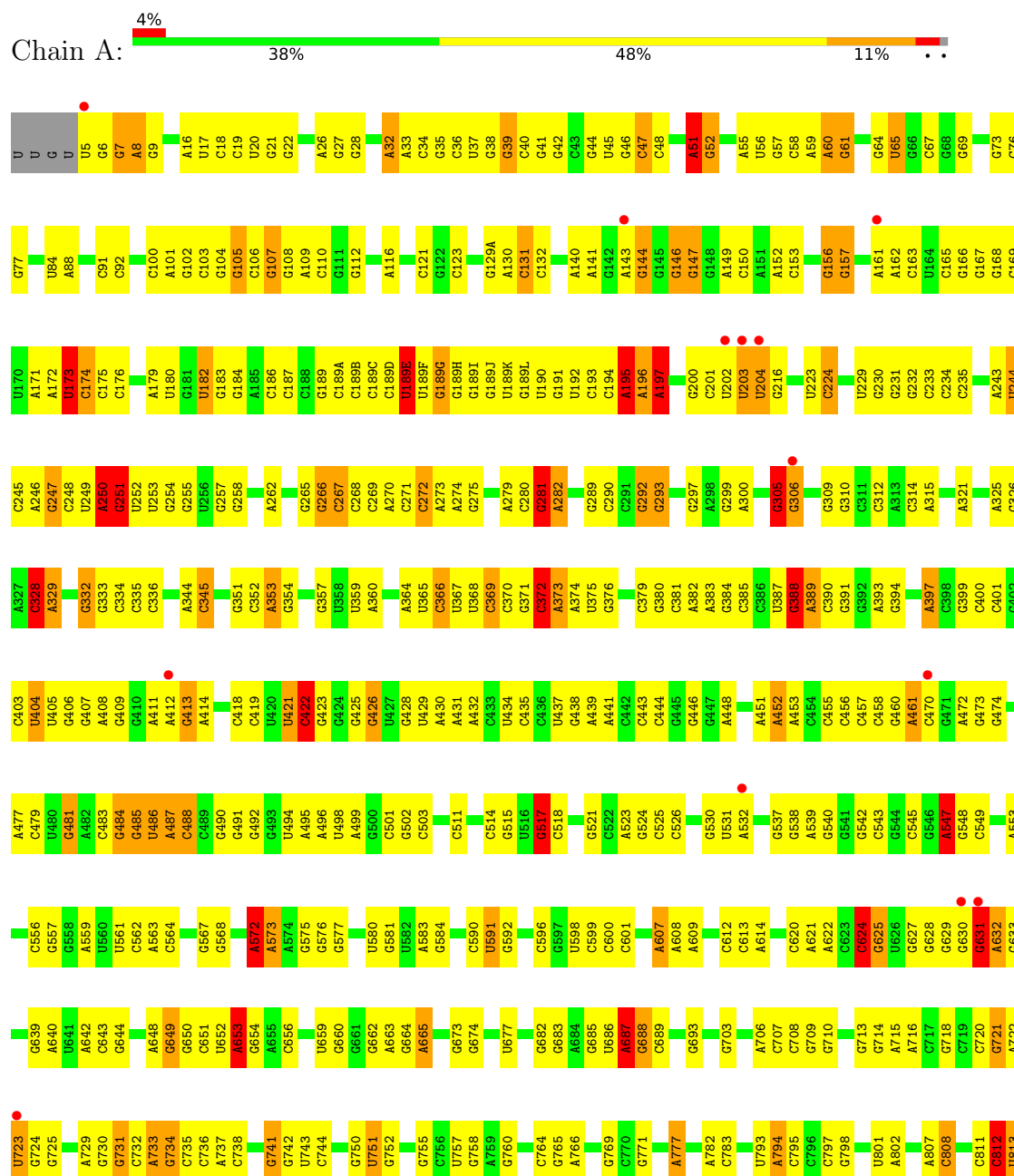
- Molecule 28 is water.

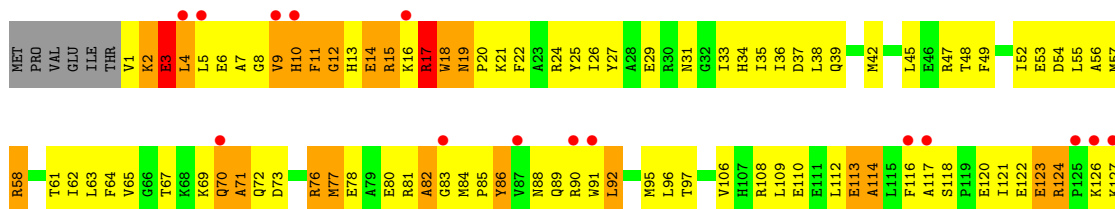
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	A	1	Total	O	0	0
			1	1		

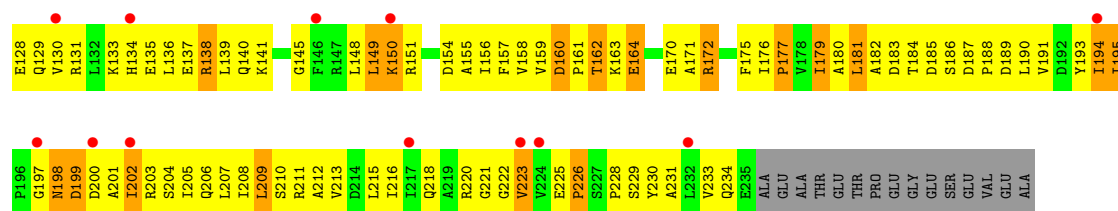
3 Residue-property plots

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.

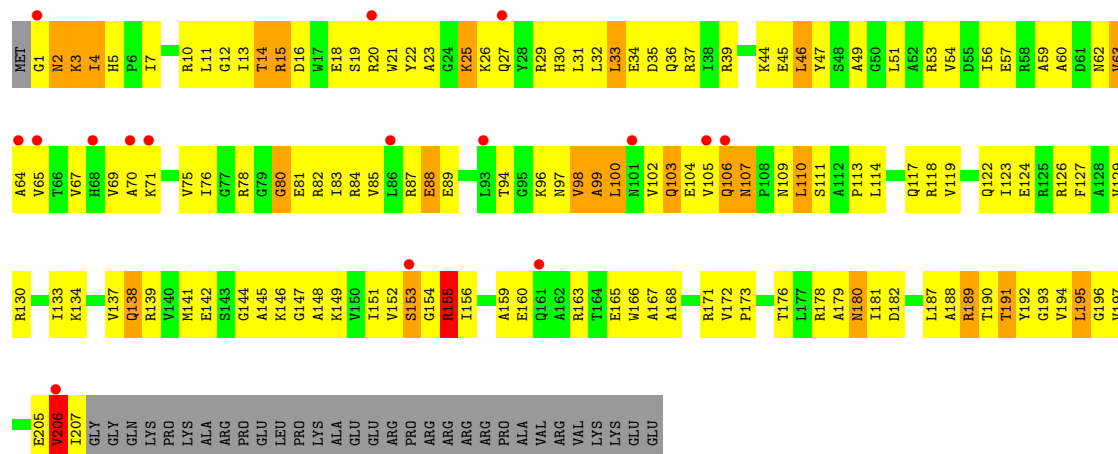
• Molecule 1: 16S RIBOSOMAL RNA



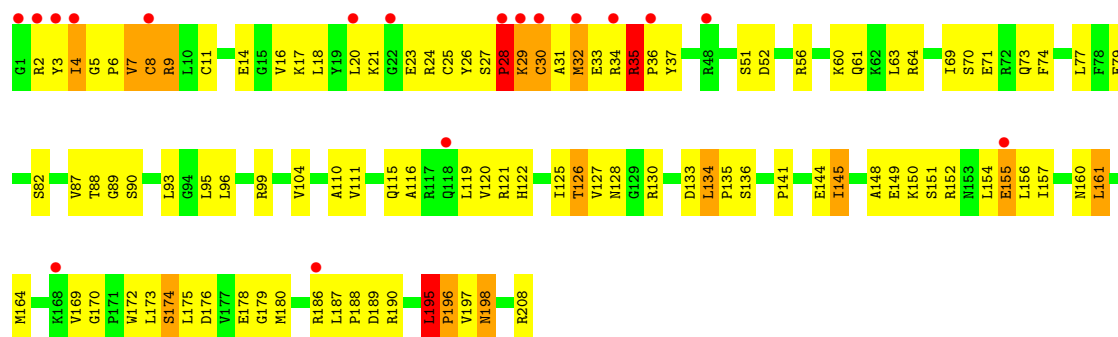




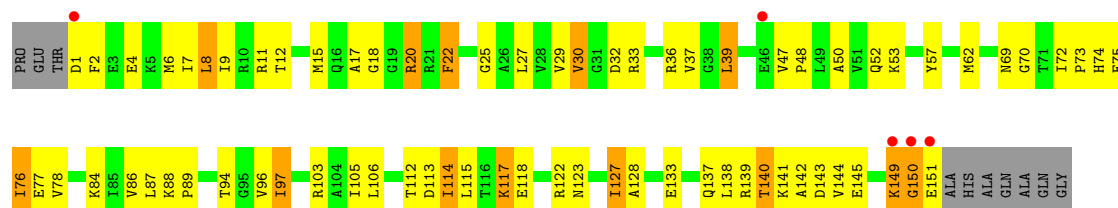
• Molecule 3: 30S RIBOSOMAL PROTEIN S3



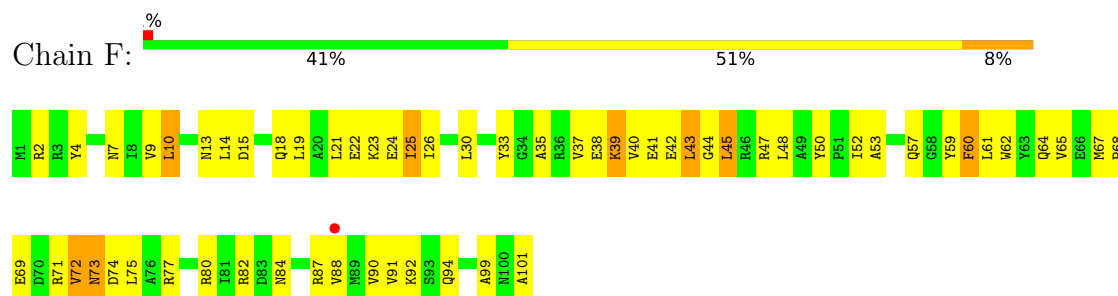
• Molecule 4: 30S RIBOSOMAL PROTEIN S4



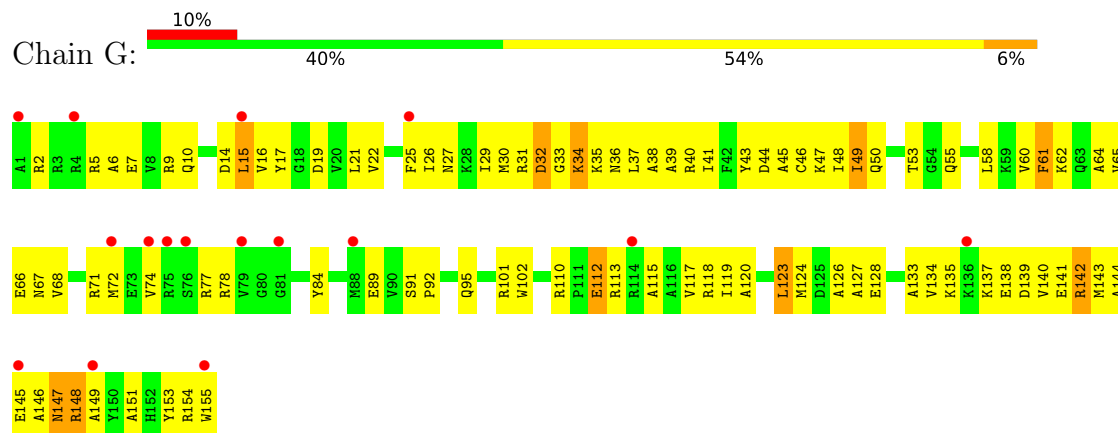
• Molecule 5: 30S RIBOSOMAL PROTEIN S5



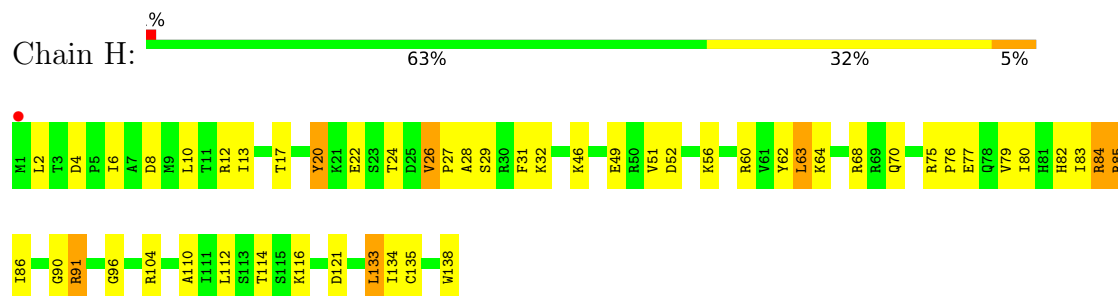
• Molecule 6: 30S RIBOSOMAL PROTEIN S6



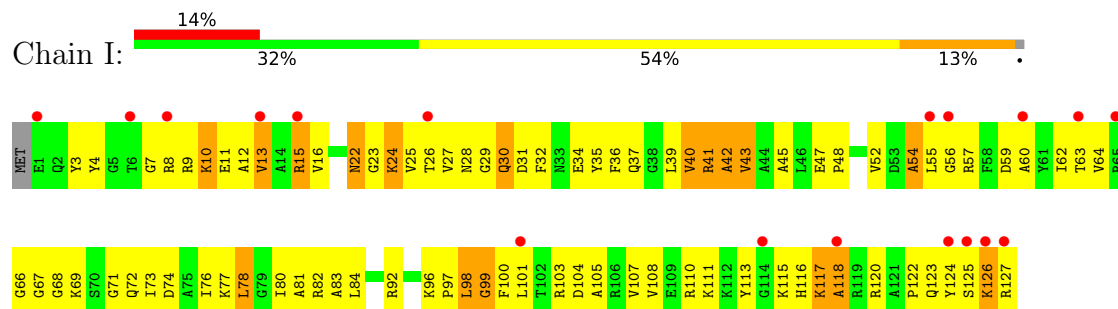
• Molecule 7: 30S RIBOSOMAL PROTEIN S7



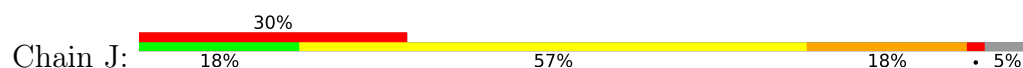
• Molecule 8: 30S RIBOSOMAL PROTEIN S8

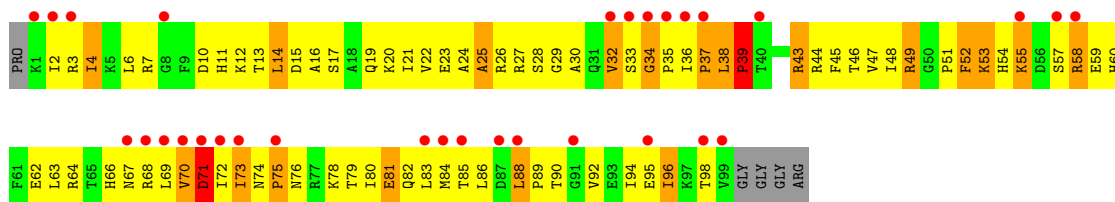


• Molecule 9: 30S RIBOSOMAL PROTEIN S9

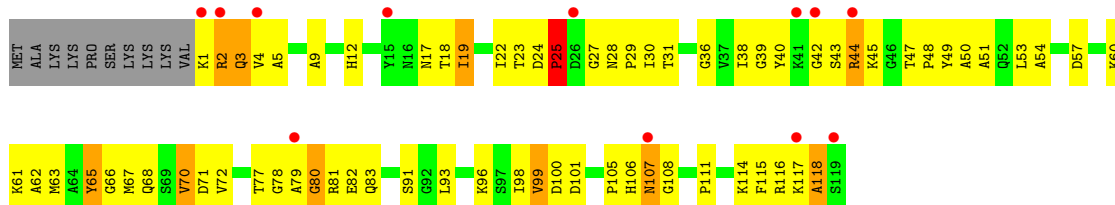


• Molecule 10: 30S RIBOSOMAL PROTEIN S10

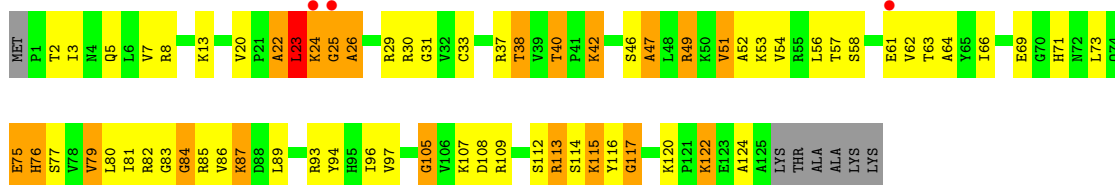
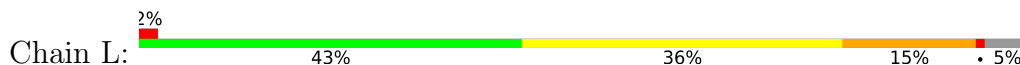




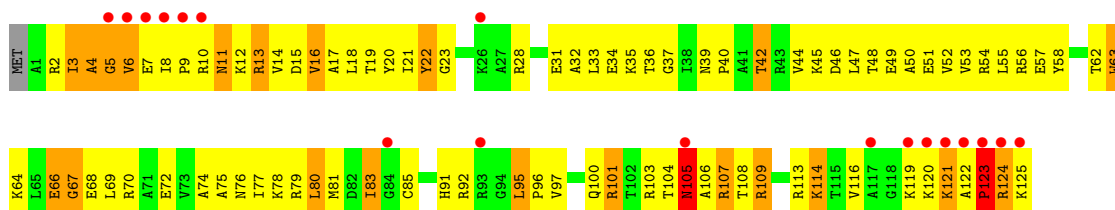
• Molecule 11: 30S RIBOSOMAL PROTEIN S11



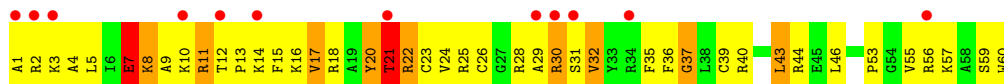
• Molecule 12: 30S RIBOSOMAL PROTEIN S12



• Molecule 13: 30S RIBOSOMAL PROTEIN S13

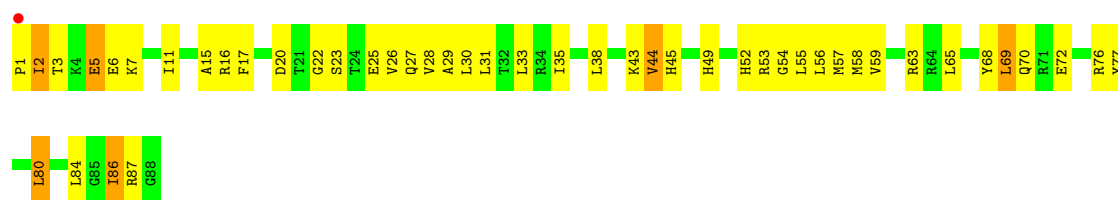


• Molecule 14: 30S RIBOSOMAL PROTEIN S14 TYPE Z

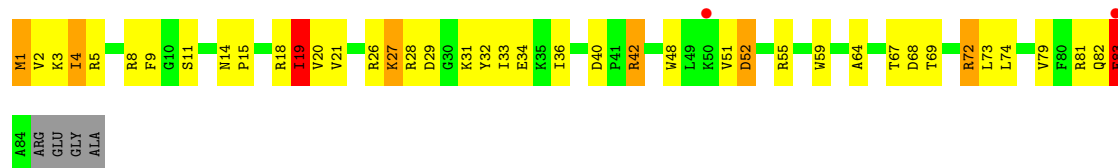


• Molecule 15: 30S RIBOSOMAL PROTEIN S15

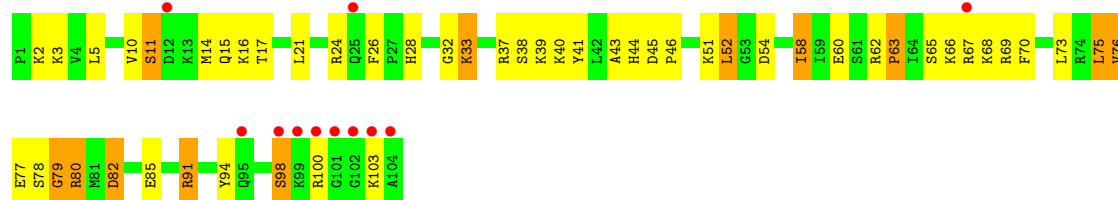




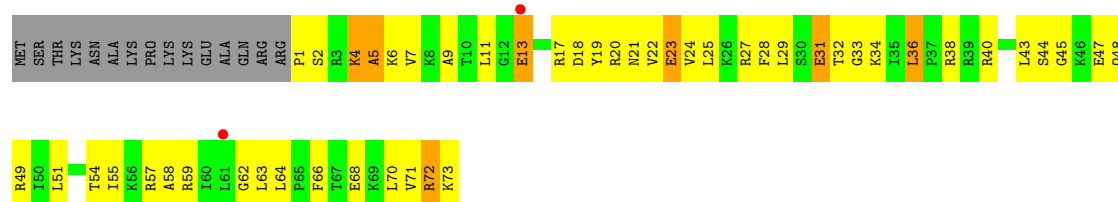
• Molecule 16: 30S RIBOSOMAL PROTEIN S16



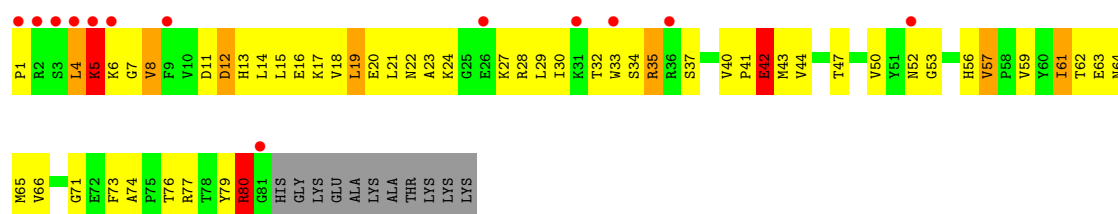
• Molecule 17: 30S RIBOSOMAL PROTEIN S17



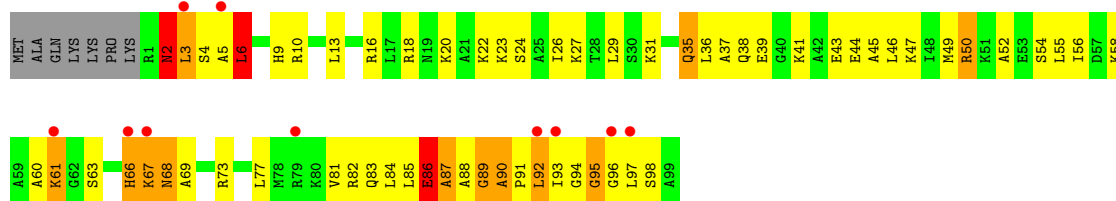
• Molecule 18: 30S RIBOSOMAL PROTEIN S18



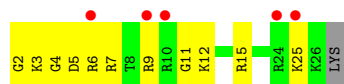
• Molecule 19: 30S RIBOSOMAL PROTEIN S19



• Molecule 20: 30S RIBOSOMAL PROTEIN S20



- Molecule 21: 30S RIBOSOMAL PROTEIN THX



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	401.73Å 401.73Å 173.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.00 40.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (40.00-3.00) 99.8 (40.00-3.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 3.01Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.210 , 0.243 0.213 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	76.5	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 69.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	52411	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.52% 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: 3TS, ZN, MG, K

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	0.42	0/36362	0.74	89/56750 (0.2%)
2	B	0.41	1/1936 (0.1%)	1.02	16/2611 (0.6%)
3	C	0.47	1/1637 (0.1%)	0.97	5/2207 (0.2%)
4	D	0.42	0/1733	0.97	9/2318 (0.4%)
5	E	0.57	1/1163 (0.1%)	1.02	2/1566 (0.1%)
6	F	0.41	0/856	0.92	4/1154 (0.3%)
7	G	0.39	0/1276	0.92	4/1709 (0.2%)
8	H	0.52	0/1136	1.09	8/1527 (0.5%)
9	I	0.42	0/1029	0.95	2/1378 (0.1%)
10	J	0.51	1/808 (0.1%)	1.02	5/1087 (0.5%)
11	K	0.50	0/900	1.06	4/1213 (0.3%)
12	L	0.55	1/987 (0.1%)	1.11	9/1322 (0.7%)
13	M	0.47	0/1008	1.05	3/1347 (0.2%)
14	N	0.48	0/501	1.11	5/664 (0.8%)
15	O	0.43	0/743	0.90	2/988 (0.2%)
16	P	0.57	1/717 (0.1%)	1.07	2/965 (0.2%)
17	Q	0.47	0/870	1.12	5/1159 (0.4%)
18	R	0.39	0/603	0.99	5/799 (0.6%)
19	S	0.52	1/662 (0.2%)	1.05	2/892 (0.2%)
20	T	0.52	0/764	1.11	5/1006 (0.5%)
21	V	0.63	1/213 (0.5%)	0.97	2/279 (0.7%)
22	W	0.37	0/87	0.69	0/133
23	Z	0.42	0/357	0.69	1/555 (0.2%)
All	All	0.44	8/56348 (0.0%)	0.84	189/83629 (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	36	35

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	S	80	ARG	C-N	-5.88	1.25	1.33
10	J	98	THR	C-N	-5.65	1.25	1.33
2	B	234	GLN	C-N	-5.62	1.25	1.33
16	P	83	GLU	C-N	-5.58	1.25	1.33
21	V	25	LYS	C-N	-5.54	1.25	1.33
3	C	206	VAL	C-N	-5.49	1.25	1.33
5	E	150	GLY	C-N	-5.47	1.25	1.33
12	L	124	ALA	C-N	-5.39	1.25	1.33

All (189) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	517	G	C2'-C3'-O3'	15.08	132.12	109.50
1	A	872	A	C2'-C3'-O3'	14.50	131.25	109.50
1	A	366	C	C2'-C3'-O3'	14.02	130.54	109.50
1	A	1345	U	C2'-C3'-O3'	13.70	130.05	109.50
1	A	189(G)	G	C2'-C3'-O3'	13.42	129.63	109.50
1	A	1085	U	C2'-C3'-O3'	13.32	129.48	109.50
1	A	653	A	C2'-C3'-O3'	12.98	128.97	109.50
1	A	47	C	C2'-C3'-O3'	12.90	128.85	109.50
1	A	1452	C	C2'-C3'-O3'	12.67	128.51	109.50
20	T	6	LEU	N-CA-C	-12.38	96.68	112.90
1	A	281	G	N9-C1'-C2'	11.31	130.96	114.00
1	A	372	C	C2'-C3'-O3'	10.51	125.26	109.50
13	M	106	ALA	N-CA-C	-10.12	98.78	112.03
1	A	1240	U	C2'-C3'-O3'	9.88	124.32	109.50
1	A	47	C	C4'-C3'-O3'	9.85	124.17	109.40
1	A	572	A	C2'-C3'-O3'	9.80	128.41	113.70
1	A	1201	A	C2'-C3'-O3'	9.67	124.00	109.50
1	A	189(G)	G	C4'-C3'-O3'	9.31	123.36	109.40
1	A	1085	U	C4'-C3'-O3'	9.20	123.19	109.40
1	A	305	G	N9-C1'-C2'	9.18	127.77	114.00
1	A	631	G	C2'-C3'-O3'	9.14	127.41	113.70
1	A	292	G	C2'-C3'-O3'	8.92	127.08	113.70
1	A	1345	U	C4'-C3'-O3'	8.59	122.29	109.40
20	T	67	LYS	N-CA-C	8.57	121.34	108.31
1	A	1452	C	C4'-C3'-O3'	8.56	122.24	109.40
1	A	366	C	C4'-C3'-O3'	8.53	122.19	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	982	U	N1-C1'-C2'	8.47	124.70	112.00
17	Q	26	PHE	N-CA-C	8.45	115.74	108.13
1	A	388	G	N9-C1'-C2'	8.18	124.28	112.00
11	K	27	GLY	N-CA-C	8.14	125.75	115.42
1	A	547	A	C2'-C3'-O3'	8.10	121.65	109.50
1	A	872	A	C4'-C3'-O3'	8.00	121.39	109.40
1	A	196	A	C2'-C3'-O3'	7.95	125.62	113.70
1	A	968	A	C2'-C3'-O3'	7.93	121.39	109.50
1	A	517	G	C4'-C3'-O3'	7.88	121.22	109.40
2	B	127	LYS	N-CA-C	-7.88	103.65	113.18
1	A	873	A	N9-C1'-C2'	7.86	125.80	114.00
1	A	884	U	C2'-C3'-O3'	7.82	121.23	109.50
1	A	1335	C	C2'-C3'-O3'	7.72	121.08	109.50
1	A	1544	U	C2'-C3'-O3'	-7.71	97.94	109.50
8	H	79	VAL	N-CA-C	-7.64	103.48	111.58
1	A	771	G	C5'-C4'-C3'	-7.50	104.75	116.00
20	T	67	LYS	CB-CA-C	-7.43	108.00	116.54
1	A	974	A	C2'-C3'-O3'	7.29	120.44	109.50
11	K	106	HIS	N-CA-C	-7.19	102.94	112.72
1	A	1400	C	C2'-C3'-O3'	7.14	120.22	109.50
12	L	115	LYS	N-CA-C	-7.11	100.95	110.55
1	A	250	A	C2'-C3'-O3'	7.10	120.15	109.50
4	D	195	LEU	CA-C-N	7.07	128.67	119.84
4	D	195	LEU	C-N-CA	7.07	128.67	119.84
6	F	43	LEU	N-CA-C	-6.98	104.65	113.72
3	C	88	GLU	N-CA-C	-6.97	103.77	112.90
14	N	32	VAL	N-CA-C	6.96	118.03	108.84
1	A	982	U	C2'-C3'-O3'	6.82	123.93	113.70
1	A	281	G	C2'-C3'-O3'	6.79	119.69	109.50
2	B	195	ILE	CA-C-N	6.79	128.32	119.84
2	B	195	ILE	C-N-CA	6.79	128.32	119.84
1	A	783	C	C5'-C4'-C3'	-6.77	105.84	116.00
1	A	1479	C	C2'-C3'-O3'	6.69	123.73	113.70
1	A	631	G	C4'-C3'-O3'	6.68	123.03	113.00
1	A	913	A	O4'-C4'-C3'	-6.65	99.45	106.10
16	P	19	ILE	N-CA-C	-6.64	100.07	108.84
1	A	1145	C	C2'-C3'-O3'	6.64	119.47	109.50
1	A	328	C	N1-C1'-C2'	6.63	123.95	114.00
6	F	72	VAL	N-CA-C	-6.63	105.37	111.67
1	A	1299	A	N9-C1'-C2'	6.61	121.92	112.00
10	J	49	ARG	N-CA-C	6.60	119.03	111.11
1	A	782	A	C5'-C4'-C3'	-6.59	106.11	116.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	T	86	GLU	N-CA-C	-6.57	99.78	109.11
12	L	87	LYS	N-CA-C	6.50	118.91	111.11
1	A	1502	A	N9-C1'-C2'	6.47	123.71	114.00
14	N	11	ARG	N-CA-C	-6.46	104.58	113.56
15	O	43	LYS	N-CA-C	-6.46	104.32	111.82
8	H	134	ILE	N-CA-C	6.46	116.62	110.42
4	D	9	ARG	N-CA-C	-6.43	106.06	114.04
1	A	896	C	C5'-C4'-C3'	-6.33	106.50	116.00
12	L	113	ARG	N-CA-C	6.25	118.90	111.71
1	A	189(E)	U	C5'-C4'-C3'	6.22	125.34	116.00
14	N	37	GLY	N-CA-C	-6.14	106.77	115.30
2	B	180	ALA	N-CA-C	6.12	118.60	108.99
1	A	1279	A	N9-C1'-C2'	6.12	121.17	112.00
18	R	36	LEU	CA-C-N	6.11	126.30	120.31
18	R	36	LEU	C-N-CA	6.11	126.30	120.31
2	B	154	ASP	N-CA-C	-6.07	104.50	113.61
9	I	59	ASP	N-CA-C	-6.07	100.27	109.85
3	C	89	GLU	N-CA-C	-6.06	104.59	112.23
1	A	547	A	C4'-C3'-O3'	6.04	118.46	109.40
1	A	173	U	N1-C1'-C2'	6.04	123.05	114.00
1	A	387	U	C5'-C4'-C3'	-6.03	106.96	116.00
1	A	687	A	C2'-C3'-O3'	6.03	118.54	109.50
18	R	4	LYS	N-CA-C	-6.03	106.18	112.93
12	L	40	THR	CA-C-N	6.01	125.97	120.21
12	L	40	THR	C-N-CA	6.01	125.97	120.21
2	B	7	ALA	N-CA-C	-6.00	106.31	113.21
3	C	98	VAL	N-CA-C	5.96	117.16	108.58
12	L	79	VAL	N-CA-C	5.94	116.72	108.23
1	A	196	A	C4'-C3'-O3'	5.91	121.87	113.00
1	A	1135	U	N1-C1'-C2'	5.91	120.86	112.00
7	G	133	ALA	N-CA-C	-5.90	104.76	111.07
1	A	624	C	C2'-C3'-O3'	5.89	122.54	113.70
12	L	22	ALA	N-CA-C	-5.89	98.26	110.80
10	J	20	LYS	N-CA-C	-5.85	104.32	112.45
17	Q	76	VAL	N-CA-C	-5.85	106.12	111.67
1	A	812	C	C2'-C3'-O3'	5.82	118.23	109.50
15	O	44	VAL	N-CA-C	-5.81	97.26	109.34
1	A	870	U	C5'-C4'-C3'	-5.81	106.49	115.20
18	R	31	GLU	N-CA-C	-5.78	105.33	112.38
7	G	49	ILE	N-CA-C	-5.76	105.23	113.07
1	A	107	G	C5'-C4'-C3'	-5.75	107.38	116.00
8	H	22	GLU	N-CA-C	-5.73	104.67	111.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J	64	ARG	N-CA-C	5.73	117.55	108.67
1	A	822	C	C5'-C4'-C3'	-5.72	107.42	116.00
2	B	113	GLU	N-CA-C	-5.68	104.91	113.89
1	A	1135	U	C2'-C3'-O3'	5.67	122.20	113.70
11	K	43	SER	N-CA-C	-5.67	106.21	113.23
13	M	107	ARG	N-CA-C	5.66	117.14	110.97
12	L	105	GLY	N-CA-C	-5.65	103.87	112.51
1	A	51	A	C2'-C3'-O3'	5.65	117.97	109.50
2	B	150	LYS	N-CA-C	-5.62	106.56	113.41
1	A	1048	G	C2'-C3'-O3'	5.62	122.12	113.70
1	A	975	A	C2'-C3'-O3'	5.59	117.89	109.50
5	E	22	PHE	N-CA-C	5.59	118.70	110.59
1	A	292	G	C4'-C3'-O3'	5.59	121.39	113.00
1	A	1182	G	C2'-C3'-O3'	5.59	117.88	109.50
2	B	58	ARG	N-CA-C	-5.58	106.29	114.39
13	M	63	TRP	N-CA-C	5.58	117.67	109.24
1	A	1335	C	C5'-C4'-C3'	-5.57	106.84	115.20
8	H	20	TYR	N-CA-C	5.55	119.09	111.54
1	A	1214	C	N1-C1'-C2'	5.55	122.32	114.00
2	B	114	ALA	N-CA-C	-5.52	104.90	111.69
8	H	96	GLY	N-CA-C	-5.50	103.99	112.85
1	A	7	G	C2'-C3'-O3'	5.50	117.75	109.50
1	A	729	A	C5'-C4'-C3'	-5.48	107.78	116.00
21	V	7	ARG	N-CA-C	5.47	118.77	112.97
8	H	28	ALA	N-CA-C	5.44	118.33	110.28
4	D	90	SER	N-CA-C	-5.43	105.25	111.07
1	A	281	G	C5'-C4'-O4'	5.43	117.25	109.10
14	N	7	GLU	N-CA-C	-5.42	106.62	113.18
1	A	1077	G	C5'-C4'-C3'	-5.42	107.87	116.00
1	A	1381	U	C5'-C4'-C3'	-5.42	107.88	116.00
14	N	20	TYR	N-CA-C	5.37	122.25	110.80
1	A	913	A	N9-C1'-C2'	5.34	122.01	114.00
8	H	75	ARG	CA-C-N	5.34	125.28	119.78
8	H	75	ARG	C-N-CA	5.34	125.28	119.78
9	I	71	GLY	N-CA-C	-5.33	106.04	112.49
1	A	1201	A	C4'-C3'-O3'	5.33	117.39	109.40
2	B	160	ASP	CA-C-N	5.33	124.78	119.24
2	B	160	ASP	C-N-CA	5.33	124.78	119.24
17	Q	98	SER	N-CA-C	5.33	116.59	108.12
1	A	193	C	C5'-C4'-C3'	-5.32	108.02	116.00
3	C	182	ASP	N-CA-C	-5.32	102.41	110.28
20	T	5	ALA	N-CA-C	-5.32	107.33	112.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	60	PHE	N-CA-C	5.30	117.87	109.24
23	Z	42	C	C4'-C3'-O3'	5.28	120.92	113.00
1	A	422	C	C5'-C4'-C3'	5.27	123.90	116.00
19	S	57	VAL	N-CA-C	5.26	113.66	107.77
12	L	84	GLY	N-CA-C	-5.26	100.72	113.18
17	Q	38	SER	N-CA-C	5.26	116.51	108.42
5	E	127	ILE	N-CA-C	-5.25	105.59	110.53
7	G	142	ARG	N-CA-C	-5.25	105.45	111.07
6	F	73	ASN	N-CA-C	-5.25	105.67	111.71
10	J	16	ALA	N-CA-C	-5.25	105.47	111.14
1	A	233	C	C5'-C4'-C3'	-5.24	108.15	116.00
2	B	202	ILE	N-CA-C	5.23	115.86	110.36
1	A	777	A	C5'-C4'-C3'	5.23	123.84	116.00
2	B	171	ALA	N-CA-C	-5.22	104.65	111.02
2	B	199	ASP	N-CA-C	-5.21	106.87	113.18
18	R	70	LEU	N-CA-C	-5.20	103.16	110.50
21	V	9	ARG	N-CA-C	-5.20	105.30	110.97
7	G	147	ASN	N-CA-C	-5.18	104.65	112.99
1	A	1479	C	C4'-C3'-O3'	5.16	120.74	113.00
1	A	1333	A	C5'-C4'-C3'	-5.16	108.26	116.00
11	K	65	TYR	N-CA-C	-5.15	106.54	114.16
16	P	4	ILE	N-CA-C	-5.13	99.30	106.53
1	A	951	G	C5'-C4'-C3'	-5.12	108.33	116.00
4	D	111	VAL	N-CA-C	5.11	115.88	110.72
19	S	53	GLY	N-CA-C	-5.11	101.06	113.18
1	A	28	G	C5'-C4'-C3'	-5.10	108.35	116.00
4	D	189	ASP	N-CA-C	-5.10	103.95	110.53
1	A	1334	G	C5'-C4'-C3'	-5.09	108.36	116.00
10	J	73	ILE	N-CA-C	-5.09	104.46	110.21
3	C	110	LEU	N-CA-C	-5.08	104.87	112.54
17	Q	82	ASP	N-CA-C	-5.08	105.75	111.28
4	D	32	MET	N-CA-C	-5.07	106.38	113.37
4	D	134	LEU	CA-C-N	5.07	125.09	119.32
4	D	134	LEU	C-N-CA	5.07	125.09	119.32
1	A	1479	C	C5'-C4'-C3'	5.05	123.58	116.00
1	A	547	A	N9-C1'-C2'	5.00	121.51	114.00
2	B	128	GLU	N-CA-C	-5.00	107.83	114.04

All (36) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	47	C	C3'

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Mol	Chain	Res	Type	Atom
1	A	173	U	C3',C4',C1'
1	A	189(E)	U	C4'
1	A	189(G)	G	C3'
1	A	196	A	C3'
1	A	281	G	C3',C4',C1'
1	A	292	G	C3'
1	A	305	G	C3',C4',C1'
1	A	366	C	C3'
1	A	388	G	C4'
1	A	422	C	C4'
1	A	517	G	C3'
1	A	547	A	C3',C4',C1'
1	A	631	G	C3'
1	A	872	A	C3'
1	A	873	A	C3',C4',C1'
1	A	913	A	C4'
1	A	982	U	C3',C4'
1	A	1048	G	C3'
1	A	1085	U	C3'
1	A	1135	U	C3',C4'
1	A	1345	U	C3'
1	A	1479	C	C3',C4'

All (35) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1048	G	Sidechain
1	A	112	G	Sidechain
1	A	1279	A	Sidechain
1	A	1289	A	Sidechain
1	A	1299	A	Sidechain
1	A	1307	U	Sidechain
1	A	1331	G	Sidechain
1	A	1405	G	Sidechain
1	A	1445	C	Sidechain
1	A	182	U	Sidechain
1	A	195	A	Sidechain
1	A	197	A	Sidechain
1	A	250	A	Sidechain
1	A	251	G	Sidechain
1	A	281	G	Sidechain
1	A	290	C	Sidechain

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Mol	Chain	Res	Type	Group
1	A	297	G	Sidechain
1	A	305	G	Sidechain
1	A	368	U	Sidechain
1	A	37	U	Sidechain
1	A	380	G	Sidechain
1	A	404	U	Sidechain
1	A	51	A	Sidechain
1	A	573	A	Sidechain
1	A	624	C	Sidechain
1	A	741	G	Sidechain
1	A	760	G	Sidechain
1	A	808	C	Sidechain
1	A	879	C	Sidechain
1	A	883	C	Sidechain
1	A	887	G	Sidechain
1	A	898	G	Sidechain
1	A	940	C	Sidechain
1	A	960	U	Sidechain
1	A	975	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	32486	0	16402	919	0
2	B	1901	0	1954	222	0
3	C	1613	0	1680	170	0
4	D	1703	0	1766	134	0
5	E	1147	0	1210	76	0
6	F	843	0	857	76	0
7	G	1257	0	1299	102	0
8	H	1116	0	1177	51	0
9	I	1011	0	1046	98	0
10	J	795	0	843	120	0
11	K	885	0	907	81	0
12	L	971	0	1059	75	0
13	M	997	0	1075	116	0
14	N	492	0	533	61	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	O	733	0	768	54	0
16	P	701	0	720	50	0
17	Q	857	0	932	55	0
18	R	597	0	670	65	0
19	S	648	0	675	83	0
20	T	762	0	862	62	0
21	V	209	0	221	15	0
22	W	79	0	44	3	0
23	Z	319	0	164	7	0
24	A	204	0	0	0	0
24	C	1	0	0	0	0
24	D	1	0	0	0	0
24	E	2	0	0	0	0
24	G	1	0	0	0	0
24	H	1	0	0	0	0
24	L	3	0	0	0	0
24	M	1	0	0	0	0
24	N	1	0	0	0	0
24	P	1	0	0	0	0
24	Q	1	0	0	0	0
24	T	2	0	0	0	0
25	A	16	0	0	0	0
25	E	1	0	0	0	0
26	A	50	0	50	6	0
27	D	1	0	0	0	0
27	N	1	0	0	0	0
28	A	1	0	0	0	0
All	All	52411	0	36914	2484	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 28.

All (2484) 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:425:G:H2'	1:A:426:G:H5''	1.22	1.17
1:A:243:A:H4'	1:A:244:U:H5'	1.19	1.13
1:A:1329:A:H2'	1:A:1330:U:H5''	1.18	1.13
4:D:17:LYS:NZ	4:D:30:CYS:HB3	1.64	1.12
3:C:190:THR:HG22	3:C:191:THR:H	1.09	1.12
1:A:872:A:H1'	1:A:873:A:H5'	1.16	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1008:C:H2'	1:A:1009:G:H5''	1.26	1.10
1:A:975:A:H5''	1:A:976:G:H5'	1.31	1.10
1:A:1271:G:H2'	1:A:1272:G:H5''	1.31	1.09
15:O:86:ILE:HG22	15:O:87:ARG:H	1.10	1.09
1:A:872:A:C1'	1:A:873:A:H5'	1.82	1.09
1:A:972:C:H4'	10:J:55:LYS:HG2	1.35	1.09
1:A:1012:U:H3'	1:A:1013:G:H5''	1.30	1.08
1:A:1029:C:H2'	1:A:1030:C:H5''	1.36	1.08
1:A:1098:C:H2'	1:A:1099:G:H5''	1.07	1.07
1:A:1054:C:O2'	1:A:1055:A:H5'	1.56	1.06
1:A:1098:C:C2'	1:A:1099:G:H5''	1.83	1.06
3:C:107:ASN:HD22	3:C:110:LEU:HG	1.20	1.06
19:S:27:LYS:HG2	19:S:28:ARG:H	1.15	1.06
1:A:223:U:H2'	1:A:224:C:H5''	1.37	1.05
1:A:1330:U:H6	1:A:1330:U:H5'	1.22	1.05
2:B:126:LYS:HA	2:B:129:GLN:HB3	1.38	1.05
10:J:43:ARG:HB3	10:J:43:ARG:HH11	1.19	1.04
1:A:1421:G:H1	1:A:1479:C:H42	1.04	1.04
10:J:36:ILE:HB	10:J:69:LEU:HB2	1.33	1.03
1:A:1329:A:C2'	1:A:1330:U:H5''	1.89	1.02
10:J:88:LEU:H	10:J:89:PRO:HD2	1.20	1.02
7:G:78:ARG:HB3	7:G:78:ARG:HH11	1.22	1.01
1:A:648:A:H2'	1:A:649:G:H5''	1.38	1.01
17:Q:91:ARG:HB3	17:Q:91:ARG:HH11	1.24	1.01
1:A:1188:A:H2'	1:A:1189:C:H5''	1.43	1.00
1:A:1276:G:H2'	1:A:1277:C:H5''	1.41	1.00
19:S:40:VAL:HG22	19:S:43:MET:HE3	1.43	0.99
1:A:1047:G:H2'	1:A:1048:G:H5''	1.39	0.99
6:F:25:ILE:H	6:F:25:ILE:HD12	1.24	0.98
1:A:1086:U:H3	1:A:1099:G:H22	1.02	0.98
1:A:1223:C:H5'	1:A:1224:G:H5''	1.45	0.98
1:A:104:G:H2'	1:A:105:G:H5''	1.42	0.97
9:I:15:ARG:HB2	9:I:63:THR:HB	1.44	0.97
1:A:1223:C:C5'	1:A:1224:G:H5''	1.93	0.96
1:A:1244:C:H2'	1:A:1245:A:H5''	1.47	0.96
2:B:78:GLU:HB3	2:B:213:VAL:HG21	1.44	0.96
11:K:44:ARG:O	11:K:47:THR:HG22	1.65	0.96
1:A:1244:C:C2'	1:A:1245:A:H5''	1.95	0.96
3:C:49:ALA:HB1	3:C:69:VAL:HG11	1.48	0.95
10:J:43:ARG:HB3	10:J:43:ARG:NH1	1.81	0.95
1:A:1271:G:C2'	1:A:1272:G:H5''	1.97	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1:VAL:HG21	2:B:215:LEU:HD23	1.46	0.94
7:G:78:ARG:HB3	7:G:78:ARG:NH1	1.82	0.94
1:A:1101:A:H4'	1:A:1102:A:H5'	1.48	0.94
3:C:2:ASN:HD22	3:C:2:ASN:H	1.14	0.93
19:S:4:LEU:O	19:S:5:LYS:HB2	1.65	0.93
1:A:1309:G:H3'	1:A:1310:G:H5''	1.47	0.93
1:A:425:G:C2'	1:A:426:G:H5''	1.98	0.92
3:C:190:THR:HG22	3:C:191:THR:N	1.83	0.92
1:A:591:U:H6	1:A:591:U:H5'	1.33	0.92
13:M:48:THR:HG22	13:M:50:ALA:H	1.34	0.92
1:A:64:G:H4'	1:A:65:U:H5'	1.51	0.91
5:E:47:VAL:HB	5:E:48:PRO:HD3	1.52	0.91
1:A:1502:A:H2	1:A:1505:G:H1	1.18	0.91
1:A:371:G:O2'	1:A:372:C:H5'	1.71	0.91
1:A:939:G:H5''	7:G:101:ARG:NH2	1.87	0.90
2:B:134:HIS:HA	2:B:137:GLU:HG2	1.53	0.90
4:D:195:LEU:HD23	4:D:195:LEU:H	1.36	0.90
1:A:1047:G:C2'	1:A:1048:G:H5''	2.01	0.89
1:A:38:G:H22	1:A:397:A:H5'	1.36	0.89
1:A:1029:C:C2'	1:A:1030:C:H5''	2.02	0.89
1:A:1442(A):G:H5''	1:A:1442(B):A:H5'	1.54	0.89
4:D:17:LYS:HZ3	4:D:30:CYS:HB3	1.30	0.89
16:P:51:VAL:O	16:P:52:ASP:HB3	1.73	0.89
1:A:1182:G:H4'	1:A:1183:A:H5'	1.54	0.89
5:E:76:ILE:CD1	5:E:87:LEU:HB2	2.03	0.89
1:A:1188:A:C2'	1:A:1189:C:H5''	2.01	0.89
1:A:1326:C:H5'	21:V:12:LYS:HZ2	1.36	0.89
3:C:25:LYS:NZ	3:C:25:LYS:H	1.71	0.88
1:A:272:C:H6	1:A:272:C:H5'	1.39	0.88
1:A:1421:G:H1	1:A:1479:C:N4	1.72	0.88
16:P:42:ARG:HG2	16:P:42:ARG:HH11	1.37	0.88
1:A:1213:A:O2'	1:A:1214:C:H5''	1.74	0.88
3:C:190:THR:CG2	3:C:191:THR:H	1.87	0.88
1:A:1231:G:O3'	9:I:125:SER:HB3	1.75	0.87
1:A:648:A:C2'	1:A:649:G:H5''	2.03	0.87
1:A:1008:C:C2'	1:A:1009:G:H5''	2.02	0.86
3:C:63:VAL:HB	3:C:98:VAL:HG23	1.57	0.86
1:A:1048:G:H5'	1:A:1048:G:H8	1.38	0.86
11:K:77:THR:HA	11:K:81:ARG:HH21	1.39	0.86
1:A:223:U:C2'	1:A:224:C:H5''	2.05	0.85
3:C:189:ARG:HB3	3:C:189:ARG:HH11	1.41	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1391:U:H2'	1:A:1392:G:C8	2.12	0.85
1:A:1329:A:H2'	1:A:1330:U:C5'	2.04	0.84
3:C:109:ASN:ND2	3:C:139:ARG:HB3	1.91	0.84
11:K:38:ILE:HG22	11:K:39:GLY:H	1.41	0.84
12:L:24:LYS:C	12:L:26:ALA:H	1.85	0.84
1:A:872:A:H1'	1:A:873:A:C5'	2.06	0.84
1:A:1276:G:C2'	1:A:1277:C:H5''	2.07	0.84
1:A:487:A:H5'	1:A:487:A:H8	1.42	0.84
13:M:39:ASN:O	13:M:42:THR:HG23	1.78	0.84
2:B:71:ALA:HB2	2:B:205:ILE:HD13	1.58	0.84
20:T:83:GLN:O	20:T:86:GLU:HB2	1.78	0.84
1:A:483:C:H3'	1:A:484:G:H5''	1.58	0.83
3:C:25:LYS:H	3:C:25:LYS:HZ3	1.26	0.83
4:D:17:LYS:HZ2	4:D:30:CYS:HB3	1.39	0.83
10:J:6:LEU:HB2	10:J:68:ARG:HB2	1.59	0.83
1:A:60:A:H4'	1:A:61:G:H5'	1.59	0.83
2:B:194:ILE:H	2:B:194:ILE:HD12	1.44	0.83
17:Q:91:ARG:HB3	17:Q:91:ARG:NH1	1.91	0.83
1:A:1012:U:C3'	1:A:1013:G:H5''	2.09	0.83
1:A:1334:G:H5'	1:A:1335:C:OP2	1.77	0.83
4:D:33:GLU:HG3	4:D:34:ARG:HH11	1.42	0.82
1:A:1330:U:H5'	1:A:1330:U:C6	2.12	0.82
14:N:26:CYS:SG	14:N:28:ARG:HB2	2.20	0.82
3:C:107:ASN:ND2	3:C:110:LEU:HG	1.92	0.82
10:J:44:ARG:HH11	10:J:44:ARG:HG2	1.43	0.82
3:C:13:ILE:HG22	3:C:14:THR:H	1.45	0.82
6:F:67:MET:HE2	6:F:72:VAL:HG22	1.62	0.82
1:A:404:U:H2'	1:A:405:U:H6	1.44	0.81
3:C:12:GLY:HA3	14:N:56:ARG:CZ	2.10	0.81
12:L:37:ARG:HH12	12:L:53:LYS:HE2	1.46	0.81
1:A:250:A:H4'	1:A:251:G:O5'	1.80	0.81
1:A:580:U:H2'	1:A:581:G:O4'	1.80	0.81
3:C:33:LEU:HG	14:N:24:VAL:HG21	1.61	0.81
1:A:1004:A:H8	1:A:1036:G:H1	1.28	0.81
1:A:1164:G:H1	1:A:1172:C:H42	1.29	0.81
2:B:118:SER:O	2:B:121:ILE:HG13	1.81	0.81
3:C:109:ASN:O	3:C:110:LEU:HD23	1.81	0.81
10:J:37:PRO:HA	10:J:68:ARG:HH11	1.46	0.81
1:A:1309:G:C3'	1:A:1310:G:H5''	2.11	0.81
4:D:25:CYS:HA	4:D:30:CYS:HB2	1.62	0.81
2:B:108:ARG:NH1	2:B:112:LEU:HG	1.96	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:82:HIS:NE2	8:H:84:ARG:HB2	1.96	0.80
11:K:12:HIS:HB3	11:K:19:ILE:CD1	2.09	0.80
1:A:1260:C:OP1	1:A:1284:C:H4'	1.82	0.80
12:L:71:HIS:HD2	12:L:73:LEU:H	1.28	0.80
1:A:189(D):C:H2'	1:A:189(E):U:H1'	1.63	0.80
10:J:88:LEU:H	10:J:89:PRO:CD	1.95	0.80
1:A:939:G:H5''	7:G:101:ARG:HH22	1.46	0.80
1:A:1256:A:H61	1:A:1278:U:H3	1.26	0.80
12:L:29:ARG:HD3	12:L:58:SER:HB3	1.64	0.79
1:A:664:G:H22	1:A:741:G:H1	1.29	0.79
1:A:1125:U:H3	10:J:3:ARG:HH21	1.30	0.79
3:C:118:ARG:HG2	3:C:139:ARG:NH2	1.97	0.79
1:A:1326:C:H5'	21:V:12:LYS:NZ	1.96	0.79
12:L:22:ALA:O	12:L:23:LEU:O	2.01	0.79
9:I:69:LYS:O	9:I:73:ILE:HG13	1.83	0.79
15:O:38:LEU:HD12	15:O:55:LEU:HB2	1.65	0.79
1:A:751:U:H1'	15:O:22:GLY:O	1.82	0.79
3:C:25:LYS:HZ2	3:C:25:LYS:HB3	1.48	0.79
12:L:37:ARG:HG2	12:L:38:THR:H	1.46	0.79
1:A:1245:A:H5'	1:A:1245:A:H8	1.46	0.78
1:A:1502:A:H2	1:A:1505:G:N1	1.82	0.78
13:M:66:GLU:HG3	13:M:67:GLY:H	1.49	0.78
3:C:103:GLN:HE21	3:C:104:GLU:H	1.31	0.78
21:V:6:ARG:HG2	21:V:15:ARG:NH1	1.99	0.78
1:A:1060:C:C5	3:C:1:GLY:HA3	2.19	0.78
4:D:28:PRO:O	4:D:29:LYS:HG3	1.84	0.78
6:F:15:ASP:H	6:F:18:GLN:NE2	1.81	0.78
6:F:48:LEU:HG	6:F:57:GLN:HA	1.66	0.78
16:P:15:PRO:HD2	16:P:42:ARG:HD2	1.66	0.78
11:K:44:ARG:NH1	11:K:44:ARG:HB3	1.98	0.78
1:A:1188:A:C3'	1:A:1189:C:H5''	2.14	0.77
3:C:2:ASN:H	3:C:2:ASN:ND2	1.81	0.77
3:C:14:THR:O	3:C:15:ARG:HB2	1.84	0.77
11:K:100:ASP:HB2	18:R:73:LYS:HD2	1.66	0.77
21:V:6:ARG:NE	21:V:15:ARG:HH12	1.83	0.77
6:F:10:LEU:CD1	6:F:59:TYR:HB3	2.13	0.77
2:B:6:GLU:HB3	2:B:10:HIS:HE1	1.49	0.77
4:D:150:LYS:H	4:D:150:LYS:HD2	1.48	0.77
7:G:53:THR:HG22	7:G:55:GLN:H	1.48	0.77
2:B:76:ARG:HA	2:B:86:TYR:CE2	2.20	0.77
1:A:613:C:O2'	1:A:614:A:H5'	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:720:C:H3'	1:A:721:G:H5''	1.66	0.77
7:G:36:ASN:ND2	9:I:40:VAL:HG23	2.00	0.77
1:A:371:G:C2'	1:A:372:C:H5'	2.16	0.76
21:V:6:ARG:HE	21:V:15:ARG:HH12	1.33	0.76
4:D:34:ARG:O	4:D:35:ARG:HB2	1.85	0.76
4:D:35:ARG:H	4:D:36:PRO:CD	1.98	0.76
4:D:178:GLU:HG3	4:D:179:GLY:H	1.49	0.76
11:K:81:ARG:CZ	18:R:73:LYS:HE2	2.15	0.76
1:A:1126:U:O2	1:A:1126:U:H2'	1.85	0.76
1:A:946:A:H2'	1:A:947:G:C8	2.21	0.76
1:A:1098:C:H2'	1:A:1099:G:C5'	2.03	0.76
1:A:1007:C:H2'	1:A:1008:C:C6	2.20	0.76
1:A:1330:U:H2'	1:A:1331:G:H5'	1.66	0.76
10:J:32:VAL:HG22	10:J:72:ILE:HG23	1.66	0.76
13:M:49:GLU:O	13:M:53:VAL:HG23	1.86	0.76
10:J:4:ILE:HD13	10:J:4:ILE:H	1.50	0.76
12:L:56:LEU:HD21	12:L:62:VAL:HG22	1.68	0.76
1:A:280:C:H4'	1:A:281:G:OP2	1.85	0.75
1:A:1435:G:H2'	1:A:1436:U:C6	2.20	0.75
4:D:186:ARG:HH22	4:D:187:LEU:HD12	1.50	0.75
1:A:1189:C:H6	1:A:1189:C:H5'	1.51	0.75
2:B:230:TYR:HD1	2:B:233:VAL:HG21	1.51	0.75
13:M:121:LYS:HG3	13:M:122:ALA:H	1.48	0.75
15:O:3:THR:HB	15:O:5:GLU:OE2	1.86	0.75
2:B:6:GLU:HB3	2:B:10:HIS:CE1	2.22	0.75
4:D:2:ARG:NH2	4:D:73:GLN:HE21	1.82	0.75
19:S:27:LYS:CG	19:S:28:ARG:H	1.96	0.75
4:D:33:GLU:HG3	4:D:34:ARG:NH1	2.02	0.75
1:A:104:G:C2'	1:A:105:G:H5''	2.16	0.75
1:A:293:G:H5'	1:A:609:A:H61	1.52	0.74
1:A:835:U:OP1	18:R:49:ARG:NH2	2.20	0.74
1:A:1223:C:H5''	1:A:1224:G:H5''	1.69	0.74
2:B:15:ARG:NH1	2:B:17:ARG:HG2	2.01	0.74
8:H:84:ARG:HH11	8:H:84:ARG:HG3	1.51	0.74
13:M:9:PRO:HB2	13:M:17:ALA:HB1	1.69	0.74
18:R:31:GLU:CD	18:R:31:GLU:H	1.94	0.74
19:S:44:VAL:HA	19:S:61:ILE:HD12	1.69	0.74
20:T:46:LEU:HB2	20:T:93:ILE:CG2	2.17	0.74
1:A:146:G:H2'	1:A:147:G:H5''	1.68	0.74
3:C:12:GLY:HA3	14:N:56:ARG:NH2	2.02	0.74
19:S:27:LYS:HG2	19:S:28:ARG:N	1.96	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:A:H2'	1:A:150:C:C6	2.23	0.74
7:G:120:ALA:O	7:G:124:MET:HG3	1.88	0.74
13:M:3:ILE:HG22	13:M:4:ALA:N	2.03	0.74
1:A:1480:G:HO2'	1:A:1481:U:H6	1.35	0.74
11:K:38:ILE:HG22	11:K:39:GLY:N	2.00	0.74
1:A:56:U:H2'	1:A:57:G:H8	1.53	0.74
15:O:35:ILE:HD13	15:O:58:MET:HE3	1.70	0.74
2:B:172:ARG:NH2	8:H:68:ARG:HH22	1.86	0.74
7:G:112:GLU:HG2	7:G:118:ARG:HG2	1.68	0.74
15:O:86:ILE:HG22	15:O:87:ARG:N	1.91	0.74
1:A:837:G:H1	1:A:849:C:H42	1.34	0.74
1:A:1474:G:C2'	1:A:1475:G:H5''	2.18	0.74
1:A:404:U:H2'	1:A:405:U:C6	2.22	0.73
10:J:59:GLU:OE1	14:N:44:ARG:NH1	2.21	0.73
17:Q:66:LYS:O	17:Q:67:ARG:HG2	1.88	0.73
1:A:624:C:H4'	1:A:625:G:OP1	1.89	0.73
1:A:751:U:H5'	1:A:752:G:OP2	1.88	0.73
1:A:1412:C:H2'	1:A:1413:A:C8	2.23	0.73
1:A:147:G:H5'	1:A:147:G:H8	1.53	0.73
1:A:818:G:O2'	1:A:819:A:H5''	1.88	0.73
4:D:173:LEU:O	4:D:174:SER:HB3	1.88	0.73
9:I:92:ARG:NH1	9:I:92:ARG:HB3	2.04	0.73
3:C:2:ASN:ND2	3:C:2:ASN:N	2.33	0.73
14:N:25:ARG:NE	14:N:46:LEU:HD21	2.04	0.73
3:C:26:LYS:HB2	3:C:27:GLN:HE21	1.53	0.73
13:M:3:ILE:HG22	13:M:4:ALA:H	1.53	0.73
19:S:32:THR:HG22	19:S:34:SER:H	1.52	0.73
2:B:78:GLU:OE2	2:B:210:SER:HA	1.88	0.73
1:A:1343:G:H2'	1:A:1344:C:C6	2.24	0.73
7:G:49:ILE:HA	7:G:124:MET:HE3	1.71	0.73
1:A:1474:G:H2'	1:A:1475:G:H5''	1.71	0.72
1:A:1065:U:C5	1:A:1190:G:H1'	2.23	0.72
11:K:12:HIS:HB3	11:K:19:ILE:HD13	1.68	0.72
1:A:998:G:H3'	1:A:999:C:H5''	1.68	0.72
6:F:101:ALA:CB	18:R:13:GLU:HG3	2.20	0.72
1:A:718:G:H5'	11:K:107:ASN:HB2	1.71	0.72
1:A:948:C:OP1	13:M:108:THR:HG22	1.89	0.72
1:A:1148:U:H2'	1:A:1149:C:O4'	1.89	0.72
20:T:3:LEU:O	20:T:6:LEU:HD13	1.88	0.72
1:A:1057:G:H5''	3:C:153:SER:HB2	1.72	0.72
1:A:1244:C:H2'	1:A:1245:A:C5'	2.18	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:4:ILE:HD13	10:J:4:ILE:N	2.05	0.72
13:M:64:LYS:HE3	13:M:68:GLU:HG2	1.71	0.72
2:B:19:ASN:C	2:B:19:ASN:HD22	1.97	0.72
12:L:33:CYS:HB2	12:L:75:GLU:O	1.90	0.72
13:M:121:LYS:CG	13:M:122:ALA:H	2.02	0.72
2:B:17:ARG:NH1	2:B:18:TRP:HA	2.04	0.72
12:L:71:HIS:CD2	12:L:73:LEU:H	2.07	0.72
18:R:23:GLU:H	18:R:23:GLU:CD	1.97	0.71
2:B:76:ARG:HA	2:B:86:TYR:HE2	1.54	0.71
17:Q:58:ILE:HG23	17:Q:70:PHE:CD2	2.25	0.71
1:A:1222:G:OP1	19:S:76:THR:HG21	1.90	0.71
1:A:1030(C):G:H2'	1:A:1030(D):A:C8	2.24	0.71
1:A:1442(A):G:C5'	1:A:1442(B):A:H5'	2.20	0.71
1:A:146:G:C2'	1:A:147:G:H5''	2.20	0.71
2:B:86:TYR:O	2:B:145:GLY:HA3	1.91	0.71
1:A:344:A:H5''	1:A:345:C:H5	1.54	0.71
1:A:1189:C:P	10:J:49:ARG:HH22	2.13	0.71
13:M:14:VAL:HG23	13:M:42:THR:O	1.91	0.71
9:I:98:LEU:HB2	9:I:100:PHE:CE1	2.26	0.71
1:A:499:A:H61	1:A:547:A:H5''	1.54	0.71
19:S:14:LEU:HA	19:S:17:LYS:HB3	1.71	0.71
19:S:61:ILE:HD13	19:S:62:THR:N	2.06	0.71
1:A:872:A:C2'	1:A:873:A:H5'	2.21	0.71
2:B:92:LEU:N	2:B:92:LEU:HD23	2.04	0.71
16:P:11:SER:HB2	16:P:14:ASN:HB3	1.73	0.71
1:A:21:G:H2'	1:A:22:G:C8	2.27	0.70
11:K:30:ILE:HG22	11:K:31:THR:HG23	1.73	0.70
11:K:47:THR:HG23	11:K:50:ALA:H	1.56	0.70
1:A:1216:G:H5''	14:N:4:ALA:CB	2.21	0.70
13:M:83:ILE:HD12	19:S:64:ASN:ND2	2.06	0.70
7:G:148:ARG:HD2	11:K:49:TYR:CE1	2.26	0.70
13:M:58:TYR:O	13:M:62:THR:HG22	1.91	0.70
1:A:1123:A:H4'	10:J:35:PRO:HD2	1.73	0.70
5:E:77:GLU:HG2	5:E:86:VAL:HG22	1.74	0.70
1:A:460:G:H2'	1:A:461:A:H5''	1.74	0.70
10:J:2:ILE:HD11	10:J:75:PRO:HA	1.73	0.70
11:K:9:ALA:HB2	11:K:70:VAL:HG11	1.73	0.70
13:M:51:GLU:HG2	13:M:54:ARG:HH21	1.57	0.70
1:A:730:G:H5'	1:A:731:G:OP2	1.90	0.70
1:A:1150:U:H4'	10:J:39:PRO:HG3	1.72	0.70
1:A:486:U:C2'	1:A:487:A:H5''	2.22	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1486:G:H2'	1:A:1487:G:O4'	1.92	0.70
4:D:186:ARG:CZ	4:D:187:LEU:H	2.05	0.70
15:O:5:GLU:H	15:O:5:GLU:CD	1.97	0.70
1:A:1005:A:H5''	1:A:1006:C:H5	1.57	0.70
9:I:16:VAL:HG22	9:I:62:ILE:HD12	1.72	0.70
1:A:1125:U:H5''	1:A:1126:U:N3	2.07	0.70
1:A:1193:G:O2'	1:A:1194:U:H5'	1.92	0.70
12:L:24:LYS:O	12:L:26:ALA:N	2.24	0.70
12:L:79:VAL:HG22	12:L:80:LEU:H	1.57	0.70
19:S:6:LYS:HG2	19:S:6:LYS:O	1.91	0.70
2:B:126:LYS:HA	2:B:129:GLN:CB	2.18	0.70
7:G:34:LYS:HD3	7:G:37:LEU:HD23	1.74	0.69
1:A:1250:A:O3'	9:I:66:GLY:HA2	1.92	0.69
2:B:81:ARG:HB3	2:B:81:ARG:HH11	1.57	0.69
2:B:194:ILE:HD12	2:B:194:ILE:N	2.06	0.69
3:C:179:ALA:O	3:C:180:ASN:HB3	1.91	0.69
10:J:14:LEU:O	10:J:14:LEU:HD13	1.92	0.69
1:A:881:G:P	12:L:8:ARG:HH22	2.15	0.69
12:L:79:VAL:HG22	12:L:80:LEU:N	2.07	0.69
5:E:74:HIS:HE1	5:E:139:ARG:H	1.37	0.69
7:G:77:ARG:HD2	7:G:155:TRP:HZ3	1.56	0.69
1:A:673:G:H2'	1:A:674:G:C8	2.28	0.69
2:B:13:HIS:NE2	2:B:200:ASP:HB3	2.07	0.69
9:I:117:LYS:HG3	9:I:120:ARG:HB3	1.75	0.69
17:Q:51:LYS:O	17:Q:54:ASP:HB2	1.92	0.69
1:A:408:A:H5'	4:D:115:GLN:HE21	1.58	0.69
1:A:460:G:H3'	1:A:461:A:C5'	2.23	0.69
1:A:1129:C:O2'	1:A:1131:G:H5''	1.93	0.69
1:A:1163:C:H2'	1:A:1164:G:H8	1.57	0.69
1:A:1504:G:OP1	1:A:1507:A:H4'	1.92	0.69
9:I:117:LYS:O	9:I:118:ALA:HB3	1.93	0.69
18:R:32:THR:HA	18:R:68:GLU:HB2	1.75	0.69
19:S:63:GLU:O	19:S:66:VAL:HG23	1.93	0.69
1:A:1305:G:N2	1:A:1331:G:H1'	2.06	0.69
3:C:18:GLU:HG2	3:C:53:ARG:HE	1.57	0.69
13:M:48:THR:HG22	13:M:50:ALA:N	2.05	0.69
1:A:1223:C:H5'	1:A:1224:G:C5'	2.22	0.69
2:B:65:VAL:HG12	2:B:164:GLU:HG2	1.75	0.69
3:C:103:GLN:HE21	3:C:104:GLU:N	1.89	0.69
1:A:56:U:H2'	1:A:57:G:C8	2.28	0.68
1:A:254:G:O2'	1:A:255:G:H5'	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:138:ARG:HA	2:B:141:LYS:HG2	1.74	0.68
5:E:106:LEU:HD13	5:E:114:ILE:HG21	1.75	0.68
1:A:172:A:O2'	1:A:173:U:H5'	1.93	0.68
13:M:3:ILE:HG23	13:M:56:ARG:HA	1.76	0.68
13:M:16:VAL:O	13:M:19:THR:HB	1.93	0.68
1:A:1048:G:H5'	1:A:1048:G:C8	2.26	0.68
3:C:122:GLN:O	3:C:127:PHE:HB2	1.93	0.68
2:B:207:LEU:HD22	2:B:208:ILE:HD13	1.75	0.68
11:K:44:ARG:HB3	11:K:44:ARG:HH11	1.54	0.68
1:A:1152:A:OP1	10:J:66:HIS:ND1	2.26	0.68
6:F:80:ARG:NH1	6:F:88:VAL:HB	2.09	0.68
16:P:26:ARG:HD2	16:P:31:LYS:O	1.94	0.68
1:A:1231:G:H4'	9:I:125:SER:CB	2.24	0.68
2:B:1:VAL:HG21	2:B:215:LEU:CD2	2.23	0.68
9:I:26:THR:HG23	9:I:29:GLY:O	1.94	0.68
10:J:11:HIS:O	10:J:15:ASP:HB2	1.94	0.68
2:B:172:ARG:HH22	8:H:68:ARG:HH22	1.40	0.67
10:J:47:VAL:O	10:J:58:ARG:HA	1.94	0.67
14:N:22:ARG:NH1	14:N:29:ALA:HB2	2.09	0.67
16:P:42:ARG:HG2	16:P:42:ARG:NH1	2.08	0.67
17:Q:52:LEU:H	17:Q:52:LEU:HD12	1.59	0.67
1:A:1352:C:H2'	1:A:1353:G:C8	2.30	0.67
5:E:76:ILE:HD12	5:E:87:LEU:HB2	1.77	0.67
13:M:10:ARG:CG	13:M:11:ASN:N	2.57	0.67
1:A:1353:G:H2'	1:A:1354:C:H6	1.58	0.67
2:B:17:ARG:HH12	2:B:185:ASP:HA	1.58	0.67
3:C:129:VAL:O	3:C:133:ILE:HG12	1.94	0.67
4:D:7:VAL:C	4:D:9:ARG:H	2.03	0.67
4:D:88:THR:HG22	4:D:88:THR:O	1.94	0.67
14:N:43:LEU:HD12	14:N:43:LEU:O	1.93	0.67
1:A:1075:C:H5'	2:B:97:THR:HG21	1.77	0.67
13:M:34:GLU:C	13:M:36:THR:H	2.02	0.67
17:Q:67:ARG:HG3	17:Q:67:ARG:O	1.93	0.67
1:A:1054:C:O2	1:A:1054:C:H3'	1.94	0.67
13:M:83:ILE:C	13:M:85:CYS:H	1.99	0.67
16:P:81:ARG:HH11	16:P:81:ARG:HB2	1.60	0.67
19:S:15:LEU:O	19:S:19:LEU:HG	1.95	0.67
3:C:84:ARG:HH11	3:C:88:GLU:HB2	1.59	0.67
4:D:2:ARG:NH1	4:D:69:ILE:HA	2.09	0.67
7:G:113:ARG:HG2	7:G:113:ARG:HH11	1.58	0.67
19:S:17:LYS:O	19:S:21:LEU:HG	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:66:HIS:O	20:T:67:LYS:HG3	1.95	0.67
4:D:29:LYS:C	4:D:31:ALA:H	2.00	0.67
3:C:18:GLU:O	3:C:39:ARG:NH2	2.28	0.66
3:C:173:PRO:O	3:C:176:THR:HG22	1.95	0.66
7:G:14:ASP:HB3	7:G:19:ASP:H	1.60	0.66
3:C:57:GLU:OE2	10:J:90:THR:HG21	1.94	0.66
11:K:38:ILE:HD13	11:K:53:LEU:HB3	1.77	0.66
14:N:8:LYS:HD3	14:N:8:LYS:C	2.21	0.66
1:A:1132:C:H2'	1:A:1133:G:H8	1.60	0.66
10:J:21:ILE:HA	10:J:83:LEU:HD21	1.77	0.66
19:S:19:LEU:HA	19:S:22:ASN:HD22	1.59	0.66
2:B:134:HIS:HA	2:B:137:GLU:CG	2.26	0.66
4:D:141:PRO:HG2	4:D:186:ARG:HH21	1.61	0.66
10:J:19:GLN:HG2	10:J:22:VAL:HG11	1.76	0.66
15:O:15:ALA:HB1	15:O:20:ASP:HB3	1.78	0.66
19:S:19:LEU:HD12	19:S:20:GLU:N	2.11	0.66
2:B:9:VAL:HG13	2:B:203:ARG:HG2	1.78	0.66
6:F:99:ALA:C	6:F:101:ALA:H	2.03	0.66
10:J:14:LEU:CD2	10:J:92:VAL:HG13	2.26	0.66
1:A:975:A:H5''	1:A:976:G:C5'	2.18	0.66
1:A:1292:U:P	7:G:40:ARG:HH22	2.19	0.66
2:B:157:PHE:HD1	2:B:179:ILE:HB	1.61	0.66
7:G:71:ARG:O	7:G:72:MET:HG2	1.96	0.66
8:H:82:HIS:HD2	8:H:83:ILE:N	1.94	0.66
2:B:209:LEU:O	2:B:213:VAL:HG23	1.96	0.66
13:M:10:ARG:HG3	13:M:11:ASN:H	1.59	0.66
1:A:224:C:H6	1:A:224:C:C5'	2.10	0.65
1:A:1054:C:N3	23:Z:34:G:O4'	2.29	0.65
7:G:47:LYS:O	7:G:50:GLN:HB3	1.95	0.65
7:G:58:LEU:O	7:G:62:LYS:HG2	1.95	0.65
10:J:78:LYS:HA	10:J:81:GLU:OE2	1.96	0.65
1:A:262:A:H5'	20:T:67:LYS:HD3	1.78	0.65
1:A:750:G:N3	15:O:22:GLY:HA3	2.11	0.65
2:B:160:ASP:OD2	2:B:163:LYS:HB2	1.96	0.65
4:D:161:LEU:HD13	4:D:180:MET:HG2	1.77	0.65
9:I:24:LYS:NZ	9:I:24:LYS:HB3	2.12	0.65
13:M:101:ARG:HB2	13:M:101:ARG:HH11	1.61	0.65
19:S:41:PRO:HG2	19:S:42:GLU:OE2	1.96	0.65
1:A:271:C:O2'	1:A:272:C:H5''	1.97	0.65
1:A:1307:U:H5'	13:M:108:THR:HG21	1.78	0.65
1:A:271:C:H2'	1:A:272:C:H5'	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1038:C:H2'	1:A:1039:C:H6	1.62	0.65
8:H:63:LEU:HD22	8:H:63:LEU:H	1.60	0.65
10:J:3:ARG:HA	10:J:71:ASP:OD1	1.96	0.65
1:A:1342:C:O2'	1:A:1343:G:H5'	1.96	0.65
26:A:2733:3TS:H1	26:A:2733:3TS:O1'	1.97	0.65
11:K:38:ILE:HD13	11:K:53:LEU:CB	2.26	0.65
13:M:53:VAL:O	13:M:57:GLU:HG2	1.96	0.65
1:A:195:A:H4'	20:T:61:LYS:HE2	1.79	0.65
1:A:1381:U:O2	1:A:1381:U:H2'	1.97	0.65
4:D:77:LEU:HD22	4:D:95:LEU:HB3	1.79	0.65
9:I:7:GLY:HA2	9:I:78:LEU:HD13	1.79	0.65
3:C:171:ARG:HB3	3:C:171:ARG:HH11	1.62	0.65
3:C:189:ARG:HH11	3:C:189:ARG:CB	2.09	0.65
13:M:83:ILE:HG22	19:S:73:PHE:HE2	1.61	0.65
19:S:12:ASP:O	19:S:16:GLU:HG2	1.97	0.65
20:T:22:LYS:O	20:T:26:ILE:HG13	1.97	0.65
1:A:486:U:H2'	1:A:487:A:C5'	2.27	0.65
1:A:975:A:H4'	1:A:976:G:O5'	1.97	0.65
1:A:1286:A:C8	1:A:1287:A:H4'	2.31	0.65
2:B:172:ARG:HH11	2:B:172:ARG:HG3	1.61	0.65
2:B:53:GLU:HB2	2:B:215:LEU:HD11	1.78	0.64
2:B:67:THR:HG21	2:B:90:ARG:NH1	2.11	0.64
6:F:47:ARG:H	6:F:47:ARG:HD2	1.61	0.64
7:G:17:TYR:CE2	7:G:58:LEU:HB2	2.32	0.64
1:A:630:G:H2'	1:A:631:G:C8	2.33	0.64
3:C:109:ASN:HD21	3:C:139:ARG:HB3	1.62	0.64
7:G:71:ARG:HG2	7:G:141:GLU:OE2	1.96	0.64
9:I:110:ARG:HG2	9:I:111:LYS:N	2.11	0.64
1:A:1129:C:H1'	1:A:1132:C:H5	1.62	0.64
4:D:178:GLU:HG3	4:D:179:GLY:N	2.11	0.64
6:F:22:GLU:O	6:F:26:ILE:HG12	1.97	0.64
7:G:41:ILE:HD12	7:G:115:ALA:HB3	1.80	0.64
1:A:369:C:O2	1:A:369:C:H2'	1.98	0.64
1:A:620:C:N1	4:D:134:LEU:HD13	2.13	0.64
1:A:1106:G:H5'	1:A:1107:C:OP2	1.97	0.64
2:B:225:GLU:H	2:B:225:GLU:CD	2.05	0.64
4:D:31:ALA:C	4:D:33:GLU:H	2.04	0.64
10:J:19:GLN:O	10:J:22:VAL:HG12	1.97	0.64
11:K:66:GLY:O	11:K:68:GLN:HG3	1.97	0.64
4:D:104:VAL:HG21	4:D:125:ILE:HD13	1.80	0.64
1:A:203:U:H4'	1:A:204:U:OP1	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1301:U:H3'	1:A:1302:U:H5'	1.79	0.64
1:A:1425:U:H2'	1:A:1426:C:H6	1.62	0.64
6:F:94:GLN:HE21	18:R:17:ARG:HH11	1.45	0.64
15:O:38:LEU:CD1	15:O:55:LEU:HB2	2.28	0.64
17:Q:43:ALA:HB2	17:Q:58:ILE:HD11	1.78	0.64
1:A:1125:U:H5''	1:A:1126:U:C4	2.33	0.64
5:E:70:GLY:HA3	5:E:112:THR:HG22	1.80	0.64
9:I:125:SER:O	9:I:127:ARG:N	2.31	0.64
11:K:105:PRO:C	11:K:107:ASN:H	2.05	0.64
6:F:94:GLN:NE2	18:R:17:ARG:HD3	2.12	0.64
7:G:74:VAL:HG13	7:G:144:ALA:HA	1.78	0.64
1:A:1256:A:O3'	1:A:1257:U:H4'	1.98	0.64
6:F:30:LEU:HB3	6:F:35:ALA:HB3	1.78	0.64
1:A:1135:U:H3	1:A:1138:G:H1	1.46	0.63
1:A:1216:G:H5''	14:N:4:ALA:HB2	1.80	0.63
3:C:100:LEU:O	3:C:100:LEU:HD13	1.95	0.63
4:D:145:ILE:HD12	4:D:145:ILE:N	2.12	0.63
10:J:44:ARG:HG2	10:J:44:ARG:NH1	2.13	0.63
1:A:722:A:H4'	1:A:723:U:C4	2.34	0.63
15:O:2:ILE:N	15:O:2:ILE:HD12	2.13	0.63
18:R:7:VAL:O	18:R:11:LEU:HD23	1.97	0.63
1:A:1026:G:H2'	1:A:1026:G:N3	2.13	0.63
1:A:1301:U:H3'	1:A:1302:U:C5'	2.28	0.63
20:T:58:LYS:O	20:T:61:LYS:HB2	1.98	0.63
1:A:590:C:C2'	1:A:591:U:H5''	2.27	0.63
1:A:1152:A:H4'	10:J:11:HIS:HD2	1.64	0.63
1:A:1442(A):G:C4'	1:A:1442(B):A:H5'	2.28	0.63
4:D:34:ARG:HD2	4:D:34:ARG:N	2.13	0.63
19:S:41:PRO:O	19:S:44:VAL:HG23	1.97	0.63
1:A:157:G:H5'	1:A:157:G:H8	1.63	0.63
1:A:1022:G:H2'	1:A:1023:G:H8	1.64	0.63
6:F:15:ASP:H	6:F:18:GLN:HE21	1.47	0.63
16:P:34:GLU:OE2	16:P:55:ARG:HD3	1.98	0.63
1:A:957:U:H3	1:A:960:U:H5''	1.62	0.63
1:A:1330:U:C2'	1:A:1331:G:H5'	2.27	0.63
1:A:1353:G:H2'	1:A:1354:C:C6	2.33	0.63
1:A:1356:G:H2'	1:A:1357:A:C8	2.34	0.63
4:D:176:ASP:OD1	4:D:178:GLU:HG3	1.98	0.63
6:F:67:MET:HB2	6:F:68:PRO:CD	2.29	0.63
10:J:88:LEU:N	10:J:89:PRO:HD2	2.02	0.63
1:A:243:A:H4'	1:A:244:U:C5'	2.12	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1271:G:H2'	1:A:1272:G:C5'	2.17	0.63
3:C:103:GLN:NE2	3:C:104:GLU:H	1.97	0.63
11:K:1:LYS:N	11:K:1:LYS:HD2	2.14	0.63
19:S:22:ASN:C	19:S:24:LYS:H	2.05	0.63
2:B:183:ASP:CG	2:B:184:THR:H	2.06	0.63
3:C:153:SER:OG	3:C:154:GLY:N	2.32	0.63
4:D:161:LEU:HD13	4:D:180:MET:HE2	1.79	0.63
5:E:97:ILE:HD12	5:E:97:ILE:N	2.14	0.63
9:I:64:VAL:HG21	9:I:72:GLN:HB3	1.81	0.63
1:A:271:C:C2'	1:A:272:C:H5''	2.29	0.62
6:F:10:LEU:HD12	6:F:59:TYR:HB3	1.81	0.62
1:A:765:G:H1	1:A:812:C:H2'	1.64	0.62
1:A:1047:G:H2'	1:A:1048:G:C5'	2.23	0.62
2:B:155:ALA:HB1	2:B:179:ILE:HD11	1.81	0.62
11:K:100:ASP:OD2	18:R:73:LYS:HD2	1.99	0.62
12:L:2:THR:OG1	12:L:5:GLN:HG3	1.99	0.62
13:M:96:PRO:HB2	13:M:100:GLN:OE1	1.99	0.62
19:S:15:LEU:O	19:S:18:VAL:HG12	1.99	0.62
20:T:82:ARG:HG3	20:T:97:LEU:HD13	1.81	0.62
1:A:1198:G:H2'	1:A:1199:U:C6	2.35	0.62
19:S:15:LEU:C	19:S:17:LYS:H	2.08	0.62
1:A:996:A:H5'	1:A:996:A:H8	1.64	0.62
1:A:1144:G:H21	1:A:1146:A:H62	1.45	0.62
2:B:12:GLY:HA2	2:B:35:ILE:HA	1.80	0.62
3:C:194:VAL:O	3:C:195:LEU:HD22	1.99	0.62
20:T:50:ARG:NE	20:T:95:GLY:HA3	2.13	0.62
4:D:82:SER:HA	4:D:88:THR:CG2	2.30	0.62
9:I:9:ARG:HD3	9:I:104:ASP:HB3	1.81	0.62
14:N:13:PRO:O	14:N:14:LYS:HB3	1.99	0.62
1:A:539:A:H2'	1:A:540:G:C8	2.35	0.62
1:A:1014:A:C2	1:A:1219:U:H1'	2.34	0.62
8:H:60:ARG:HH11	8:H:60:ARG:HG3	1.65	0.62
1:A:64:G:C4'	1:A:65:U:H5'	2.28	0.62
1:A:1301:U:O2'	1:A:1302:U:H5''	2.00	0.62
1:A:1314:C:C5	19:S:5:LYS:HD3	2.34	0.62
2:B:91:TRP:CZ2	2:B:96:LEU:HD13	2.35	0.62
4:D:2:ARG:NH2	4:D:73:GLN:NE2	2.48	0.62
4:D:35:ARG:H	4:D:36:PRO:HD3	1.63	0.62
10:J:4:ILE:HG22	10:J:96:ILE:HG23	1.80	0.62
10:J:80:ILE:O	10:J:84:MET:HB2	1.99	0.62
19:S:32:THR:HG22	19:S:34:SER:N	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1229:A:H2'	1:A:1230:C:H6	1.64	0.62
2:B:126:LYS:O	2:B:130:VAL:HG23	2.00	0.62
2:B:133:LYS:O	2:B:133:LYS:HD3	2.00	0.62
12:L:122:LYS:HD2	12:L:122:LYS:C	2.24	0.62
14:N:43:LEU:HD12	14:N:43:LEU:C	2.25	0.62
1:A:451:A:H61	1:A:481:G:H5'	1.65	0.62
4:D:2:ARG:HH21	4:D:73:GLN:HE21	1.48	0.62
4:D:82:SER:HA	4:D:88:THR:HG21	1.80	0.62
4:D:149:GLU:CD	4:D:149:GLU:H	2.08	0.62
6:F:74:ASP:CG	6:F:77:ARG:HH21	2.08	0.62
1:A:370:C:O2'	1:A:371:G:H5'	2.00	0.61
1:A:1189:C:OP1	10:J:49:ARG:NH2	2.20	0.61
4:D:150:LYS:HD2	4:D:150:LYS:N	2.14	0.61
7:G:74:VAL:HG21	7:G:143:MET:HE3	1.81	0.61
12:L:107:LYS:O	12:L:108:ASP:HB2	2.00	0.61
2:B:71:ALA:HB2	2:B:205:ILE:CD1	2.29	0.61
5:E:48:PRO:O	5:E:52:GLN:HG2	2.00	0.61
10:J:30:ALA:C	10:J:32:VAL:H	2.08	0.61
20:T:29:LEU:HD12	20:T:55:LEU:HD12	1.80	0.61
20:T:60:ALA:HA	20:T:66:HIS:H	1.65	0.61
1:A:335:C:O2'	1:A:336:C:H5'	2.00	0.61
12:L:83:GLY:HA2	12:L:94:TYR:HA	1.81	0.61
1:A:156:G:H2'	1:A:157:G:H5''	1.81	0.61
3:C:138:GLN:HA	3:C:138:GLN:HE21	1.65	0.61
17:Q:44:HIS:CD2	17:Q:46:PRO:HG3	2.34	0.61
20:T:43:GLU:H	20:T:92:LEU:HD12	1.65	0.61
1:A:953:G:H1'	13:M:124:ARG:HA	1.82	0.61
1:A:999:C:OP1	1:A:999:C:H4'	2.00	0.61
2:B:120:GLU:HA	2:B:123:GLU:CG	2.31	0.61
1:A:487:A:H5'	1:A:487:A:C8	2.31	0.61
1:A:1060:C:C4	3:C:1:GLY:HA3	2.35	0.61
1:A:1163:C:H2'	1:A:1164:G:C8	2.36	0.61
1:A:1178:G:N2	1:A:1180:A:H3'	2.15	0.61
1:A:1510:U:H2'	1:A:1511:G:C8	2.36	0.61
3:C:98:VAL:HG22	3:C:99:ALA:O	2.00	0.61
4:D:2:ARG:HH21	4:D:73:GLN:HG3	1.65	0.61
10:J:46:THR:OG1	10:J:60:HIS:CD2	2.53	0.61
1:A:271:C:H2'	1:A:272:C:C5'	2.30	0.61
1:A:1140:C:O2	1:A:1140:C:H2'	1.99	0.61
1:A:1306:A:O2'	13:M:108:THR:HG21	2.01	0.61
3:C:63:VAL:HG12	3:C:65:VAL:HG23	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:82:ARG:HG3	12:L:82:ARG:HH11	1.66	0.61
14:N:11:ARG:C	14:N:13:PRO:HD3	2.26	0.61
1:A:499:A:H61	1:A:547:A:C5'	2.13	0.61
1:A:1425:U:H2'	1:A:1426:C:C6	2.35	0.61
1:A:1427:U:H2'	1:A:1428:A:C8	2.36	0.61
12:L:20:VAL:HG23	12:L:20:VAL:O	2.00	0.61
16:P:81:ARG:HG3	16:P:83:GLU:OE1	2.00	0.61
1:A:709:G:O2'	1:A:710:G:H5'	2.01	0.61
1:A:948:C:O2'	1:A:949:A:H5'	2.01	0.61
1:A:1420:C:H2'	1:A:1421:G:H8	1.66	0.61
2:B:77:MET:HG3	2:B:229:SER:HB3	1.82	0.61
3:C:124:GLU:HG2	3:C:189:ARG:O	2.00	0.61
10:J:13:THR:C	10:J:15:ASP:H	2.08	0.61
10:J:37:PRO:HA	10:J:68:ARG:NH1	2.16	0.61
10:J:37:PRO:O	10:J:38:LEU:HB2	2.00	0.61
14:N:8:LYS:HE2	14:N:21:THR:O	2.01	0.61
1:A:1420:C:H2'	1:A:1421:G:C8	2.36	0.60
4:D:186:ARG:HH22	4:D:187:LEU:CD1	2.14	0.60
6:F:7:ASN:HD21	18:R:19:TYR:HE1	1.49	0.60
13:M:39:ASN:HD22	13:M:40:PRO:CD	2.13	0.60
15:O:69:LEU:HD13	15:O:77:TYR:HA	1.82	0.60
15:O:87:ARG:N	15:O:87:ARG:HE	1.99	0.60
4:D:198:ASN:HD22	4:D:198:ASN:C	2.08	0.60
16:P:28:ARG:HG2	16:P:29:ASP:OD1	2.01	0.60
21:V:6:ARG:HG2	21:V:15:ARG:HH12	1.66	0.60
1:A:693:G:C6	1:A:1539:C:H1'	2.35	0.60
1:A:1405:G:O2'	1:A:1406:U:H5'	2.01	0.60
3:C:13:ILE:O	3:C:15:ARG:N	2.34	0.60
3:C:171:ARG:HH12	3:C:173:PRO:HG3	1.66	0.60
6:F:2:ARG:CD	6:F:69:GLU:HG2	2.31	0.60
13:M:95:LEU:HB3	13:M:96:PRO:HD2	1.83	0.60
1:A:165:C:H2'	1:A:166:G:H8	1.64	0.60
1:A:591:U:H6	1:A:591:U:C5'	2.12	0.60
14:N:30:ARG:HH11	14:N:30:ARG:HG3	1.66	0.60
10:J:6:LEU:CD2	10:J:94:ILE:HG12	2.31	0.60
12:L:24:LYS:C	12:L:26:ALA:N	2.51	0.60
16:P:26:ARG:CD	16:P:31:LYS:O	2.50	0.60
1:A:439:A:H2'	1:A:441:A:H5'	1.83	0.60
1:A:620:C:H2'	1:A:621:A:O4'	2.02	0.60
17:Q:3:LYS:HE3	17:Q:5:LEU:HD21	1.84	0.60
17:Q:77:GLU:OE1	17:Q:80:ARG:HD2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:62:THR:HG23	19:S:65:MET:HE3	1.84	0.60
1:A:689:C:P	11:K:36:GLY:HA3	2.41	0.60
1:A:1222:G:P	19:S:76:THR:HG21	2.41	0.60
2:B:230:TYR:CD1	2:B:233:VAL:HG21	2.36	0.60
5:E:117:LYS:HD3	5:E:118:GLU:N	2.16	0.60
7:G:119:ILE:HD12	7:G:119:ILE:N	2.17	0.60
13:M:83:ILE:HD12	19:S:64:ASN:HD22	1.65	0.60
13:M:121:LYS:HG3	13:M:122:ALA:N	2.16	0.60
1:A:591:U:H5'	1:A:591:U:C6	2.24	0.60
1:A:677:U:H3	1:A:713:G:H22	1.48	0.60
1:A:968:A:H8	1:A:968:A:O5'	1.85	0.60
1:A:998:G:H2'	1:A:999:C:C4'	2.32	0.60
2:B:81:ARG:HB3	2:B:81:ARG:NH1	2.16	0.60
3:C:113:PRO:O	3:C:117:GLN:HG3	2.01	0.60
12:L:23:LEU:C	12:L:25:GLY:H	2.10	0.60
1:A:1392:G:N2	1:A:1502:A:H8	1.99	0.60
2:B:21:LYS:HD2	2:B:187:ASP:OD2	2.02	0.60
1:A:969:A:H61	13:M:125:LYS:HB2	1.66	0.60
1:A:1300:G:O2'	1:A:1301:U:H5''	2.00	0.60
1:A:1474:G:H2'	1:A:1475:G:C5'	2.32	0.60
2:B:72:GLN:HE21	2:B:89:GLN:HA	1.67	0.60
2:B:108:ARG:NH2	2:B:112:LEU:HD21	2.16	0.60
4:D:7:VAL:HG13	4:D:20:LEU:HD12	1.84	0.60
1:A:8:A:H5'	5:E:97:ILE:HG22	1.84	0.59
1:A:590:C:H2'	1:A:591:U:H5''	1.83	0.59
1:A:998:G:C3'	1:A:999:C:H5''	2.32	0.59
1:A:1213:A:C2'	1:A:1214:C:H5''	2.32	0.59
2:B:11:PHE:HB3	2:B:38:LEU:HD21	1.83	0.59
7:G:53:THR:HG22	7:G:55:GLN:N	2.17	0.59
1:A:820:U:H4'	1:A:821:G:OP2	2.00	0.59
2:B:21:LYS:HD3	2:B:189:ASP:OD2	2.02	0.59
2:B:216:ILE:O	2:B:220:ARG:HG3	2.02	0.59
12:L:23:LEU:O	12:L:25:GLY:N	2.35	0.59
12:L:66:ILE:HD13	12:L:73:LEU:HD12	1.82	0.59
16:P:36:ILE:O	16:P:51:VAL:O	2.20	0.59
18:R:18:ASP:OD2	18:R:21:ASN:HB2	2.02	0.59
2:B:63:LEU:HD23	2:B:64:PHE:N	2.17	0.59
13:M:4:ALA:O	13:M:5:GLY:C	2.45	0.59
1:A:477:A:O2'	1:A:479:C:H5'	2.03	0.59
1:A:953:G:H5'	1:A:965:A:H61	1.68	0.59
11:K:57:ASP:OD1	11:K:61:LYS:HE3	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:3:THR:OG1	15:O:6:GLU:HB2	2.02	0.59
2:B:70:GLN:HG3	2:B:200:ASP:OD1	2.02	0.59
3:C:25:LYS:HZ2	3:C:25:LYS:CB	2.15	0.59
5:E:114:ILE:HD13	5:E:115:LEU:N	2.17	0.59
1:A:35:G:H2'	1:A:36:C:C6	2.37	0.59
1:A:51:A:H4'	1:A:52:G:O5'	2.03	0.59
1:A:1132:C:H2'	1:A:1133:G:C8	2.37	0.59
2:B:6:GLU:C	2:B:8:GLY:H	2.08	0.59
2:B:12:GLY:CA	2:B:35:ILE:HA	2.33	0.59
9:I:7:GLY:HA2	9:I:78:LEU:HB3	1.84	0.59
13:M:72:GLU:O	13:M:75:ALA:HB3	2.03	0.59
1:A:179:A:H2'	1:A:180:U:C6	2.37	0.59
3:C:49:ALA:HB1	3:C:69:VAL:CG1	2.30	0.59
16:P:9:PHE:CD2	16:P:18:ARG:HG3	2.38	0.59
4:D:21:LYS:HB2	4:D:25:CYS:SG	2.42	0.59
9:I:68:GLY:O	9:I:72:GLN:HG3	2.02	0.59
1:A:1326:C:C5'	21:V:12:LYS:HZ2	2.11	0.59
3:C:99:ALA:O	3:C:100:LEU:HB2	2.01	0.59
10:J:23:GLU:C	10:J:25:ALA:H	2.11	0.59
19:S:40:VAL:HB	19:S:41:PRO:HD2	1.85	0.59
20:T:89:GLY:O	20:T:90:ALA:HB3	2.02	0.59
1:A:1117:G:H5''	9:I:103:ARG:NH2	2.18	0.59
3:C:138:GLN:HA	3:C:138:GLN:NE2	2.18	0.59
10:J:46:THR:HG1	10:J:60:HIS:CD2	2.20	0.59
19:S:61:ILE:HD13	19:S:61:ILE:C	2.27	0.59
20:T:84:LEU:C	20:T:86:GLU:H	2.11	0.59
22:W:2:U:H2'	22:W:3:C:H6	1.68	0.59
1:A:896:C:H5'	1:A:897:C:OP2	2.02	0.58
1:A:967:C:H4'	9:I:127:ARG:HG3	1.84	0.58
1:A:1135:U:O2	1:A:1135:U:H2'	2.02	0.58
2:B:212:ALA:O	2:B:216:ILE:HG12	2.03	0.58
3:C:76:ILE:HA	3:C:83:ILE:HB	1.84	0.58
3:C:180:ASN:C	3:C:181:ILE:HD12	2.27	0.58
3:C:190:THR:HG21	3:C:192:TYR:CZ	2.38	0.58
7:G:145:GLU:C	7:G:147:ASN:H	2.09	0.58
3:C:5:HIS:HD2	3:C:7:ILE:H	1.51	0.58
18:R:40:ARG:NH1	18:R:40:ARG:HB3	2.18	0.58
18:R:59:ARG:HB3	18:R:66:PHE:CE1	2.39	0.58
19:S:13:HIS:O	19:S:17:LYS:HE3	2.03	0.58
1:A:67:C:O2'	1:A:171:A:H1'	2.03	0.58
1:A:881:G:OP2	12:L:8:ARG:NH2	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:149:GLU:HG3	4:D:152:ARG:NH1	2.17	0.58
23:Z:41:C:H2'	23:Z:42:C:C6	2.38	0.58
1:A:824:C:H2'	1:A:825:G:H8	1.68	0.58
1:A:1022:G:H2'	1:A:1023:G:C8	2.39	0.58
11:K:99:VAL:HG22	18:R:71:VAL:HA	1.86	0.58
19:S:41:PRO:C	19:S:43:MET:H	2.11	0.58
1:A:452:A:H4'	16:P:72:ARG:NE	2.19	0.58
2:B:157:PHE:CD1	2:B:179:ILE:HB	2.39	0.58
12:L:71:HIS:HD2	12:L:73:LEU:N	2.00	0.58
5:E:8:LEU:CD1	5:E:27:LEU:HB2	2.33	0.58
6:F:60:PHE:C	6:F:61:LEU:HD12	2.29	0.58
7:G:71:ARG:HH12	7:G:137:LYS:NZ	2.01	0.58
12:L:64:ALA:HB1	12:L:96:ILE:HG13	1.85	0.58
20:T:46:LEU:O	20:T:50:ARG:HD2	2.03	0.58
1:A:403:C:O2'	1:A:404:U:H5'	2.04	0.58
1:A:794:A:H2'	1:A:795:C:C6	2.39	0.58
1:A:1277:C:H6	1:A:1277:C:H5'	1.67	0.58
10:J:4:ILE:CG2	10:J:96:ILE:HG23	2.32	0.58
18:R:21:ASN:O	18:R:25:LEU:HG	2.03	0.58
18:R:38:ARG:HH11	18:R:44:SER:HA	1.68	0.58
1:A:662:G:H2'	1:A:663:A:C8	2.39	0.58
1:A:1005:A:H5''	1:A:1006:C:C5	2.39	0.58
1:A:1487:G:O2'	1:A:1488:G:H5'	2.04	0.58
3:C:81:GLU:O	3:C:85:VAL:HG23	2.04	0.58
10:J:22:VAL:O	10:J:26:ARG:HG3	2.03	0.58
1:A:384:G:H2'	1:A:385:C:C6	2.39	0.58
1:A:1001:A:N3	1:A:1001(A):G:H5'	2.19	0.58
2:B:24:ARG:HG3	2:B:25:TYR:CD1	2.39	0.58
2:B:31:ASN:O	2:B:33:ILE:HG12	2.03	0.58
3:C:54:VAL:O	3:C:54:VAL:HG12	2.03	0.58
11:K:17:ASN:ND2	11:K:45:LYS:HD2	2.18	0.58
1:A:1391:U:H2'	1:A:1392:G:H8	1.64	0.58
10:J:19:GLN:HG2	10:J:22:VAL:CG1	2.33	0.58
12:L:13:LYS:HA	12:L:13:LYS:HE2	1.86	0.58
20:T:50:ARG:NH1	20:T:50:ARG:HG2	2.19	0.58
1:A:353:A:H5'	1:A:353:A:H8	1.69	0.57
1:A:743:U:H2'	1:A:744:C:C6	2.39	0.57
3:C:176:THR:HG23	3:C:179:ALA:HB2	1.86	0.57
9:I:92:ARG:HB3	9:I:92:ARG:HH11	1.68	0.57
14:N:32:VAL:HA	14:N:39:CYS:HA	1.85	0.57
1:A:920:U:H2'	1:A:921:U:C6	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1314:C:H5	19:S:5:LYS:HD3	1.69	0.57
9:I:8:ARG:HG3	9:I:13:VAL:HG13	1.86	0.57
13:M:123:PRO:C	13:M:125:LYS:H	2.12	0.57
1:A:26:A:H2'	1:A:27:G:H5'	1.86	0.57
1:A:946:A:H2'	1:A:947:G:H8	1.70	0.57
1:A:1245:A:O2'	1:A:1246:C:H5'	2.03	0.57
1:A:1263:C:H2'	1:A:1264:C:C6	2.39	0.57
2:B:13:HIS:HB2	2:B:198:ASN:OD1	2.05	0.57
6:F:2:ARG:NE	6:F:69:GLU:HG2	2.19	0.57
7:G:144:ALA:C	7:G:146:ALA:H	2.12	0.57
1:A:486:U:H2'	1:A:487:A:H5''	1.85	0.57
2:B:63:LEU:HD12	2:B:149:LEU:HD11	1.87	0.57
10:J:19:GLN:C	10:J:22:VAL:HG12	2.29	0.57
15:O:25:GLU:HG3	15:O:80:LEU:HG	1.86	0.57
1:A:147:G:H5'	1:A:147:G:C8	2.38	0.57
1:A:837:G:H1	1:A:849:C:N4	2.02	0.57
1:A:1001(A):G:C2'	1:A:1002:G:H5'	2.34	0.57
1:A:1299:A:C8	1:A:1301:U:H1'	2.39	0.57
1:A:1346:A:C6	7:G:9:ARG:NH1	2.72	0.57
1:A:1364:U:O2'	1:A:1365:G:H5''	2.04	0.57
2:B:120:GLU:HA	2:B:123:GLU:HG2	1.86	0.57
3:C:57:GLU:H	3:C:64:ALA:HB3	1.69	0.57
3:C:154:GLY:O	3:C:155:ARG:HB2	2.03	0.57
7:G:119:ILE:HD12	7:G:119:ILE:H	1.69	0.57
8:H:29:SER:OG	8:H:32:LYS:HG3	2.03	0.57
8:H:84:ARG:HG3	8:H:84:ARG:NH1	2.20	0.57
10:J:2:ILE:N	10:J:2:ILE:HD12	2.19	0.57
10:J:82:GLN:O	10:J:86:LEU:HD22	2.04	0.57
12:L:79:VAL:HG21	12:L:96:ILE:HG23	1.85	0.57
21:V:6:ARG:HE	21:V:15:ARG:NH1	2.01	0.57
1:A:1296:C:H4'	1:A:1302:U:C4	2.40	0.57
1:A:1330:U:H6	1:A:1330:U:C5'	2.08	0.57
6:F:99:ALA:C	6:F:101:ALA:N	2.60	0.57
9:I:9:ARG:CD	9:I:104:ASP:HB3	2.35	0.57
13:M:22:TYR:HB3	13:M:66:GLU:HA	1.87	0.57
13:M:119:LYS:HG2	13:M:120:LYS:N	2.20	0.57
1:A:44:G:C2	1:A:45:U:H1'	2.40	0.57
1:A:314:C:O2'	1:A:315:A:H5'	2.05	0.57
1:A:649:G:H5'	1:A:649:G:H8	1.68	0.57
1:A:1480:G:O2'	1:A:1481:U:H6	1.87	0.57
2:B:135:GLU:O	2:B:139:LEU:HG	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:C:H2'	1:A:270:A:C8	2.40	0.57
2:B:134:HIS:CA	2:B:137:GLU:HG2	2.32	0.57
5:E:47:VAL:HB	5:E:48:PRO:CD	2.30	0.57
7:G:144:ALA:O	7:G:146:ALA:N	2.35	0.57
11:K:63:MET:C	11:K:65:TYR:H	2.13	0.57
12:L:37:ARG:NH1	12:L:53:LYS:HE2	2.18	0.57
15:O:16:ARG:HD3	15:O:25:GLU:OE1	2.04	0.57
1:A:797:C:O2'	1:A:798:G:H5'	2.04	0.57
5:E:72:ILE:HG22	5:E:74:HIS:H	1.70	0.57
5:E:140:THR:HG22	5:E:142:ALA:N	2.20	0.57
1:A:1259:C:H5'	1:A:1260:C:OP2	2.05	0.57
2:B:172:ARG:HH22	8:H:68:ARG:NH2	2.03	0.57
13:M:39:ASN:HD22	13:M:40:PRO:HD2	1.70	0.57
13:M:121:LYS:CG	13:M:122:ALA:N	2.68	0.57
1:A:57:G:H2'	1:A:58:C:C6	2.39	0.56
1:A:721:G:H8	1:A:721:G:OP1	1.88	0.56
1:A:1012:U:H3'	1:A:1013:G:C5'	2.20	0.56
1:A:1151:A:HO2'	1:A:1152:A:H8	1.51	0.56
5:E:15:MET:SD	5:E:20:ARG:HB3	2.44	0.56
13:M:8:ILE:O	13:M:8:ILE:HG22	2.04	0.56
19:S:16:GLU:HA	19:S:19:LEU:HD11	1.86	0.56
1:A:1349:A:P	9:I:117:LYS:HE2	2.45	0.56
1:A:1394:A:C5	1:A:1501:C:H4'	2.40	0.56
1:A:1442(A):G:H5''	1:A:1442(B):A:C5'	2.33	0.56
3:C:57:GLU:HB2	3:C:64:ALA:HB2	1.86	0.56
3:C:194:VAL:HG12	3:C:195:LEU:N	2.20	0.56
13:M:48:THR:HB	13:M:51:GLU:HG3	1.87	0.56
13:M:95:LEU:O	13:M:109:ARG:NH1	2.38	0.56
17:Q:2:LYS:HD3	17:Q:60:GLU:O	2.05	0.56
1:A:411:A:H2'	1:A:412:A:H5''	1.87	0.56
1:A:1216:G:O2'	1:A:1217:C:H5'	2.04	0.56
1:A:1249:C:H2'	1:A:1250:A:H5''	1.86	0.56
2:B:6:GLU:CB	2:B:10:HIS:HE1	2.18	0.56
7:G:84:TYR:HD2	7:G:153:TYR:HE2	1.53	0.56
10:J:48:ILE:HD12	10:J:48:ILE:H	1.70	0.56
11:K:81:ARG:NE	18:R:73:LYS:HE2	2.21	0.56
17:Q:39:LYS:HG2	17:Q:41:TYR:CE1	2.41	0.56
1:A:1276:G:C3'	1:A:1277:C:H5''	2.35	0.56
3:C:57:GLU:CD	10:J:90:THR:HG21	2.30	0.56
9:I:111:LYS:HG3	9:I:117:LYS:HA	1.87	0.56
10:J:79:THR:HG22	10:J:83:LEU:HD12	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:486:U:O2'	1:A:487:A:H5''	2.05	0.56
1:A:812:C:O2'	1:A:813:U:P	2.63	0.56
1:A:1245:A:H5'	1:A:1245:A:C8	2.34	0.56
1:A:1442(A):G:H4'	1:A:1442(B):A:H5'	1.87	0.56
2:B:172:ARG:HG3	2:B:172:ARG:NH1	2.21	0.56
3:C:30:HIS:C	3:C:32:LEU:H	2.13	0.56
9:I:42:ALA:N	9:I:73:ILE:HD13	2.20	0.56
11:K:38:ILE:CG2	11:K:39:GLY:H	2.18	0.56
11:K:67:MET:HE1	11:K:70:VAL:HG22	1.87	0.56
13:M:12:LYS:O	13:M:44:VAL:HG23	2.06	0.56
1:A:812:C:O2'	1:A:813:U:OP2	2.24	0.56
1:A:872:A:C3'	1:A:873:A:H5'	2.36	0.56
1:A:1232:U:OP1	9:I:123:GLN:HG2	2.05	0.56
2:B:22:PHE:CD2	2:B:184:THR:HA	2.40	0.56
2:B:175:PHE:HD2	8:H:70:GLN:HB3	1.71	0.56
6:F:10:LEU:HD12	6:F:10:LEU:H	1.70	0.56
6:F:94:GLN:HE21	18:R:17:ARG:HD3	1.70	0.56
15:O:86:ILE:CG2	15:O:87:ARG:H	1.94	0.56
16:P:81:ARG:HB2	16:P:81:ARG:NH1	2.21	0.56
1:A:156:G:C2'	1:A:157:G:H5''	2.35	0.56
1:A:245:C:O2'	1:A:246:A:H5'	2.05	0.56
1:A:501:C:H2'	1:A:502:G:H8	1.71	0.56
1:A:1244:C:O2'	1:A:1245:A:H5''	2.05	0.56
13:M:33:LEU:HD13	13:M:40:PRO:HA	1.88	0.56
1:A:1366:C:H2'	1:A:1367:C:C6	2.41	0.56
12:L:23:LEU:C	12:L:25:GLY:N	2.59	0.56
2:B:215:LEU:O	2:B:215:LEU:HD13	2.06	0.56
4:D:30:CYS:SG	4:D:30:CYS:O	2.64	0.56
4:D:195:LEU:H	4:D:195:LEU:CD2	2.16	0.56
6:F:40:VAL:HG22	6:F:41:GLU:N	2.20	0.56
13:M:13:ARG:HB2	13:M:16:VAL:HG12	1.88	0.56
16:P:28:ARG:HG2	16:P:28:ARG:HH11	1.71	0.56
1:A:243:A:C4'	1:A:244:U:H5'	2.12	0.56
1:A:1540:U:H3'	1:A:1540:U:OP2	2.06	0.56
2:B:81:ARG:O	2:B:82:ALA:HB2	2.04	0.56
3:C:18:GLU:CG	3:C:53:ARG:HE	2.18	0.56
10:J:4:ILE:HA	10:J:95:GLU:O	2.06	0.56
13:M:10:ARG:CG	13:M:11:ASN:H	2.16	0.56
16:P:20:VAL:CG1	16:P:32:TYR:HB2	2.36	0.56
1:A:409:G:OP1	4:D:23:GLU:HB3	2.06	0.55
1:A:1095:U:H2'	1:A:1096:C:C6	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1164:G:H1	1:A:1172:C:N4	1.99	0.55
1:A:1229:A:H2'	1:A:1230:C:C6	2.41	0.55
6:F:91:VAL:HG11	18:R:57:ARG:NH1	2.22	0.55
6:F:101:ALA:HB1	18:R:13:GLU:HG3	1.87	0.55
7:G:15:LEU:HD22	7:G:15:LEU:N	2.22	0.55
9:I:117:LYS:O	9:I:118:ALA:CB	2.54	0.55
17:Q:39:LYS:HE3	17:Q:41:TYR:CZ	2.40	0.55
1:A:1007:C:H2'	1:A:1008:C:H6	1.65	0.55
1:A:1053:G:C4'	1:A:1054:C:H5'	2.37	0.55
1:A:1228:C:OP1	13:M:114:LYS:HE3	2.07	0.55
9:I:92:ARG:HH11	9:I:92:ARG:CB	2.20	0.55
11:K:44:ARG:HH11	11:K:44:ARG:CB	2.19	0.55
11:K:78:GLY:O	11:K:80:GLY:N	2.38	0.55
21:V:6:ARG:CG	21:V:15:ARG:HH12	2.19	0.55
1:A:146:G:C3'	1:A:147:G:H5''	2.36	0.55
11:K:12:HIS:HB3	11:K:19:ILE:HD11	1.86	0.55
11:K:67:MET:CE	11:K:70:VAL:HG22	2.36	0.55
12:L:56:LEU:CD2	12:L:62:VAL:HG22	2.33	0.55
18:R:38:ARG:NH1	18:R:44:SER:HA	2.20	0.55
3:C:130:ARG:O	3:C:134:LYS:HG3	2.06	0.55
4:D:30:CYS:C	4:D:32:MET:H	2.14	0.55
8:H:8:ASP:O	8:H:12:ARG:HG3	2.06	0.55
8:H:63:LEU:HD22	8:H:63:LEU:N	2.20	0.55
1:A:413:G:O2'	1:A:428:G:N2	2.40	0.55
1:A:860:A:H2'	1:A:861:G:O4'	2.07	0.55
1:A:977:A:O2'	1:A:978:A:C5'	2.54	0.55
1:A:1330:U:OP1	13:M:22:TYR:O	2.23	0.55
26:A:2733:3TS:OAI	26:A:2733:3TS:H1'	2.06	0.55
2:B:11:PHE:HD1	2:B:12:GLY:N	2.04	0.55
2:B:48:THR:O	2:B:52:ILE:HG12	2.07	0.55
5:E:114:ILE:HD13	5:E:115:LEU:H	1.72	0.55
8:H:68:ARG:HG2	8:H:68:ARG:HH11	1.72	0.55
12:L:75:GLU:O	12:L:77:SER:N	2.40	0.55
17:Q:77:GLU:CD	17:Q:80:ARG:HD2	2.31	0.55
1:A:131:C:H2'	1:A:132:C:C6	2.42	0.55
1:A:421:U:H4'	1:A:422:C:OP2	2.06	0.55
1:A:553:A:H5''	12:L:20:VAL:HG21	1.88	0.55
1:A:1392:G:H21	1:A:1502:A:H8	1.54	0.55
2:B:207:LEU:HD23	2:B:207:LEU:C	2.30	0.55
4:D:195:LEU:HD23	4:D:195:LEU:N	2.13	0.55
10:J:25:ALA:C	10:J:27:ARG:H	2.14	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:U:H2'	1:A:197:A:C5	2.42	0.55
1:A:224:C:H6	1:A:224:C:H5'	1.72	0.55
1:A:591:U:O2'	1:A:592:G:H5'	2.07	0.55
1:A:1062:U:H2'	1:A:1063:C:C6	2.42	0.55
1:A:1136:U:H5''	1:A:1137:C:OP2	2.07	0.55
2:B:91:TRP:HZ2	2:B:96:LEU:HD13	1.70	0.55
3:C:69:VAL:HG12	3:C:70:ALA:N	2.22	0.55
9:I:24:LYS:HB3	9:I:24:LYS:HZ3	1.72	0.55
15:O:26:VAL:O	15:O:30:LEU:HD13	2.07	0.55
1:A:100:C:H2'	1:A:101:A:C8	2.42	0.55
1:A:271:C:C2'	1:A:272:C:C5'	2.84	0.55
1:A:272:C:H5'	1:A:272:C:C6	2.30	0.55
1:A:1141:C:O2'	1:A:1142:G:H5'	2.07	0.55
1:A:1168:A:O2'	1:A:1169:A:C8	2.58	0.55
2:B:76:ARG:NH2	2:B:86:TYR:OH	2.38	0.55
3:C:84:ARG:NH1	3:C:88:GLU:HB2	2.22	0.55
4:D:99:ARG:HH12	4:D:136:SER:HB3	1.72	0.55
15:O:16:ARG:HH11	15:O:16:ARG:HG3	1.72	0.55
15:O:55:LEU:HA	15:O:58:MET:HE2	1.88	0.55
1:A:1004:A:H8	1:A:1036:G:N1	2.02	0.55
1:A:1074:G:O3'	2:B:97:THR:CG2	2.55	0.55
1:A:1125:U:H3	10:J:3:ARG:NH2	2.03	0.55
1:A:1392:G:O2'	1:A:1502:A:H5''	2.06	0.55
1:A:1491:G:H2'	26:A:2733:3TS:HAUA	1.88	0.55
5:E:117:LYS:HD3	5:E:118:GLU:H	1.72	0.55
7:G:44:ASP:O	7:G:48:ILE:HG13	2.07	0.55
10:J:13:THR:C	10:J:15:ASP:N	2.65	0.55
17:Q:69:ARG:HD2	17:Q:69:ARG:N	2.22	0.55
20:T:60:ALA:O	20:T:66:HIS:ND1	2.40	0.55
1:A:818:G:H3'	1:A:819:A:C5'	2.37	0.55
1:A:967:C:C4'	9:I:127:ARG:HG3	2.37	0.55
1:A:972:C:H4'	10:J:55:LYS:CG	2.23	0.55
1:A:972:C:OP1	10:J:55:LYS:HE2	2.07	0.55
2:B:65:VAL:CG1	2:B:164:GLU:HG2	2.36	0.55
2:B:106:VAL:O	2:B:110:GLU:HG3	2.07	0.55
3:C:138:GLN:HE21	3:C:138:GLN:CA	2.19	0.55
5:E:9:ILE:O	5:E:9:ILE:HG13	2.06	0.55
6:F:33:TYR:HA	6:F:71:ARG:NH2	2.22	0.55
6:F:38:GLU:O	6:F:39:LYS:HB3	2.05	0.55
6:F:45:LEU:HD22	6:F:45:LEU:N	2.22	0.55
7:G:67:ASN:ND2	7:G:127:ALA:HA	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:67:ASN:O	10:J:68:ARG:HD3	2.06	0.55
1:A:448:A:C4	1:A:487:A:C2	2.95	0.54
1:A:530:G:O6	22:W:3:C:H1'	2.07	0.54
1:A:1038:C:H2'	1:A:1039:C:C6	2.42	0.54
1:A:1053:G:C3'	1:A:1054:C:H5'	2.36	0.54
2:B:10:HIS:HB3	2:B:204:SER:OG	2.07	0.54
2:B:200:ASP:O	2:B:201:ALA:HB3	2.07	0.54
6:F:22:GLU:OE1	6:F:22:GLU:HA	2.06	0.54
21:V:2:GLY:C	21:V:4:GLY:H	2.14	0.54
1:A:255:G:H1'	17:Q:15:GLN:NE2	2.22	0.54
6:F:94:GLN:HB3	18:R:17:ARG:HH11	1.71	0.54
10:J:37:PRO:O	10:J:67:ASN:O	2.25	0.54
10:J:58:ARG:HG2	10:J:58:ARG:HH11	1.73	0.54
13:M:64:LYS:CE	13:M:68:GLU:HG2	2.37	0.54
1:A:446:G:H1	1:A:488:C:H42	1.56	0.54
1:A:1252:A:H61	1:A:1285:A:H61	1.55	0.54
1:A:1475:G:H2'	1:A:1476:G:O4'	2.06	0.54
7:G:27:ASN:O	7:G:30:MET:HB3	2.08	0.54
15:O:53:ARG:O	15:O:57:MET:HG3	2.06	0.54
1:A:1251:A:H4'	9:I:11:GLU:OE2	2.08	0.54
3:C:65:VAL:O	3:C:65:VAL:HG12	2.07	0.54
4:D:3:TYR:O	4:D:4:ILE:HB	2.07	0.54
5:E:1:ASP:CG	5:E:2:PHE:H	2.15	0.54
5:E:75:GLU:HG3	5:E:89:PRO:HD3	1.89	0.54
7:G:31:ARG:O	7:G:33:GLY:N	2.41	0.54
8:H:20:TYR:CE1	8:H:76:PRO:HG2	2.42	0.54
9:I:9:ARG:O	9:I:10:LYS:C	2.50	0.54
1:A:426:G:H5'	1:A:426:G:H8	1.73	0.54
1:A:1188:A:C3'	1:A:1189:C:C5'	2.84	0.54
2:B:126:LYS:HE3	2:B:129:GLN:HE22	1.72	0.54
20:T:49:MET:HE3	20:T:81:VAL:HG11	1.88	0.54
1:A:268:C:O2'	1:A:269:C:H5'	2.08	0.54
1:A:403:C:O3'	4:D:121:ARG:HD2	2.07	0.54
1:A:954:G:H2'	1:A:955:U:C6	2.43	0.54
4:D:31:ALA:C	4:D:33:GLU:N	2.65	0.54
4:D:150:LYS:H	4:D:150:LYS:CD	2.17	0.54
15:O:87:ARG:NE	15:O:87:ARG:HA	2.22	0.54
1:A:612:C:O2'	1:A:613:C:H5'	2.08	0.54
1:A:1301:U:C3'	1:A:1302:U:C5'	2.85	0.54
2:B:231:ALA:C	2:B:233:VAL:H	2.15	0.54
6:F:47:ARG:HD2	6:F:47:ARG:N	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:8:LYS:HD3	14:N:9:ALA:N	2.22	0.54
18:R:4:LYS:O	18:R:5:ALA:HB3	2.06	0.54
20:T:50:ARG:HG2	20:T:50:ARG:HH11	1.72	0.54
4:D:56:ARG:HH11	4:D:56:ARG:HG3	1.73	0.54
8:H:82:HIS:CD2	8:H:83:ILE:N	2.75	0.54
13:M:119:LYS:C	13:M:120:LYS:HD2	2.33	0.54
20:T:87:ALA:O	20:T:88:ALA:HB3	2.08	0.54
1:A:682:G:O2'	1:A:683:G:H5'	2.08	0.54
1:A:1077:G:H5'	1:A:1078:U:OP2	2.07	0.54
1:A:1251:A:O2'	1:A:1370:G:H5'	2.07	0.54
4:D:157:ILE:O	4:D:161:LEU:HB2	2.08	0.54
5:E:8:LEU:HD13	5:E:27:LEU:HB2	1.89	0.54
5:E:76:ILE:HD12	5:E:76:ILE:N	2.23	0.54
13:M:13:ARG:NH1	13:M:15:ASP:OD2	2.41	0.54
16:P:20:VAL:HG13	16:P:32:TYR:HB2	1.90	0.54
1:A:129(A):G:N1	1:A:189(E):U:O2'	2.40	0.54
1:A:439:A:C2'	1:A:441:A:H5'	2.37	0.54
1:A:1286:A:H8	1:A:1287:A:H4'	1.72	0.54
2:B:15:ARG:HH11	2:B:17:ARG:HG2	1.73	0.54
5:E:33:ARG:HG2	5:E:33:ARG:HH11	1.72	0.54
12:L:37:ARG:HH22	12:L:53:LYS:CE	2.20	0.54
1:A:262:A:C5'	20:T:67:LYS:HD3	2.37	0.53
1:A:486:U:H2'	1:A:487:A:H5'	1.89	0.53
2:B:163:LYS:HD3	2:B:163:LYS:C	2.33	0.53
4:D:149:GLU:HG3	4:D:152:ARG:CZ	2.38	0.53
13:M:101:ARG:HB2	13:M:101:ARG:NH1	2.23	0.53
18:R:58:ALA:HB3	18:R:64:LEU:HD12	1.89	0.53
1:A:353:A:H5'	1:A:353:A:C8	2.43	0.53
1:A:1030:C:H6	1:A:1030:C:H5'	1.73	0.53
1:A:1315:U:H2'	1:A:1316:G:O4'	2.08	0.53
5:E:94:THR:HG22	5:E:97:ILE:CD1	2.38	0.53
10:J:29:GLY:HA2	10:J:76:ASN:ND2	2.22	0.53
23:Z:31:A:H2'	23:Z:32:U:O4'	2.08	0.53
1:A:1047:G:H5''	14:N:3:LYS:HD2	1.89	0.53
2:B:16:LYS:HD2	2:B:29:GLU:OE2	2.09	0.53
2:B:47:ARG:NH1	2:B:193:TYR:CD1	2.75	0.53
3:C:106:GLN:NE2	3:C:106:GLN:H	2.07	0.53
3:C:109:ASN:C	3:C:110:LEU:HD23	2.34	0.53
3:C:109:ASN:HD22	3:C:139:ARG:HB3	1.72	0.53
6:F:15:ASP:N	6:F:18:GLN:HE21	2.05	0.53
6:F:25:ILE:H	6:F:25:ILE:CD1	2.02	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:45:ALA:HB1	9:I:76:ILE:CG2	2.38	0.53
11:K:17:ASN:HD22	11:K:45:LYS:CE	2.21	0.53
13:M:14:VAL:HG21	13:M:47:LEU:HD21	1.89	0.53
13:M:36:THR:HG22	13:M:36:THR:O	2.08	0.53
13:M:83:ILE:C	13:M:85:CYS:N	2.66	0.53
18:R:32:THR:C	18:R:34:LYS:H	2.16	0.53
1:A:1001:A:N3	1:A:1001:A:H2'	2.24	0.53
1:A:1218:C:H2'	1:A:1219:U:C6	2.43	0.53
1:A:1447:A:O2'	1:A:1452:C:OP1	2.26	0.53
11:K:17:ASN:ND2	11:K:45:LYS:HB3	2.23	0.53
19:S:29:LEU:HD23	19:S:47:THR:HG22	1.89	0.53
1:A:254:G:OP1	17:Q:66:LYS:O	2.26	0.53
1:A:1014:A:H2	1:A:1219:U:O2	1.90	0.53
1:A:1112:C:H5'	1:A:1113:C:OP2	2.08	0.53
4:D:208:ARG:HG2	4:D:208:ARG:HH11	1.74	0.53
11:K:100:ASP:CB	18:R:73:LYS:HD2	2.38	0.53
14:N:10:LYS:C	14:N:12:THR:H	2.15	0.53
1:A:460:G:O6	1:A:470:C:H5''	2.09	0.53
1:A:523:A:C2	12:L:87:LYS:HB3	2.44	0.53
2:B:191:VAL:HB	2:B:194:ILE:HG13	1.89	0.53
4:D:29:LYS:C	4:D:31:ALA:N	2.67	0.53
5:E:139:ARG:NH1	8:H:77:GLU:OE2	2.39	0.53
10:J:30:ALA:C	10:J:32:VAL:N	2.67	0.53
19:S:4:LEU:O	19:S:4:LEU:HD23	2.08	0.53
1:A:166:G:O2'	1:A:167:G:H5'	2.08	0.53
1:A:189(J):G:O2'	1:A:189(K):U:H5'	2.09	0.53
1:A:390:C:H2'	1:A:391:G:C8	2.43	0.53
1:A:1118:C:H1'	1:A:1179:A:C4	2.44	0.53
5:E:7:ILE:HB	5:E:27:LEU:HB3	1.91	0.53
5:E:29:VAL:HG11	5:E:105:ILE:HA	1.91	0.53
7:G:71:ARG:HH12	7:G:137:LYS:HZ3	1.56	0.53
10:J:36:ILE:HB	10:J:69:LEU:CB	2.22	0.53
1:A:526:C:OP1	1:A:913:A:H4'	2.09	0.53
1:A:542:G:OP1	4:D:9:ARG:NH2	2.42	0.53
1:A:1245:A:H2'	1:A:1246:C:O4'	2.09	0.53
2:B:175:PHE:CD2	8:H:70:GLN:HB3	2.44	0.53
7:G:14:ASP:OD1	7:G:43:TYR:OH	2.25	0.53
7:G:64:ALA:CB	7:G:123:LEU:HD23	2.38	0.53
10:J:7:ARG:HB3	10:J:7:ARG:NH1	2.23	0.53
19:S:32:THR:HG22	19:S:33:TRP:N	2.23	0.53
1:A:460:G:C6	1:A:470:C:H5''	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:818:G:C2'	1:A:819:A:H5''	2.38	0.53
1:A:1129:C:H1'	1:A:1132:C:C5	2.42	0.53
1:A:1263:C:H2'	1:A:1264:C:H6	1.74	0.53
1:A:1296:C:H4'	1:A:1302:U:C5	2.44	0.53
6:F:21:LEU:O	6:F:24:GLU:HB3	2.08	0.53
10:J:29:GLY:HA2	10:J:76:ASN:CG	2.34	0.53
11:K:3:GLN:HA	11:K:65:TYR:O	2.08	0.53
13:M:83:ILE:HG21	19:S:65:MET:HB3	1.90	0.53
17:Q:10:VAL:O	17:Q:11:SER:HB2	2.09	0.53
1:A:1014:A:H2'	1:A:1015:A:C8	2.44	0.53
1:A:1149:C:H2'	1:A:1150:U:C6	2.44	0.53
1:A:1250:A:H4'	9:I:67:GLY:N	2.24	0.53
1:A:1369:C:H2'	1:A:1370:G:C8	2.44	0.53
1:A:1479:C:H2'	1:A:1480:G:H5'	1.90	0.53
2:B:85:PRO:HB3	2:B:148:LEU:HB2	1.91	0.53
5:E:76:ILE:HD12	5:E:76:ILE:H	1.74	0.53
9:I:62:ILE:HG21	9:I:76:ILE:HG13	1.91	0.53
10:J:43:ARG:O	10:J:62:GLU:HA	2.09	0.53
14:N:2:ARG:NH1	14:N:5:LEU:HD11	2.24	0.53
18:R:28:PHE:O	18:R:36:LEU:HG	2.09	0.53
1:A:17:U:H2'	1:A:18:C:C6	2.44	0.52
1:A:818:G:C3'	1:A:819:A:C5'	2.86	0.52
1:A:1278:U:H5''	1:A:1279:A:O4'	2.09	0.52
1:A:1481:U:H2'	1:A:1482:G:O4'	2.09	0.52
5:E:77:GLU:OE1	5:E:84:LYS:HE2	2.10	0.52
9:I:117:LYS:CG	9:I:120:ARG:HB3	2.39	0.52
14:N:10:LYS:C	14:N:12:THR:N	2.67	0.52
16:P:72:ARG:HG3	16:P:73:LEU:N	2.22	0.52
1:A:706:A:H4'	11:K:19:ILE:HD11	1.90	0.52
1:A:1371:G:OP1	9:I:10:LYS:O	2.27	0.52
2:B:96:LEU:N	2:B:96:LEU:HD12	2.24	0.52
15:O:87:ARG:NE	15:O:87:ARG:CA	2.72	0.52
16:P:74:LEU:HD22	16:P:79:VAL:HG21	1.91	0.52
17:Q:39:LYS:HE3	17:Q:41:TYR:OH	2.08	0.52
1:A:486:U:C2'	1:A:487:A:C5'	2.86	0.52
1:A:1230:C:H1'	13:M:125:LYS:HA	1.90	0.52
1:A:1468:A:H2'	1:A:1469:G:O4'	2.09	0.52
2:B:17:ARG:O	2:B:18:TRP:O	2.27	0.52
3:C:179:ALA:O	3:C:180:ASN:CB	2.57	0.52
3:C:187:LEU:HG	3:C:188:ALA:H	1.73	0.52
4:D:63:LEU:HD12	4:D:74:PHE:CZ	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:88:LYS:HB3	5:E:115:LEU:HB2	1.91	0.52
7:G:74:VAL:CG1	7:G:144:ALA:HA	2.40	0.52
10:J:46:THR:HG23	10:J:60:HIS:CD2	2.44	0.52
12:L:37:ARG:HH22	12:L:53:LYS:HE2	1.74	0.52
23:Z:34:G:H2'	23:Z:35:A:C8	2.43	0.52
1:A:818:G:H3'	1:A:819:A:H5'	1.91	0.52
1:A:1256:A:O3'	1:A:1257:U:C4'	2.57	0.52
4:D:104:VAL:CG2	4:D:125:ILE:HD13	2.39	0.52
12:L:109:ARG:HG2	12:L:109:ARG:HH11	1.73	0.52
20:T:38:GLN:HG2	20:T:84:LEU:HD13	1.91	0.52
20:T:41:LYS:O	20:T:45:ALA:HB2	2.10	0.52
1:A:737:A:H1'	6:F:73:ASN:OD1	2.08	0.52
1:A:818:G:C3'	1:A:819:A:H5''	2.39	0.52
7:G:68:VAL:HG12	7:G:68:VAL:O	2.09	0.52
10:J:73:ILE:O	10:J:74:ASN:HB3	2.09	0.52
10:J:74:ASN:O	10:J:76:ASN:N	2.40	0.52
18:R:72:ARG:HG2	18:R:72:ARG:HH11	1.75	0.52
3:C:25:LYS:NZ	3:C:25:LYS:N	2.52	0.52
7:G:14:ASP:OD1	7:G:15:LEU:N	2.42	0.52
9:I:78:LEU:HD22	9:I:82:ARG:HD2	1.91	0.52
11:K:17:ASN:OD1	11:K:18:THR:N	2.42	0.52
1:A:757:U:H2'	1:A:758:G:O4'	2.09	0.52
1:A:1064:G:H21	1:A:1190:G:H2'	1.75	0.52
2:B:194:ILE:H	2:B:194:ILE:CD1	2.20	0.52
4:D:161:LEU:HD13	4:D:180:MET:CG	2.40	0.52
9:I:7:GLY:HA2	9:I:78:LEU:CD1	2.39	0.52
12:L:113:ARG:NH2	12:L:120:LYS:HB2	2.24	0.52
18:R:22:VAL:CG1	18:R:63:LEU:HB3	2.39	0.52
19:S:79:TYR:O	19:S:80:ARG:C	2.52	0.52
1:A:1256:A:N1	1:A:1278:U:O2	2.43	0.52
2:B:45:LEU:HD22	2:B:49:PHE:CE1	2.45	0.52
2:B:191:VAL:CG1	2:B:194:ILE:HG13	2.39	0.52
3:C:26:LYS:HB2	3:C:27:GLN:NE2	2.22	0.52
6:F:19:LEU:HD11	6:F:23:LYS:HE3	1.92	0.52
7:G:25:PHE:CE2	7:G:29:ILE:HD11	2.45	0.52
10:J:85:THR:C	10:J:86:LEU:HD12	2.35	0.52
1:A:101:A:O2'	1:A:102:G:H5'	2.10	0.51
1:A:632:A:C2'	1:A:633:G:H5'	2.40	0.51
1:A:1189:C:P	10:J:49:ARG:NH2	2.83	0.51
1:A:1508:G:O2'	1:A:1509:C:H5'	2.10	0.51
2:B:2:LYS:HD2	2:B:2:LYS:C	2.35	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:61:THR:HA	2:B:84:MET:HE1	1.91	0.51
9:I:126:LYS:HB2	13:M:125:LYS:NZ	2.26	0.51
11:K:17:ASN:HD21	11:K:45:LYS:HD2	1.74	0.51
17:Q:75:LEU:HD23	17:Q:76:VAL:N	2.25	0.51
19:S:42:GLU:H	19:S:42:GLU:CD	2.18	0.51
1:A:723:U:O2	1:A:723:U:H2'	2.10	0.51
2:B:172:ARG:HH21	2:B:190:LEU:HA	1.75	0.51
3:C:33:LEU:CG	14:N:24:VAL:HG21	2.36	0.51
8:H:80:ILE:O	8:H:80:ILE:HG22	2.09	0.51
9:I:9:ARG:O	9:I:11:GLU:N	2.43	0.51
20:T:50:ARG:HH11	20:T:50:ARG:CG	2.23	0.51
1:A:248:C:O2'	1:A:249:U:H5'	2.10	0.51
1:A:269:C:H2'	1:A:270:A:H8	1.76	0.51
1:A:514:C:O2'	1:A:515:G:H5'	2.09	0.51
2:B:172:ARG:NH2	8:H:68:ARG:NH2	2.55	0.51
2:B:181:LEU:HD23	2:B:195:ILE:O	2.09	0.51
4:D:11:CYS:SG	4:D:18:LEU:HB2	2.51	0.51
6:F:23:LYS:NZ	6:F:42:GLU:OE2	2.39	0.51
9:I:45:ALA:HB2	9:I:73:ILE:HG23	1.92	0.51
12:L:25:GLY:O	12:L:26:ALA:C	2.52	0.51
17:Q:62:ARG:HG2	17:Q:63:PRO:HD2	1.92	0.51
19:S:50:VAL:O	19:S:56:HIS:HA	2.11	0.51
19:S:76:THR:HG22	19:S:77:ARG:HG3	1.91	0.51
20:T:20:LYS:O	20:T:24:SER:HB2	2.11	0.51
1:A:157:G:H5'	1:A:157:G:C8	2.45	0.51
1:A:344:A:H5''	1:A:345:C:C5	2.41	0.51
1:A:627:G:O2'	1:A:628:G:H5'	2.10	0.51
1:A:629:G:O2'	1:A:630:G:H5'	2.10	0.51
26:A:2733:3TS:CLA	12:L:40:THR:HG21	2.47	0.51
2:B:112:LEU:HD11	2:B:135:GLU:OE1	2.11	0.51
2:B:206:GLN:NE2	2:B:210:SER:HB3	2.25	0.51
6:F:44:GLY:O	6:F:59:TYR:HA	2.10	0.51
8:H:26:VAL:O	8:H:27:PRO:C	2.52	0.51
12:L:109:ARG:HH12	12:L:112:SER:H	1.56	0.51
1:A:174:C:H6	1:A:174:C:H5'	1.75	0.51
1:A:325:A:OP2	20:T:63:SER:HB3	2.10	0.51
1:A:983:A:H5'	1:A:984:C:OP2	2.09	0.51
1:A:1004:A:N3	1:A:1004:A:H5''	2.25	0.51
1:A:1124:G:N7	1:A:1145:C:H2'	2.26	0.51
1:A:1262:C:H2'	1:A:1263:C:C6	2.45	0.51
4:D:35:ARG:HD2	4:D:37:TYR:OH	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:66:HIS:C	20:T:67:LYS:CG	2.83	0.51
1:A:1054:C:O2	1:A:1054:C:C3'	2.59	0.51
2:B:56:ALA:C	2:B:58:ARG:H	2.19	0.51
3:C:173:PRO:HB2	3:C:176:THR:HG22	1.93	0.51
6:F:38:GLU:HB2	6:F:64:GLN:O	2.11	0.51
7:G:22:VAL:HG12	7:G:26:ILE:HD11	1.93	0.51
9:I:7:GLY:CA	9:I:78:LEU:HB3	2.40	0.51
9:I:126:LYS:CD	9:I:126:LYS:H	2.23	0.51
9:I:126:LYS:N	9:I:126:LYS:HD2	2.25	0.51
12:L:79:VAL:CG2	12:L:80:LEU:H	2.24	0.51
1:A:1039:C:H2'	1:A:1040:U:C6	2.46	0.51
1:A:1140:C:H2'	1:A:1141:C:H5''	1.93	0.51
2:B:233:VAL:O	2:B:233:VAL:HG12	2.11	0.51
4:D:130:ARG:HH11	4:D:130:ARG:HG3	1.75	0.51
6:F:37:VAL:HA	6:F:65:VAL:HG12	1.91	0.51
9:I:98:LEU:CB	9:I:100:PHE:CE1	2.94	0.51
10:J:14:LEU:HD23	10:J:92:VAL:HG13	1.93	0.51
12:L:105:GLY:HA3	12:L:117:GLY:O	2.11	0.51
13:M:123:PRO:C	13:M:125:LYS:N	2.69	0.51
1:A:152:A:H2'	1:A:153:C:H5'	1.92	0.51
1:A:418:C:O2'	1:A:419:C:H5'	2.11	0.51
1:A:501:C:H2'	1:A:502:G:C8	2.46	0.51
1:A:1206:G:O2'	1:A:1207:G:H5'	2.11	0.51
5:E:6:MET:SD	5:E:9:ILE:HG23	2.51	0.51
6:F:22:GLU:OE1	6:F:82:ARG:HD3	2.10	0.51
10:J:80:ILE:O	10:J:80:ILE:HG22	2.11	0.51
13:M:77:ILE:O	13:M:80:LEU:HD23	2.11	0.51
1:A:1190:G:OP1	3:C:3:LYS:HA	2.10	0.51
2:B:62:ILE:HG12	2:B:155:ALA:HB3	1.92	0.51
13:M:81:MET:HE2	13:M:91:HIS:CB	2.41	0.51
1:A:976:G:C8	1:A:1358:U:C2	2.99	0.51
1:A:1231:G:H4'	9:I:125:SER:HB3	1.93	0.51
2:B:14:GLU:HG2	2:B:183:ASP:OD2	2.11	0.51
1:A:1001(A):G:H2'	1:A:1002:G:H5'	1.93	0.50
3:C:181:ILE:HD12	3:C:181:ILE:N	2.25	0.50
4:D:161:LEU:CD1	4:D:180:MET:HE2	2.41	0.50
7:G:91:SER:O	7:G:95:GLN:HG3	2.10	0.50
12:L:46:SER:O	12:L:47:ALA:HB2	2.11	0.50
13:M:81:MET:HE2	13:M:91:HIS:HB3	1.92	0.50
1:A:1064:G:H4'	1:A:1065:U:OP1	2.11	0.50
7:G:16:VAL:O	7:G:16:VAL:HG12	2.09	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:49:ILE:HA	7:G:124:MET:CE	2.39	0.50
16:P:20:VAL:HG11	16:P:32:TYR:CB	2.41	0.50
1:A:140:A:O2'	1:A:141:A:H5'	2.10	0.50
1:A:407:G:H2'	1:A:408:A:H8	1.77	0.50
1:A:556:C:O2'	1:A:557:G:H5'	2.11	0.50
1:A:945:G:C2	1:A:946:A:C8	2.98	0.50
1:A:1161:C:H2'	1:A:1162:C:H6	1.76	0.50
1:A:1402:C:O2	1:A:1500:A:N1	2.45	0.50
2:B:17:ARG:HH12	2:B:185:ASP:CA	2.24	0.50
3:C:13:ILE:HG22	3:C:14:THR:N	2.22	0.50
3:C:69:VAL:C	3:C:105:VAL:HG23	2.35	0.50
14:N:7:GLU:C	14:N:7:GLU:OE1	2.55	0.50
17:Q:78:SER:O	17:Q:79:GLY:O	2.29	0.50
1:A:262:A:H5'	20:T:67:LYS:CD	2.40	0.50
1:A:404:U:O2'	1:A:405:U:H5'	2.11	0.50
1:A:1102:A:H2'	1:A:1103:C:C6	2.45	0.50
1:A:1272:G:H5'	1:A:1272:G:H8	1.76	0.50
2:B:11:PHE:CD1	2:B:12:GLY:N	2.79	0.50
2:B:83:GLY:O	2:B:84:MET:HE2	2.11	0.50
2:B:86:TYR:CE1	2:B:145:GLY:HA2	2.46	0.50
6:F:33:TYR:CD2	6:F:75:LEU:HD23	2.46	0.50
12:L:76:HIS:ND1	12:L:76:HIS:N	2.60	0.50
15:O:54:GLY:O	15:O:58:MET:HG3	2.12	0.50
1:A:162:A:H2'	1:A:163:C:O4'	2.11	0.50
1:A:952:U:H2'	1:A:953:G:H8	1.77	0.50
1:A:1254:C:OP1	10:J:43:ARG:HD2	2.11	0.50
1:A:1277:C:H2'	1:A:1278:U:H5'	1.94	0.50
2:B:82:ALA:C	2:B:84:MET:H	2.19	0.50
2:B:126:LYS:HE3	2:B:129:GLN:NE2	2.26	0.50
3:C:83:ILE:O	3:C:83:ILE:HG12	2.11	0.50
11:K:23:THR:HG22	11:K:29:PRO:HA	1.92	0.50
20:T:52:ALA:O	20:T:56:ILE:HG13	2.11	0.50
1:A:58:C:H1'	1:A:388:G:N7	2.26	0.50
1:A:1176:A:H2'	1:A:1177:G:O4'	2.11	0.50
2:B:86:TYR:N	2:B:86:TYR:CD1	2.80	0.50
5:E:73:PRO:O	5:E:74:HIS:HB3	2.11	0.50
7:G:36:ASN:HD21	9:I:40:VAL:H	1.60	0.50
10:J:6:LEU:HD23	10:J:94:ILE:HG12	1.93	0.50
11:K:22:ILE:HD12	11:K:62:ALA:HB2	1.93	0.50
14:N:28:ARG:HB3	14:N:39:CYS:HB3	1.94	0.50
16:P:59:TRP:HB3	16:P:64:ALA:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:V:6:ARG:CD	21:V:15:ARG:HH12	2.24	0.50
1:A:192:U:H1'	20:T:96:GLY:HA2	1.94	0.50
1:A:1098:C:C3'	1:A:1099:G:H5''	2.40	0.50
3:C:82:ARG:C	3:C:84:ARG:H	2.18	0.50
13:M:22:TYR:CB	13:M:66:GLU:HA	2.42	0.50
1:A:393:A:O2'	1:A:394:G:H5'	2.12	0.50
1:A:738:C:H5''	6:F:69:GLU:HB3	1.93	0.50
1:A:983:A:H2	1:A:984:C:C6	2.30	0.50
1:A:1057:G:H5''	3:C:153:SER:CB	2.39	0.50
1:A:1203:C:OP1	14:N:1:ALA:HB3	2.12	0.50
1:A:1314:C:OP2	19:S:5:LYS:HD2	2.12	0.50
7:G:40:ARG:O	7:G:41:ILE:C	2.55	0.50
10:J:86:LEU:HD12	10:J:86:LEU:N	2.26	0.50
13:M:10:ARG:HG2	13:M:11:ASN:N	2.26	0.50
19:S:4:LEU:HD23	19:S:4:LEU:C	2.37	0.50
1:A:961:U:C2'	1:A:962:C:H5'	2.42	0.50
1:A:1334:G:C5'	1:A:1335:C:OP2	2.55	0.50
2:B:73:ASP:O	2:B:76:ARG:HB3	2.12	0.50
2:B:131:ARG:HB3	2:B:131:ARG:HH11	1.76	0.50
5:E:33:ARG:HG2	5:E:33:ARG:NH1	2.27	0.50
5:E:39:LEU:HD11	5:E:128:ALA:HB1	1.93	0.50
5:E:140:THR:HB	5:E:143:ASP:OD2	2.11	0.50
7:G:144:ALA:O	7:G:145:GLU:HB3	2.11	0.50
13:M:3:ILE:CG2	13:M:4:ALA:H	2.16	0.50
15:O:23:SER:HB2	15:O:26:VAL:HG23	1.94	0.50
1:A:460:G:C3'	1:A:461:A:C5'	2.90	0.49
1:A:1144:G:N2	1:A:1146:A:H62	2.09	0.49
1:A:1201:A:H4'	1:A:1202:G:O5'	2.12	0.49
2:B:70:GLN:O	2:B:202:ILE:HD13	2.12	0.49
2:B:112:LEU:O	2:B:136:LEU:HD11	2.12	0.49
4:D:7:VAL:C	4:D:9:ARG:N	2.70	0.49
17:Q:65:SER:OG	17:Q:68:LYS:CB	2.60	0.49
20:T:46:LEU:HD12	20:T:93:ILE:HG22	1.93	0.49
22:W:2:U:H2'	22:W:3:C:C6	2.46	0.49
1:A:165:C:H2'	1:A:166:G:C8	2.45	0.49
1:A:189(B):C:H2'	1:A:189(C):C:C6	2.47	0.49
1:A:431:A:O2'	1:A:432:A:H5'	2.12	0.49
1:A:741:G:O2'	1:A:742:G:H5'	2.11	0.49
1:A:1213:A:C3'	1:A:1214:C:H5''	2.42	0.49
1:A:1400:C:O5'	1:A:1400:C:H6	1.95	0.49
3:C:114:LEU:HD23	3:C:117:GLN:NE2	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:35:ARG:N	4:D:36:PRO:CD	2.69	0.49
12:L:49:ARG:HB3	12:L:89:LEU:HD11	1.94	0.49
18:R:73:LYS:HG2	18:R:73:LYS:OXT	2.12	0.49
1:A:229:U:H5''	16:P:33:ILE:HD13	1.94	0.49
1:A:390:C:H2'	1:A:391:G:H8	1.77	0.49
1:A:632:A:O2'	1:A:633:G:H5'	2.13	0.49
1:A:743:U:H2'	1:A:744:C:H6	1.76	0.49
1:A:1138:G:C8	1:A:1140:C:H1'	2.47	0.49
1:A:1495:U:H2'	1:A:1496:C:H6	1.76	0.49
3:C:118:ARG:HG2	3:C:139:ARG:HH21	1.77	0.49
3:C:166:TRP:O	3:C:167:ALA:HB3	2.12	0.49
9:I:25:VAL:HG13	9:I:60:ALA:HB3	1.95	0.49
12:L:79:VAL:HG21	12:L:96:ILE:CG2	2.41	0.49
13:M:66:GLU:HG3	13:M:67:GLY:N	2.23	0.49
17:Q:65:SER:OG	17:Q:68:LYS:HB3	2.12	0.49
18:R:22:VAL:HG12	18:R:63:LEU:HB3	1.94	0.49
1:A:485:G:C2'	1:A:486:U:OP2	2.60	0.49
1:A:631:G:H2'	1:A:632:A:C8	2.48	0.49
1:A:650:G:O2'	1:A:651:C:H5'	2.12	0.49
1:A:979:C:H2'	1:A:980:C:H5'	1.94	0.49
1:A:1052:U:H2'	1:A:1055:A:OP1	2.12	0.49
1:A:1072:G:H2'	1:A:1073:U:C6	2.46	0.49
1:A:1119:C:O2'	1:A:1120:G:H5'	2.12	0.49
2:B:63:LEU:HB3	2:B:156:ILE:HD13	1.94	0.49
3:C:103:GLN:HE21	3:C:103:GLN:CA	2.24	0.49
4:D:99:ARG:NH1	4:D:136:SER:HA	2.28	0.49
13:M:2:ARG:HE	13:M:6:VAL:HA	1.77	0.49
1:A:720:C:H2'	1:A:721:G:C8	2.48	0.49
7:G:124:MET:O	7:G:128:GLU:HG2	2.12	0.49
9:I:116:HIS:CD2	9:I:122:PRO:HA	2.48	0.49
13:M:119:LYS:HG2	13:M:120:LYS:H	1.78	0.49
14:N:4:ALA:O	14:N:7:GLU:HG2	2.11	0.49
16:P:42:ARG:NH1	16:P:42:ARG:CG	2.75	0.49
19:S:62:THR:OG1	19:S:65:MET:HG2	2.11	0.49
1:A:305:G:H4'	1:A:306:G:OP1	2.12	0.49
1:A:431:A:C2'	1:A:432:A:H5'	2.42	0.49
1:A:600:C:O2'	1:A:601:C:H5'	2.13	0.49
1:A:733:A:H4'	1:A:734:G:OP1	2.12	0.49
3:C:31:LEU:O	3:C:35:ASP:HB2	2.13	0.49
14:N:13:PRO:O	14:N:14:LYS:CB	2.60	0.49
17:Q:17:THR:HG23	17:Q:68:LYS:HE3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:976:G:N7	1:A:1358:U:C2	2.81	0.49
5:E:11:ARG:HD3	5:E:22:PHE:CD1	2.47	0.49
6:F:61:LEU:HD12	6:F:61:LEU:N	2.27	0.49
11:K:66:GLY:O	11:K:67:MET:C	2.56	0.49
19:S:62:THR:CG2	19:S:65:MET:HE3	2.43	0.49
1:A:51:A:H4'	1:A:52:G:C5'	2.43	0.49
1:A:223:U:C3'	1:A:224:C:H5''	2.42	0.49
1:A:397:A:H3'	1:A:397:A:N3	2.27	0.49
1:A:653:A:OP1	8:H:56:LYS:NZ	2.41	0.49
1:A:1029:C:C3'	1:A:1030:C:H5''	2.42	0.49
1:A:1128:C:H2'	1:A:1129:C:H5''	1.93	0.49
1:A:1188:A:H3'	1:A:1189:C:C5'	2.43	0.49
1:A:1286:A:C8	1:A:1286:A:H3'	2.48	0.49
1:A:1309:G:H3'	1:A:1310:G:C5'	2.32	0.49
1:A:1343:G:OP1	9:I:124:TYR:HE1	1.95	0.49
2:B:26:ILE:HD12	2:B:34:HIS:HB3	1.95	0.49
5:E:4:GLU:HG2	5:E:30:VAL:HG13	1.95	0.49
5:E:53:LYS:O	5:E:57:TYR:HD1	1.95	0.49
1:A:189(I):G:O2'	1:A:189(J):G:H5'	2.11	0.49
1:A:332:G:O2'	1:A:333:G:H5'	2.12	0.49
1:A:521:G:OP1	12:L:69:GLU:O	2.30	0.49
1:A:918:A:H2'	1:A:919:A:C8	2.47	0.49
1:A:1125:U:H5''	1:A:1126:U:H3	1.78	0.49
1:A:1225:A:H2'	1:A:1226:C:C5	2.48	0.49
2:B:108:ARG:HH22	2:B:112:LEU:HD21	1.75	0.49
2:B:162:THR:HG22	2:B:186:SER:HB3	1.94	0.49
3:C:178:ARG:CG	3:C:178:ARG:O	2.61	0.49
7:G:145:GLU:C	7:G:145:GLU:CD	2.81	0.49
9:I:4:TYR:O	9:I:83:ALA:HA	2.12	0.49
10:J:17:SER:OG	10:J:89:PRO:HG3	2.13	0.49
12:L:37:ARG:HH12	12:L:53:LYS:CE	2.20	0.49
13:M:34:GLU:C	13:M:36:THR:N	2.70	0.49
17:Q:2:LYS:HB3	17:Q:60:GLU:HB3	1.94	0.49
1:A:913:A:H2'	1:A:914:A:C1'	2.43	0.49
1:A:1061:G:H1'	10:J:54:HIS:CE1	2.48	0.49
1:A:1221:G:H4'	19:S:52:ASN:O	2.13	0.49
1:A:1232:U:H5''	9:I:123:GLN:O	2.13	0.49
1:A:1401:G:OP1	1:A:1544:U:O2'	2.31	0.49
1:A:1479:C:H2'	1:A:1480:G:C5'	2.42	0.49
3:C:34:GLU:O	3:C:37:ARG:N	2.45	0.49
11:K:24:ASP:OD2	11:K:28:ASN:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:34:GLU:O	13:M:36:THR:N	2.46	0.49
15:O:38:LEU:HD12	15:O:55:LEU:HD13	1.95	0.49
17:Q:94:TYR:N	17:Q:94:TYR:CD1	2.80	0.49
1:A:162:A:H2'	1:A:163:C:C4'	2.43	0.48
1:A:472:A:H2'	1:A:473:G:O4'	2.13	0.48
1:A:977:A:N6	1:A:1224:G:O5'	2.46	0.48
1:A:1207:G:H2'	1:A:1208:C:H6	1.77	0.48
7:G:138:GLU:O	7:G:142:ARG:HG3	2.13	0.48
1:A:19:C:H2'	1:A:20:U:H6	1.78	0.48
16:P:20:VAL:CG1	16:P:32:TYR:CB	2.91	0.48
19:S:14:LEU:O	19:S:18:VAL:N	2.46	0.48
1:A:376:G:OP2	16:P:67:THR:HG21	2.13	0.48
1:A:434:U:H2'	1:A:435:C:C6	2.48	0.48
1:A:1040:U:H2'	1:A:1041:A:C8	2.48	0.48
1:A:1256:A:H3'	3:C:26:LYS:HE2	1.94	0.48
1:A:1335:C:H4'	1:A:1336:C:O5'	2.12	0.48
1:A:1540:U:O2'	1:A:1541:U:H5'	2.13	0.48
4:D:190:ARG:O	4:D:190:ARG:HD3	2.13	0.48
7:G:134:VAL:O	7:G:138:GLU:HG3	2.12	0.48
9:I:126:LYS:O	13:M:125:LYS:NZ	2.45	0.48
12:L:51:VAL:CG1	12:L:52:ALA:N	2.76	0.48
13:M:83:ILE:HD13	13:M:83:ILE:N	2.28	0.48
15:O:52:HIS:CE1	15:O:56:LEU:HD13	2.48	0.48
15:O:70:GLN:HG3	15:O:77:TYR:CD2	2.48	0.48
18:R:44:SER:O	18:R:45:GLY:C	2.56	0.48
1:A:131:C:H2'	1:A:132:C:H6	1.77	0.48
1:A:149:A:H2'	1:A:150:C:H6	1.77	0.48
1:A:538:G:O2'	1:A:539:A:H5'	2.13	0.48
1:A:913:A:O5'	1:A:913:A:H1'	2.14	0.48
1:A:1416:G:H1	1:A:1484:C:H42	1.60	0.48
2:B:15:ARG:HH12	2:B:17:ARG:HG2	1.77	0.48
2:B:19:ASN:ND2	2:B:21:LYS:H	2.12	0.48
2:B:131:ARG:C	2:B:133:LYS:H	2.20	0.48
3:C:29:ARG:O	3:C:32:LEU:HB3	2.14	0.48
3:C:46:LEU:N	3:C:46:LEU:HD12	2.27	0.48
4:D:164:MET:HE2	4:D:175:LEU:HD22	1.94	0.48
7:G:84:TYR:HD2	7:G:153:TYR:CE2	2.31	0.48
10:J:4:ILE:N	10:J:4:ILE:CD1	2.73	0.48
12:L:75:GLU:C	12:L:77:SER:H	2.21	0.48
13:M:39:ASN:HB3	13:M:42:THR:CG2	2.43	0.48
1:A:590:C:C3'	1:A:591:U:H5''	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1090:U:H2'	1:A:1091:U:H6	1.76	0.48
1:A:1170:A:H2'	1:A:1171:G:O4'	2.13	0.48
1:A:1368:G:O2'	1:A:1369:C:H5'	2.12	0.48
2:B:55:LEU:O	2:B:55:LEU:HD13	2.13	0.48
3:C:119:VAL:HB	3:C:197:VAL:HG11	1.96	0.48
4:D:198:ASN:C	4:D:198:ASN:ND2	2.71	0.48
7:G:27:ASN:OD1	7:G:35:LYS:NZ	2.47	0.48
9:I:74:ASP:O	9:I:77:LYS:HB3	2.13	0.48
12:L:79:VAL:CG2	12:L:80:LEU:N	2.75	0.48
14:N:11:ARG:C	14:N:13:PRO:CD	2.87	0.48
14:N:35:PHE:O	14:N:35:PHE:CD1	2.67	0.48
16:P:19:ILE:HG22	16:P:36:ILE:CG1	2.44	0.48
17:Q:94:TYR:N	17:Q:94:TYR:HD1	2.11	0.48
1:A:1057:G:H2'	1:A:1058:G:O4'	2.14	0.48
7:G:77:ARG:HD2	7:G:155:TRP:CZ3	2.42	0.48
7:G:110:ARG:HB3	7:G:112:GLU:OE2	2.13	0.48
8:H:91:ARG:O	8:H:91:ARG:HG3	2.14	0.48
9:I:29:GLY:O	9:I:30:GLN:O	2.31	0.48
20:T:3:LEU:N	20:T:3:LEU:HD23	2.29	0.48
1:A:166:G:H2'	1:A:167:G:H8	1.78	0.48
1:A:1320:C:C2	19:S:71:GLY:HA3	2.49	0.48
1:A:1393:U:O4'	1:A:1502:A:H5'	2.14	0.48
1:A:1466:C:H2'	1:A:1467:G:O4'	2.14	0.48
6:F:26:ILE:O	6:F:30:LEU:HG	2.14	0.48
7:G:41:ILE:HD12	7:G:115:ALA:CB	2.43	0.48
7:G:153:TYR:O	7:G:154:ARG:C	2.56	0.48
8:H:114:THR:C	8:H:116:LYS:H	2.21	0.48
10:J:30:ALA:H	10:J:76:ASN:HD21	1.61	0.48
16:P:20:VAL:HG11	16:P:32:TYR:HB3	1.96	0.48
1:A:401:C:H1'	1:A:622:A:H1'	1.95	0.48
2:B:213:VAL:O	2:B:216:ILE:HB	2.13	0.48
2:B:231:ALA:C	2:B:233:VAL:N	2.70	0.48
4:D:64:ARG:O	4:D:64:ARG:HG2	2.14	0.48
4:D:195:LEU:CD2	4:D:195:LEU:N	2.77	0.48
20:T:50:ARG:HE	20:T:95:GLY:HA3	1.77	0.48
1:A:376:G:H5''	16:P:5:ARG:HB2	1.95	0.48
1:A:738:C:OP1	6:F:92:LYS:HE2	2.13	0.48
3:C:156:ILE:HG21	3:C:163:ARG:HH21	1.78	0.48
3:C:179:ALA:HB1	3:C:181:ILE:HD11	1.96	0.48
4:D:56:ARG:HG3	4:D:56:ARG:NH1	2.29	0.48
7:G:17:TYR:HE2	7:G:58:LEU:HB2	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:69:LEU:O	10:J:70:VAL:HB	2.13	0.48
11:K:24:ASP:HB2	11:K:25:PRO:HD2	1.96	0.48
14:N:2:ARG:O	14:N:3:LYS:C	2.57	0.48
19:S:22:ASN:C	19:S:24:LYS:N	2.72	0.48
21:V:2:GLY:C	21:V:4:GLY:N	2.72	0.48
1:A:502:G:P	12:L:114:SER:HG	2.37	0.48
1:A:1365:G:H5'	1:A:1365:G:H8	1.78	0.48
2:B:86:TYR:N	2:B:86:TYR:HD1	2.12	0.48
2:B:108:ARG:NH1	2:B:112:LEU:CG	2.72	0.48
5:E:27:LEU:HD22	5:E:39:LEU:HD22	1.95	0.48
7:G:22:VAL:O	7:G:26:ILE:HG13	2.14	0.48
9:I:41:ARG:O	9:I:43:VAL:N	2.46	0.48
18:R:44:SER:OG	18:R:47:GLU:HG3	2.13	0.48
20:T:16:ARG:NH1	20:T:16:ARG:HG2	2.29	0.48
20:T:49:MET:CE	20:T:81:VAL:HG11	2.42	0.48
1:A:272:C:H6	1:A:272:C:C5'	2.20	0.47
1:A:939:G:H2'	1:A:940:C:C6	2.49	0.47
3:C:149:LYS:HG3	3:C:168:ALA:HB2	1.95	0.47
4:D:176:ASP:OD1	4:D:178:GLU:CG	2.62	0.47
11:K:38:ILE:HD11	11:K:54:ALA:N	2.29	0.47
1:A:38:G:N2	1:A:397:A:H5'	2.17	0.47
1:A:182:U:C4	1:A:183:G:H1'	2.50	0.47
1:A:390:C:O3'	16:P:28:ARG:NH2	2.47	0.47
1:A:460:G:C2'	1:A:461:A:H5''	2.42	0.47
1:A:607:A:O2'	1:A:608:A:H5'	2.13	0.47
1:A:1064:G:H1'	1:A:1190:G:N2	2.29	0.47
1:A:1286:A:H8	1:A:1286:A:H3'	1.79	0.47
1:A:1346:A:N1	1:A:1374:A:H5''	2.29	0.47
2:B:122:GLU:O	2:B:123:GLU:C	2.58	0.47
3:C:190:THR:HG21	3:C:192:TYR:CE1	2.48	0.47
4:D:120:VAL:O	4:D:133:ASP:HA	2.14	0.47
4:D:127:VAL:HG12	4:D:128:ASN:ND2	2.28	0.47
5:E:74:HIS:CE1	5:E:139:ARG:H	2.25	0.47
7:G:36:ASN:HD21	9:I:40:VAL:HG23	1.77	0.47
10:J:2:ILE:O	10:J:71:ASP:HA	2.14	0.47
10:J:30:ALA:HB2	10:J:74:ASN:HB3	1.95	0.47
10:J:59:GLU:OE2	14:N:57:LYS:NZ	2.44	0.47
19:S:41:PRO:O	19:S:43:MET:N	2.47	0.47
1:A:106:C:O2	1:A:379:C:H4'	2.14	0.47
1:A:184:G:H5'	1:A:224:C:O2'	2.14	0.47
1:A:389:A:H2'	1:A:389:A:N3	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:868:C:H2'	1:A:869:G:O4'	2.14	0.47
1:A:1118:C:O4'	1:A:1179:A:H1'	2.14	0.47
3:C:71:LYS:NZ	3:C:71:LYS:HB3	2.29	0.47
3:C:189:ARG:HB3	3:C:189:ARG:NH1	2.21	0.47
6:F:99:ALA:O	6:F:101:ALA:N	2.47	0.47
9:I:98:LEU:HB2	9:I:100:PHE:HE1	1.79	0.47
11:K:38:ILE:HD11	11:K:54:ALA:HA	1.95	0.47
11:K:71:ASP:OD1	11:K:96:LYS:HB2	2.14	0.47
13:M:122:ALA:O	13:M:123:PRO:C	2.57	0.47
14:N:59:SER:O	14:N:60:TRP:HB3	2.14	0.47
17:Q:100:ARG:NE	17:Q:100:ARG:HA	2.29	0.47
19:S:7:GLY:O	19:S:8:VAL:C	2.57	0.47
1:A:5:U:H5''	1:A:5:U:O2	2.15	0.47
1:A:123:C:OP1	1:A:312:C:H5'	2.14	0.47
1:A:299:G:H2'	1:A:300:A:C8	2.49	0.47
1:A:411:A:H2'	1:A:412:A:C5'	2.44	0.47
1:A:721:G:OP2	18:R:38:ARG:HG3	2.15	0.47
1:A:922:G:H2'	1:A:923:A:C8	2.49	0.47
1:A:1366:C:H2'	1:A:1367:C:H6	1.79	0.47
7:G:144:ALA:C	7:G:146:ALA:N	2.73	0.47
13:M:124:ARG:HH11	13:M:124:ARG:HG3	1.79	0.47
1:A:328:C:O2	1:A:328:C:H2'	2.15	0.47
1:A:649:G:H8	1:A:649:G:C5'	2.27	0.47
1:A:959:A:C2	1:A:1222:G:O4'	2.68	0.47
1:A:1013:G:N2	1:A:1016:A:OP2	2.48	0.47
10:J:51:PRO:O	10:J:52:PHE:O	2.33	0.47
11:K:4:VAL:CG2	11:K:67:MET:HG2	2.45	0.47
11:K:48:PRO:O	11:K:51:ALA:HB3	2.14	0.47
14:N:5:LEU:C	14:N:7:GLU:H	2.23	0.47
1:A:109:A:H2'	1:A:326:G:N2	2.29	0.47
1:A:143:A:H5'	1:A:144:G:O5'	2.15	0.47
1:A:643:C:H2'	1:A:644:G:H8	1.78	0.47
1:A:997:U:H2'	1:A:998:G:O4'	2.13	0.47
1:A:1126:U:O2	1:A:1126:U:C2'	2.61	0.47
2:B:63:LEU:HD23	2:B:63:LEU:C	2.39	0.47
7:G:112:GLU:HG3	7:G:117:VAL:HG12	1.97	0.47
9:I:9:ARG:HD2	9:I:10:LYS:H	1.80	0.47
9:I:105:ALA:O	9:I:107:VAL:HG23	2.14	0.47
10:J:25:ALA:HA	10:J:79:THR:HG23	1.97	0.47
14:N:25:ARG:CZ	14:N:46:LEU:HD21	2.44	0.47
19:S:15:LEU:C	19:S:17:LYS:N	2.73	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Z:31:A:O2'	23:Z:32:U:H5'	2.14	0.47
1:A:359:U:O2'	1:A:360:A:H5'	2.14	0.47
1:A:382:A:C2	1:A:383:A:C4	3.02	0.47
1:A:407:G:H2'	1:A:408:A:C8	2.49	0.47
1:A:1054:C:H42	23:Z:34:G:C1'	2.28	0.47
1:A:1111:A:N1	3:C:176:THR:HB	2.29	0.47
1:A:1277:C:H5'	1:A:1277:C:C6	2.47	0.47
1:A:1351:U:O4'	7:G:32:ASP:HB3	2.14	0.47
2:B:2:LYS:O	2:B:3:GLU:HB2	2.13	0.47
2:B:36:ILE:HD12	2:B:197:GLY:HA2	1.97	0.47
2:B:123:GLU:O	2:B:124:ARG:HB2	2.15	0.47
3:C:7:ILE:HG23	3:C:15:ARG:HG2	1.97	0.47
3:C:154:GLY:O	3:C:155:ARG:CB	2.62	0.47
4:D:61:GLN:HA	4:D:61:GLN:NE2	2.30	0.47
5:E:76:ILE:HD13	5:E:87:LEU:HD12	1.96	0.47
8:H:6:ILE:HD11	8:H:31:PHE:CD2	2.50	0.47
8:H:24:THR:HG22	8:H:63:LEU:HD21	1.97	0.47
13:M:51:GLU:HG2	13:M:54:ARG:NH2	2.27	0.47
14:N:13:PRO:C	14:N:15:PHE:H	2.23	0.47
19:S:4:LEU:O	19:S:5:LYS:CB	2.50	0.47
19:S:11:ASP:H	19:S:37:SER:HB3	1.80	0.47
20:T:92:LEU:C	20:T:94:GLY:H	2.23	0.47
1:A:1414:U:H2'	1:A:1415:G:H8	1.80	0.47
1:A:1423:G:O2'	1:A:1424:C:H5'	2.15	0.47
3:C:163:ARG:NH2	3:C:165:GLU:OE1	2.44	0.47
5:E:32:ASP:O	5:E:33:ARG:HB2	2.15	0.47
6:F:9:VAL:HB	6:F:87:ARG:HB2	1.97	0.47
10:J:96:ILE:H	10:J:96:ILE:HD12	1.80	0.47
13:M:5:GLY:O	13:M:7:GLU:N	2.48	0.47
14:N:9:ALA:O	14:N:10:LYS:C	2.58	0.47
1:A:279:A:H5'	1:A:279:A:C8	2.50	0.47
1:A:1275:A:O2'	1:A:1276:G:H5'	2.15	0.47
1:A:1390:U:H2'	1:A:1391:U:C6	2.50	0.47
2:B:13:HIS:HD2	2:B:199:ASP:OD1	1.97	0.47
3:C:69:VAL:O	3:C:105:VAL:HG23	2.15	0.47
4:D:172:TRP:CD2	4:D:188:PRO:HB3	2.50	0.47
5:E:72:ILE:HD12	5:E:138:LEU:HD11	1.96	0.47
6:F:18:GLN:O	6:F:21:LEU:HB3	2.15	0.47
8:H:4:ASP:CG	8:H:85:ARG:HH11	2.23	0.47
10:J:30:ALA:H	10:J:76:ASN:ND2	2.13	0.47
14:N:8:LYS:C	14:N:8:LYS:CD	2.87	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:G:H2'	1:A:42:G:C8	2.50	0.47
1:A:73:G:O2'	1:A:76:C:H5'	2.15	0.47
1:A:224:C:H5'	1:A:224:C:C6	2.48	0.47
1:A:542:G:O2'	1:A:543:C:H5'	2.15	0.47
1:A:872:A:C3'	1:A:873:A:C5'	2.92	0.47
1:A:1074:G:O3'	2:B:97:THR:HG22	2.15	0.47
1:A:1349:A:OP1	9:I:117:LYS:HE2	2.15	0.47
2:B:126:LYS:HG2	2:B:129:GLN:CD	2.40	0.47
2:B:156:ILE:HG22	2:B:158:VAL:HG23	1.97	0.47
3:C:178:ARG:O	3:C:178:ARG:HG2	2.15	0.47
3:C:188:ALA:HB3	3:C:195:LEU:HB2	1.97	0.47
4:D:29:LYS:O	4:D:31:ALA:N	2.47	0.47
9:I:29:GLY:O	9:I:30:GLN:C	2.58	0.47
11:K:81:ARG:NH1	18:R:73:LYS:HE2	2.30	0.47
13:M:15:ASP:OD1	13:M:16:VAL:N	2.46	0.47
17:Q:3:LYS:CE	17:Q:5:LEU:HD21	2.45	0.47
20:T:39:GLU:OE1	20:T:41:LYS:NZ	2.48	0.47
1:A:18:C:H5''	5:E:123:ASN:HD21	1.79	0.46
1:A:627:G:H2'	1:A:628:G:H8	1.80	0.46
1:A:1203:C:H2'	1:A:1204:A:H8	1.79	0.46
1:A:1252:A:H61	1:A:1285:A:N6	2.13	0.46
1:A:1353:G:O2'	1:A:1354:C:H5'	2.15	0.46
2:B:1:VAL:CG2	2:B:215:LEU:HD23	2.31	0.46
2:B:189:ASP:O	8:H:68:ARG:NH2	2.47	0.46
3:C:57:GLU:HB2	3:C:64:ALA:CB	2.45	0.46
6:F:101:ALA:HA	18:R:13:GLU:OE1	2.15	0.46
8:H:82:HIS:CD2	8:H:82:HIS:C	2.93	0.46
16:P:20:VAL:CG1	16:P:21:VAL:N	2.77	0.46
17:Q:3:LYS:HE3	17:Q:5:LEU:CD2	2.44	0.46
1:A:109:A:H5'	1:A:110:C:C5	2.50	0.46
1:A:384:G:H2'	1:A:385:C:H6	1.79	0.46
1:A:539:A:H2'	1:A:540:G:H8	1.78	0.46
1:A:687:A:H4'	1:A:688:G:O5'	2.15	0.46
1:A:824:C:H2'	1:A:825:G:C8	2.47	0.46
3:C:148:ALA:O	3:C:168:ALA:HB1	2.15	0.46
4:D:17:LYS:HZ3	4:D:30:CYS:CB	2.15	0.46
7:G:102:TRP:CH2	7:G:140:VAL:HG21	2.50	0.46
7:G:151:ALA:C	7:G:153:TYR:H	2.24	0.46
9:I:31:ASP:O	9:I:34:GLU:HB3	2.15	0.46
11:K:24:ASP:C	11:K:24:ASP:OD1	2.58	0.46
15:O:86:ILE:O	15:O:87:ARG:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:40:ARG:HH11	18:R:40:ARG:CA	2.29	0.46
19:S:76:THR:HG22	19:S:77:ARG:N	2.29	0.46
1:A:156:G:C3'	1:A:157:G:H5''	2.45	0.46
1:A:945:G:H2'	1:A:945:G:N3	2.30	0.46
1:A:954:G:H2'	1:A:955:U:H6	1.80	0.46
1:A:970:C:N4	9:I:125:SER:OG	2.48	0.46
1:A:1124:G:H4'	10:J:36:ILE:HD11	1.97	0.46
1:A:1151:A:O2'	1:A:1152:A:H8	1.98	0.46
3:C:82:ARG:C	3:C:84:ARG:N	2.70	0.46
4:D:33:GLU:O	4:D:34:ARG:HB2	2.13	0.46
4:D:63:LEU:HD23	4:D:197:VAL:HG21	1.97	0.46
4:D:93:LEU:HA	4:D:96:LEU:HD12	1.98	0.46
12:L:115:LYS:O	12:L:116:TYR:HB2	2.15	0.46
13:M:76:ASN:O	13:M:79:ARG:HB3	2.15	0.46
15:O:49:HIS:O	15:O:52:HIS:HB3	2.15	0.46
16:P:82:GLN:O	16:P:83:GLU:C	2.58	0.46
17:Q:91:ARG:NH1	17:Q:91:ARG:CB	2.72	0.46
20:T:67:LYS:HB2	20:T:68:ASN:H	1.32	0.46
21:V:2:GLY:O	21:V:4:GLY:N	2.48	0.46
1:A:484:G:H8	1:A:484:G:OP1	1.98	0.46
1:A:737:A:H2'	1:A:738:C:C6	2.50	0.46
1:A:1175:G:O2'	1:A:1176:A:H5'	2.15	0.46
5:E:70:GLY:CA	5:E:112:THR:HG22	2.46	0.46
7:G:61:PHE:HD1	7:G:123:LEU:HD21	1.81	0.46
8:H:112:LEU:HD12	8:H:112:LEU:N	2.30	0.46
14:N:30:ARG:HG3	14:N:30:ARG:NH1	2.31	0.46
1:A:129(A):G:C6	1:A:189(E):U:O2'	2.66	0.46
1:A:583:A:H2'	1:A:584:G:O4'	2.16	0.46
1:A:1082:G:O2'	1:A:1083:U:H5'	2.15	0.46
1:A:1281:U:O2	1:A:1281:U:O4'	2.33	0.46
1:A:1539:C:O5'	1:A:1540:U:OP2	2.28	0.46
5:E:9:ILE:HA	5:E:25:GLY:O	2.16	0.46
6:F:67:MET:HB2	6:F:68:PRO:HD2	1.95	0.46
7:G:16:VAL:HG12	7:G:17:TYR:CE1	2.51	0.46
9:I:39:LEU:O	9:I:41:ARG:N	2.49	0.46
12:L:37:ARG:HG2	12:L:38:THR:N	2.24	0.46
15:O:25:GLU:OE2	15:O:76:ARG:HD2	2.16	0.46
16:P:52:ASP:C	16:P:52:ASP:OD1	2.58	0.46
17:Q:66:LYS:O	17:Q:67:ARG:CG	2.62	0.46
19:S:12:ASP:HA	19:S:15:LEU:HB3	1.98	0.46
19:S:21:LEU:HD12	19:S:30:ILE:HD11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:28:ARG:O	19:S:29:LEU:HB2	2.15	0.46
20:T:37:ALA:HA	20:T:85:LEU:HD21	1.98	0.46
1:A:364:A:N6	12:L:24:LYS:NZ	2.63	0.46
1:A:607:A:H5'	1:A:607:A:H8	1.80	0.46
1:A:651:C:O2'	1:A:652:U:H5'	2.16	0.46
1:A:1428:A:H2'	1:A:1429:C:C6	2.51	0.46
1:A:1483:A:H2'	1:A:1484:C:O4'	2.16	0.46
2:B:176:ILE:O	2:B:177:PRO:C	2.58	0.46
3:C:19:SER:O	14:N:53:PRO:HB3	2.15	0.46
3:C:137:VAL:O	3:C:141:MET:HB2	2.16	0.46
4:D:195:LEU:HB2	4:D:196:PRO:HD2	1.97	0.46
5:E:36:ARG:HG2	5:E:36:ARG:HH11	1.80	0.46
5:E:47:VAL:O	5:E:50:ALA:HB3	2.16	0.46
7:G:45:ALA:O	7:G:49:ILE:HG13	2.15	0.46
7:G:91:SER:HB2	7:G:92:PRO:HD2	1.98	0.46
7:G:135:LYS:HD2	7:G:135:LYS:C	2.40	0.46
9:I:36:PHE:HB3	9:I:42:ALA:HB2	1.96	0.46
9:I:48:PRO:HB3	9:I:81:ALA:HB2	1.96	0.46
10:J:84:MET:O	10:J:84:MET:HE3	2.16	0.46
16:P:1:MET:HE3	16:P:3:LYS:HD3	1.96	0.46
16:P:74:LEU:CD2	16:P:79:VAL:HG21	2.44	0.46
17:Q:16:LYS:HA	17:Q:45:ASP:O	2.14	0.46
19:S:18:VAL:HG13	19:S:19:LEU:N	2.31	0.46
20:T:88:ALA:O	20:T:89:GLY:C	2.58	0.46
1:A:293:G:H5'	1:A:609:A:N6	2.26	0.46
1:A:653:A:C8	8:H:56:LYS:HG2	2.51	0.46
1:A:1126:U:H6	1:A:1280:A:N7	2.12	0.46
6:F:22:GLU:C	6:F:24:GLU:H	2.23	0.46
6:F:62:TRP:CG	18:R:20:ARG:NH1	2.83	0.46
10:J:24:ALA:O	10:J:83:LEU:HG	2.16	0.46
17:Q:68:LYS:C	17:Q:69:ARG:HD2	2.40	0.46
18:R:71:VAL:O	18:R:72:ARG:HG2	2.15	0.46
23:Z:34:G:H2'	23:Z:35:A:H8	1.81	0.46
2:B:72:GLN:O	2:B:88:ASN:OD1	2.33	0.46
6:F:40:VAL:CG2	6:F:41:GLU:N	2.79	0.46
10:J:55:LYS:HD2	10:J:55:LYS:C	2.41	0.46
10:J:73:ILE:HG22	10:J:74:ASN:N	2.31	0.46
11:K:60:LYS:O	11:K:61:LYS:C	2.59	0.46
12:L:24:LYS:HD3	12:L:29:ARG:HH12	1.80	0.46
13:M:45:LYS:HG3	13:M:46:ASP:N	2.31	0.46
17:Q:80:ARG:HG3	17:Q:80:ARG:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:C:H5''	5:E:123:ASN:ND2	2.31	0.46
1:A:107:G:C2'	1:A:108:G:H5'	2.46	0.46
1:A:310:G:H5''	16:P:31:LYS:HB2	1.98	0.46
2:B:4:LEU:O	2:B:6:GLU:N	2.49	0.46
2:B:183:ASP:OD2	2:B:199:ASP:OD1	2.34	0.46
3:C:27:GLN:HA	3:C:30:HIS:HD2	1.81	0.46
10:J:4:ILE:O	10:J:4:ILE:HG12	2.15	0.46
10:J:96:ILE:HD12	10:J:96:ILE:N	2.31	0.46
12:L:31:GLY:HA3	12:L:54:VAL:CG1	2.46	0.46
15:O:65:LEU:O	15:O:68:TYR:HB3	2.16	0.46
17:Q:32:GLY:O	17:Q:33:LYS:C	2.58	0.46
1:A:439:A:H2'	1:A:441:A:C5'	2.45	0.46
1:A:714:G:H2'	1:A:715:A:C8	2.50	0.46
1:A:1044:A:H2'	1:A:1045:C:C4'	2.46	0.46
1:A:1144:G:H21	1:A:1146:A:N6	2.13	0.46
1:A:1471:G:O2'	1:A:1472:U:H5'	2.16	0.46
3:C:22:TYR:CD1	3:C:23:ALA:N	2.84	0.46
3:C:142:GLU:C	3:C:144:GLY:H	2.23	0.46
5:E:72:ILE:HG23	5:E:138:LEU:HD13	1.98	0.46
9:I:63:THR:HG22	9:I:64:VAL:N	2.31	0.46
11:K:38:ILE:HD13	11:K:53:LEU:HB2	1.97	0.46
11:K:81:ARG:CZ	18:R:73:LYS:CE	2.92	0.46
12:L:30:ARG:O	12:L:57:THR:HG23	2.15	0.46
13:M:64:LYS:HE3	13:M:68:GLU:CG	2.40	0.46
19:S:57:VAL:O	19:S:59:VAL:HG23	2.16	0.46
1:A:413:G:H21	1:A:428:G:H1'	1.80	0.45
1:A:1129:C:O5'	1:A:1130:A:H5'	2.16	0.45
1:A:1460:A:H2'	1:A:1461:G:O4'	2.16	0.45
2:B:24:ARG:NH2	2:B:188:PRO:HB2	2.31	0.45
2:B:229:SER:C	2:B:231:ALA:H	2.24	0.45
3:C:106:GLN:H	3:C:106:GLN:CD	2.21	0.45
6:F:101:ALA:HA	18:R:13:GLU:CD	2.41	0.45
9:I:31:ASP:O	9:I:32:PHE:C	2.58	0.45
11:K:36:GLY:O	11:K:38:ILE:O	2.34	0.45
15:O:7:LYS:O	15:O:11:ILE:HD12	2.16	0.45
15:O:35:ILE:HD12	15:O:59:VAL:HG23	1.97	0.45
1:A:55:A:O2'	1:A:56:U:H5'	2.16	0.45
1:A:253:U:H2'	1:A:254:G:H8	1.78	0.45
1:A:334:C:H2'	1:A:335:C:C6	2.52	0.45
1:A:455:C:H2'	1:A:456:C:C6	2.52	0.45
1:A:1037:C:H2'	1:A:1038:C:C6	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:44:LYS:HE3	3:C:44:LYS:HB2	1.66	0.45
3:C:153:SER:CB	3:C:196:GLY:H	2.29	0.45
4:D:69:ILE:HG22	4:D:73:GLN:HB2	1.98	0.45
13:M:2:ARG:O	13:M:2:ARG:HG2	2.16	0.45
13:M:10:ARG:HA	13:M:44:VAL:HB	1.97	0.45
14:N:25:ARG:HE	14:N:46:LEU:HD21	1.80	0.45
1:A:483:C:C3'	1:A:484:G:H5''	2.38	0.45
1:A:639:G:O2'	1:A:640:A:H5'	2.16	0.45
1:A:715:A:H2'	1:A:716:A:C8	2.52	0.45
1:A:880:C:O2'	1:A:881:G:H5'	2.16	0.45
1:A:1161:C:H2'	1:A:1162:C:C6	2.51	0.45
2:B:11:PHE:O	2:B:12:GLY:C	2.59	0.45
2:B:222:GLY:O	2:B:223:VAL:C	2.58	0.45
5:E:112:THR:HG23	5:E:113:ASP:OD2	2.16	0.45
7:G:38:ALA:O	7:G:39:ALA:C	2.59	0.45
7:G:123:LEU:O	7:G:126:ALA:HB3	2.15	0.45
16:P:67:THR:HG22	16:P:69:THR:H	1.81	0.45
17:Q:100:ARG:HA	17:Q:100:ARG:HE	1.81	0.45
19:S:18:VAL:HG21	19:S:43:MET:HG2	1.98	0.45
1:A:175:C:H2'	1:A:176:C:H6	1.81	0.45
1:A:982:U:O4	1:A:1223:C:N3	2.50	0.45
1:A:1142:G:C2'	1:A:1143:G:H5'	2.47	0.45
1:A:1249:C:H4'	9:I:35:TYR:OH	2.17	0.45
1:A:1346:A:C2	7:G:9:ARG:NH1	2.84	0.45
2:B:22:PHE:HD1	2:B:188:PRO:HG3	1.81	0.45
2:B:37:ASP:OD1	2:B:39:GLN:HB2	2.15	0.45
2:B:150:LYS:O	2:B:150:LYS:HD3	2.15	0.45
4:D:175:LEU:HG	4:D:176:ASP:N	2.31	0.45
12:L:84:GLY:H	12:L:94:TYR:HA	1.81	0.45
14:N:7:GLU:O	14:N:8:LYS:C	2.59	0.45
14:N:28:ARG:HG2	14:N:39:CYS:HB2	1.98	0.45
21:V:6:ARG:CG	21:V:15:ARG:NH1	2.74	0.45
1:A:921:U:O2	5:E:15:MET:HB2	2.17	0.45
1:A:977:A:O2'	1:A:978:A:H5''	2.16	0.45
1:A:1032:G:H2'	1:A:1033:G:C8	2.52	0.45
1:A:1256:A:N6	1:A:1278:U:H3	2.05	0.45
3:C:46:LEU:CD2	3:C:67:VAL:HG11	2.47	0.45
4:D:60:LYS:NZ	4:D:71:GLU:OE1	2.50	0.45
4:D:154:LEU:O	4:D:155:GLU:C	2.59	0.45
6:F:43:LEU:HD22	6:F:43:LEU:N	2.32	0.45
10:J:30:ALA:HB2	10:J:74:ASN:CB	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:80:LEU:O	13:M:85:CYS:HB3	2.16	0.45
1:A:161:A:O2'	1:A:162:A:H5'	2.17	0.45
1:A:807:A:H2'	1:A:808:C:C6	2.51	0.45
1:A:952:U:H2'	1:A:953:G:C8	2.52	0.45
1:A:1040:U:H2'	1:A:1041:A:H8	1.82	0.45
1:A:1109:C:H2'	1:A:1110:A:O4'	2.17	0.45
1:A:1168:A:O2'	1:A:1169:A:H8	1.99	0.45
1:A:1335:C:H6	1:A:1335:C:H5''	1.81	0.45
1:A:1402:C:H2'	1:A:1403:C:O4'	2.16	0.45
2:B:3:GLU:HG2	2:B:211:ARG:HH12	1.81	0.45
2:B:9:VAL:HG12	2:B:204:SER:HA	1.99	0.45
2:B:19:ASN:HD22	2:B:21:LYS:H	1.65	0.45
3:C:118:ARG:CG	3:C:139:ARG:NH2	2.76	0.45
3:C:147:GLY:HA3	3:C:171:ARG:O	2.16	0.45
5:E:94:THR:HG22	5:E:97:ILE:HD11	1.98	0.45
11:K:4:VAL:O	11:K:5:ALA:HB3	2.16	0.45
1:A:19:C:H2'	1:A:20:U:C6	2.51	0.45
1:A:253:U:H2'	1:A:254:G:C8	2.52	0.45
1:A:572:A:H5''	1:A:917:G:H4'	1.99	0.45
1:A:954:G:H21	1:A:1227:A:H62	1.65	0.45
1:A:1231:G:H4'	9:I:125:SER:HB2	1.98	0.45
2:B:11:PHE:CD1	2:B:11:PHE:C	2.95	0.45
2:B:81:ARG:HD3	2:B:228:PRO:HD2	1.98	0.45
2:B:129:GLN:O	2:B:133:LYS:HB2	2.16	0.45
2:B:130:VAL:HG12	2:B:134:HIS:CD2	2.52	0.45
4:D:63:LEU:HD12	4:D:74:PHE:HZ	1.82	0.45
5:E:78:VAL:HG22	5:E:137:GLN:NE2	2.31	0.45
6:F:72:VAL:CG1	6:F:90:VAL:HG11	2.47	0.45
6:F:94:GLN:HE21	18:R:17:ARG:NH1	2.12	0.45
12:L:25:GLY:O	12:L:26:ALA:O	2.34	0.45
18:R:38:ARG:HG2	18:R:48:GLN:OE1	2.17	0.45
19:S:12:ASP:OD1	19:S:12:ASP:N	2.49	0.45
1:A:173:U:H2'	1:A:197:A:N7	2.32	0.45
1:A:1438:G:H2'	1:A:1439:C:C6	2.51	0.45
2:B:109:LEU:HD11	2:B:140:GLN:NE2	2.32	0.45
4:D:110:ALA:HB2	4:D:119:LEU:HD12	1.99	0.45
5:E:149:LYS:O	5:E:151:GLU:N	2.50	0.45
6:F:50:TYR:CE1	18:R:62:GLY:HA2	2.51	0.45
8:H:56:LYS:HD2	8:H:56:LYS:N	2.31	0.45
8:H:60:ARG:HG3	8:H:60:ARG:NH1	2.30	0.45
10:J:44:ARG:NH1	10:J:44:ARG:CG	2.76	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:116:ARG:O	11:K:117:LYS:HB2	2.17	0.45
12:L:85:ARG:HD2	12:L:86:VAL:C	2.42	0.45
1:A:892:A:H2'	1:A:893:C:C6	2.52	0.45
1:A:1305:G:H22	1:A:1331:G:H1'	1.80	0.45
3:C:4:ILE:HD12	3:C:4:ILE:O	2.16	0.45
4:D:24:ARG:C	4:D:26:TYR:H	2.25	0.45
10:J:43:ARG:NH2	14:N:35:PHE:CD2	2.85	0.45
11:K:100:ASP:OD1	11:K:101:ASP:N	2.50	0.45
13:M:121:LYS:CD	13:M:122:ALA:H	2.29	0.45
15:O:16:ARG:HG3	15:O:16:ARG:NH1	2.32	0.45
20:T:36:LEU:HD13	20:T:44:GLU:HG3	1.99	0.45
1:A:838:G:H1	1:A:848:C:N4	2.15	0.45
2:B:52:ILE:HD11	2:B:179:ILE:HD13	1.98	0.45
2:B:77:MET:HG3	2:B:229:SER:CB	2.45	0.45
4:D:110:ALA:HB1	4:D:115:GLN:HG2	1.99	0.45
8:H:4:ASP:OD2	8:H:85:ARG:NH1	2.49	0.45
11:K:40:TYR:HB3	11:K:44:ARG:HB2	1.97	0.45
18:R:32:THR:HG22	18:R:33:GLY:N	2.31	0.45
20:T:16:ARG:HG2	20:T:16:ARG:HH11	1.80	0.45
1:A:130:A:C8	17:Q:62:ARG:HG3	2.52	0.44
1:A:279:A:H5'	1:A:279:A:H8	1.83	0.44
1:A:1099:G:H5'	1:A:1099:G:H8	1.81	0.44
2:B:151:ARG:HH11	2:B:151:ARG:HG3	1.82	0.44
4:D:7:VAL:HG13	4:D:20:LEU:CD1	2.47	0.44
5:E:140:THR:HG22	5:E:142:ALA:H	1.81	0.44
7:G:5:ARG:O	7:G:5:ARG:HG2	2.17	0.44
10:J:32:VAL:HG12	10:J:33:SER:N	2.31	0.44
13:M:20:TYR:N	13:M:20:TYR:CD1	2.84	0.44
14:N:23:CYS:HA	14:N:37:GLY:O	2.16	0.44
1:A:107:G:C3'	1:A:108:G:H5'	2.47	0.44
1:A:328:C:O2	1:A:328:C:C2'	2.63	0.44
1:A:1036:G:O2'	1:A:1037:C:H5'	2.17	0.44
1:A:1128:C:O2'	1:A:1129:C:P	2.75	0.44
2:B:18:TRP:CD1	2:B:18:TRP:N	2.85	0.44
2:B:39:GLN:O	2:B:42:MET:HB2	2.17	0.44
2:B:47:ARG:HG2	2:B:47:ARG:HH11	1.82	0.44
4:D:186:ARG:NH2	4:D:187:LEU:HG	2.32	0.44
8:H:46:LYS:HG3	8:H:64:LYS:HG2	1.99	0.44
10:J:85:THR:H	10:J:86:LEU:HD12	1.81	0.44
11:K:2:ARG:O	11:K:3:GLN:HB2	2.17	0.44
20:T:46:LEU:HB2	20:T:93:ILE:HG21	1.96	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:485:G:O2'	1:A:486:U:P	2.75	0.44
1:A:949:A:H2'	1:A:950:U:O4'	2.18	0.44
1:A:1241:G:H2'	1:A:1242:C:C6	2.52	0.44
2:B:1:VAL:HG11	2:B:215:LEU:HD23	2.00	0.44
2:B:194:ILE:HG22	2:B:195:ILE:N	2.32	0.44
4:D:30:CYS:O	4:D:31:ALA:HB3	2.17	0.44
5:E:140:THR:O	5:E:141:LYS:C	2.58	0.44
7:G:15:LEU:HD22	7:G:15:LEU:H	1.82	0.44
7:G:119:ILE:H	7:G:119:ILE:CD1	2.31	0.44
13:M:28:ARG:HB3	13:M:63:TRP:CH2	2.53	0.44
18:R:38:ARG:HD2	18:R:43:LEU:O	2.17	0.44
19:S:14:LEU:HD23	19:S:14:LEU:H	1.82	0.44
19:S:19:LEU:HA	19:S:22:ASN:ND2	2.31	0.44
20:T:66:HIS:C	20:T:67:LYS:HG3	2.41	0.44
1:A:39:G:O2'	1:A:40:C:H5'	2.17	0.44
1:A:76:C:O2'	1:A:77:G:H5'	2.17	0.44
1:A:1236:A:H2'	1:A:1237:C:C6	2.52	0.44
2:B:13:HIS:CE1	2:B:200:ASP:HB3	2.51	0.44
5:E:140:THR:O	5:E:144:VAL:HG23	2.18	0.44
8:H:86:ILE:HG13	8:H:133:LEU:HD22	1.99	0.44
8:H:110:ALA:HB3	8:H:121:ASP:HB3	1.99	0.44
15:O:52:HIS:HE1	15:O:56:LEU:HD13	1.81	0.44
1:A:146:G:C3'	1:A:147:G:C5'	2.96	0.44
1:A:613:C:C2'	1:A:614:A:H5'	2.48	0.44
1:A:911:U:H2'	1:A:912:C:C6	2.52	0.44
1:A:1226:C:H4'	1:A:1227:A:OP1	2.18	0.44
1:A:1346:A:N1	7:G:9:ARG:NH1	2.65	0.44
2:B:96:LEU:N	2:B:96:LEU:CD1	2.81	0.44
3:C:35:ASP:OD1	3:C:56:ILE:HD12	2.17	0.44
8:H:83:ILE:HG23	8:H:83:ILE:O	2.18	0.44
9:I:99:GLY:C	9:I:101:LEU:N	2.73	0.44
11:K:105:PRO:C	11:K:107:ASN:N	2.74	0.44
13:M:83:ILE:CG2	19:S:73:PHE:HE2	2.28	0.44
14:N:20:TYR:O	14:N:21:THR:C	2.59	0.44
16:P:72:ARG:HG2	16:P:72:ARG:HH11	1.82	0.44
18:R:22:VAL:HG23	18:R:23:GLU:N	2.33	0.44
1:A:224:C:C5'	1:A:224:C:C6	2.95	0.44
1:A:364:A:N6	12:L:24:LYS:HZ1	2.14	0.44
1:A:438:G:O2'	1:A:494:U:O4	2.35	0.44
1:A:965:A:C2	1:A:969:A:C2	3.06	0.44
1:A:1238:A:OP1	1:A:1335:C:H1'	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:69:ILE:HG22	4:D:70:SER:N	2.32	0.44
6:F:22:GLU:C	6:F:24:GLU:N	2.73	0.44
1:A:46:G:O2'	1:A:365:U:H1'	2.18	0.44
1:A:55:A:C2'	1:A:56:U:H5'	2.47	0.44
1:A:189(E):U:O2	1:A:189(E):U:C2'	2.66	0.44
1:A:200:G:H2'	1:A:201:C:O4'	2.18	0.44
1:A:1027:C:H2'	1:A:1028:C:H6	1.82	0.44
2:B:91:TRP:CZ3	2:B:170:GLU:OE2	2.71	0.44
3:C:96:LYS:O	3:C:97:ASN:C	2.59	0.44
3:C:172:VAL:N	3:C:173:PRO:CD	2.80	0.44
3:C:194:VAL:HG12	3:C:195:LEU:H	1.82	0.44
12:L:54:VAL:O	12:L:61:GLU:HA	2.17	0.44
12:L:79:VAL:CG2	12:L:96:ILE:HG23	2.48	0.44
1:A:35:G:H2'	1:A:36:C:H6	1.83	0.44
1:A:487:A:H2'	1:A:488:C:O4'	2.18	0.44
1:A:1054:C:O2'	1:A:1055:A:C5'	2.46	0.44
2:B:6:GLU:C	2:B:8:GLY:N	2.75	0.44
2:B:27:TYR:HB2	2:B:37:ASP:HA	1.99	0.44
2:B:215:LEU:HD13	2:B:215:LEU:C	2.42	0.44
4:D:6:PRO:HG2	4:D:9:ARG:HD2	1.99	0.44
4:D:156:LEU:HD11	4:D:160:ASN:HD21	1.83	0.44
5:E:78:VAL:CG2	5:E:137:GLN:HE21	2.31	0.44
14:N:22:ARG:HA	14:N:32:VAL:HG21	1.99	0.44
1:A:194:C:OP1	20:T:54:SER:OG	2.29	0.44
1:A:567:G:H2'	1:A:568:G:O4'	2.18	0.44
1:A:735:C:O2'	1:A:736:C:H5'	2.17	0.44
1:A:1300:G:H1'	1:A:1301:U:H5	1.83	0.44
1:A:1479:C:H2'	1:A:1480:G:O5'	2.18	0.44
2:B:136:LEU:O	2:B:140:GLN:OE1	2.36	0.44
1:A:923:A:OP1	5:E:17:ALA:HB2	2.18	0.43
1:A:1392:G:N2	1:A:1502:A:C8	2.83	0.43
2:B:52:ILE:CD1	2:B:179:ILE:HD13	2.48	0.43
4:D:7:VAL:O	4:D:9:ARG:N	2.48	0.43
8:H:91:ARG:NH1	17:Q:32:GLY:HA3	2.33	0.43
11:K:1:LYS:HD2	11:K:1:LYS:H3	1.81	0.43
11:K:98:ILE:O	11:K:99:VAL:HG23	2.18	0.43
13:M:69:LEU:O	13:M:72:GLU:N	2.51	0.43
13:M:97:VAL:O	13:M:97:VAL:HG12	2.17	0.43
20:T:69:ALA:O	20:T:73:ARG:CG	2.66	0.43
1:A:273:A:H1'	17:Q:15:GLN:OE1	2.18	0.43
1:A:524:G:H2'	1:A:525:C:C6	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:36:ILE:CD1	2:B:197:GLY:HA2	2.48	0.43
2:B:186:SER:O	2:B:188:PRO:HD3	2.18	0.43
4:D:148:ALA:O	4:D:149:GLU:C	2.61	0.43
6:F:10:LEU:HD12	6:F:59:TYR:O	2.18	0.43
6:F:52:ILE:O	6:F:53:ALA:HB3	2.18	0.43
9:I:42:ALA:H	9:I:73:ILE:HD13	1.83	0.43
11:K:42:GLY:H	11:K:45:LYS:HG3	1.83	0.43
13:M:39:ASN:HD22	13:M:40:PRO:N	2.16	0.43
17:Q:67:ARG:O	17:Q:67:ARG:CG	2.63	0.43
20:T:92:LEU:C	20:T:94:GLY:N	2.74	0.43
1:A:234:C:H2'	1:A:235:C:C6	2.53	0.43
1:A:490:G:O2'	1:A:491:G:H5'	2.18	0.43
1:A:974:A:OP2	14:N:31:SER:HB3	2.18	0.43
2:B:2:LYS:O	2:B:211:ARG:NH1	2.50	0.43
3:C:22:TYR:CD1	3:C:22:TYR:C	2.96	0.43
3:C:30:HIS:C	3:C:32:LEU:N	2.76	0.43
3:C:67:VAL:HG12	3:C:69:VAL:HG23	2.00	0.43
3:C:111:SER:HB3	3:C:114:LEU:HD12	1.98	0.43
3:C:146:LYS:NZ	3:C:205:GLU:HB2	2.33	0.43
6:F:22:GLU:OE2	6:F:84:ASN:HB2	2.19	0.43
8:H:104:ARG:NH2	8:H:138:TRP:CZ3	2.86	0.43
9:I:116:HIS:O	9:I:117:LYS:HB3	2.18	0.43
10:J:13:THR:HG22	10:J:92:VAL:CG2	2.48	0.43
10:J:47:VAL:CG1	14:N:40:ARG:HB2	2.48	0.43
1:A:189:G:H2'	1:A:189(A):C:C6	2.53	0.43
1:A:813:U:OP1	1:A:904:C:H5'	2.18	0.43
1:A:1399:C:C2	1:A:1502:A:N6	2.87	0.43
2:B:148:LEU:O	2:B:149:LEU:C	2.61	0.43
3:C:14:THR:O	3:C:15:ARG:CB	2.58	0.43
3:C:69:VAL:CG1	3:C:70:ALA:N	2.81	0.43
3:C:171:ARG:HB3	3:C:171:ARG:NH1	2.30	0.43
4:D:51:SER:O	4:D:52:ASP:C	2.59	0.43
7:G:147:ASN:C	7:G:149:ALA:N	2.76	0.43
10:J:47:VAL:HG12	14:N:40:ARG:HB2	2.00	0.43
11:K:1:LYS:HD2	11:K:1:LYS:H1	1.83	0.43
15:O:2:ILE:N	15:O:2:ILE:CD1	2.81	0.43
15:O:68:TYR:CE1	15:O:72:GLU:HG3	2.54	0.43
15:O:87:ARG:HE	15:O:87:ARG:CA	2.31	0.43
1:A:656:C:O2'	15:O:27:GLN:OE1	2.30	0.43
1:A:913:A:H2'	1:A:914:A:H1'	2.01	0.43
1:A:1381:U:O2	1:A:1381:U:C2'	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1516:G:H2'	1:A:1518:A:OP2	2.18	0.43
2:B:210:SER:O	2:B:213:VAL:N	2.52	0.43
4:D:69:ILE:HG22	4:D:70:SER:H	1.84	0.43
5:E:72:ILE:HG23	5:E:138:LEU:CD1	2.49	0.43
5:E:76:ILE:HD13	5:E:87:LEU:HB2	1.97	0.43
9:I:54:ALA:O	9:I:56:GLY:N	2.49	0.43
9:I:99:GLY:C	9:I:101:LEU:H	2.26	0.43
9:I:126:LYS:H	9:I:126:LYS:HD2	1.81	0.43
11:K:38:ILE:CD1	11:K:54:ALA:N	2.82	0.43
13:M:2:ARG:HA	13:M:7:GLU:O	2.19	0.43
14:N:12:THR:O	14:N:12:THR:HG22	2.18	0.43
20:T:31:LYS:O	20:T:35:GLN:HB2	2.18	0.43
1:A:234:C:H2'	1:A:235:C:H6	1.83	0.43
1:A:517:G:H8	1:A:517:G:OP2	2.02	0.43
1:A:1272:G:H2'	1:A:1273:G:O4'	2.19	0.43
2:B:13:HIS:ND1	2:B:198:ASN:ND2	2.66	0.43
3:C:7:ILE:HD12	3:C:15:ARG:CZ	2.48	0.43
3:C:45:GLU:C	3:C:47:TYR:H	2.26	0.43
3:C:78:ARG:HH21	3:C:81:GLU:HG2	1.82	0.43
11:K:114:LYS:HD3	11:K:115:PHE:CE1	2.53	0.43
16:P:72:ARG:HG2	16:P:72:ARG:NH1	2.33	0.43
17:Q:82:ASP:O	17:Q:85:GLU:HB2	2.19	0.43
1:A:247:G:OP2	17:Q:98:SER:HB2	2.18	0.43
1:A:598:U:H2'	1:A:599:C:C6	2.54	0.43
1:A:996:A:H5'	1:A:996:A:C8	2.50	0.43
3:C:179:ALA:CB	3:C:181:ILE:HD11	2.49	0.43
7:G:142:ARG:O	7:G:146:ALA:CB	2.67	0.43
11:K:23:THR:HB	11:K:28:ASN:C	2.43	0.43
16:P:27:LYS:NZ	16:P:27:LYS:HB3	2.34	0.43
1:A:374:A:C6	1:A:375:U:C4	3.07	0.43
1:A:659:U:H2'	1:A:660:G:C8	2.53	0.43
1:A:1203:C:O2'	1:A:1204:A:H5'	2.19	0.43
1:A:1310:G:N7	19:S:1:PRO:HG3	2.33	0.43
1:A:1425:U:H3	1:A:1475:G:H1	1.65	0.43
3:C:51:LEU:H	3:C:51:LEU:CD2	2.32	0.43
3:C:133:ILE:HD12	3:C:152:VAL:HG23	2.00	0.43
4:D:120:VAL:HG22	4:D:125:ILE:HD12	2.00	0.43
5:E:96:VAL:O	5:E:103:ARG:NH2	2.52	0.43
10:J:45:PHE:CE2	14:N:36:PHE:HE2	2.36	0.43
13:M:107:ARG:HD3	13:M:113:ARG:NH1	2.34	0.43
14:N:20:TYR:O	14:N:20:TYR:CD1	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:79:GLY:O	17:Q:80:ARG:HB3	2.19	0.43
20:T:89:GLY:O	20:T:90:ALA:CB	2.67	0.43
1:A:501:C:H1'	1:A:549:C:O2'	2.19	0.43
1:A:985:C:H2'	1:A:986:A:C8	2.53	0.43
1:A:1296:C:H5''	13:M:13:ARG:HD2	2.01	0.43
1:A:1527:C:O2'	1:A:1528:U:H5'	2.19	0.43
2:B:63:LEU:C	2:B:63:LEU:CD2	2.92	0.43
3:C:159:ALA:O	3:C:160:GLU:C	2.62	0.43
4:D:125:ILE:HG22	4:D:126:THR:N	2.33	0.43
8:H:49:GLU:HG2	8:H:62:TYR:HE2	1.84	0.43
10:J:58:ARG:HG2	10:J:58:ARG:NH1	2.33	0.43
11:K:91:SER:C	11:K:93:LEU:H	2.26	0.43
12:L:51:VAL:HG13	12:L:52:ALA:N	2.34	0.43
13:M:69:LEU:O	13:M:70:ARG:C	2.62	0.43
16:P:21:VAL:HG21	16:P:59:TRP:CD1	2.54	0.43
18:R:19:TYR:HA	18:R:54:THR:HG23	1.99	0.43
18:R:29:LEU:CD1	18:R:64:LEU:HD22	2.49	0.43
19:S:35:ARG:HH21	19:S:74:ALA:HB3	1.84	0.43
1:A:231:G:C2'	1:A:232:G:H5'	2.48	0.43
1:A:707:C:H2'	1:A:708:C:H6	1.83	0.43
1:A:1060:C:N4	3:C:1:GLY:HA3	2.34	0.43
1:A:1355:G:O2'	1:A:1356:G:H5'	2.19	0.43
1:A:1486:G:H5'	1:A:1486:G:H8	1.84	0.43
2:B:131:ARG:HB3	2:B:131:ARG:NH1	2.33	0.43
2:B:131:ARG:CB	2:B:131:ARG:NH1	2.82	0.43
4:D:27:SER:O	4:D:28:PRO:C	2.62	0.43
4:D:79:GLU:OE1	4:D:79:GLU:HA	2.18	0.43
5:E:11:ARG:HD3	5:E:22:PHE:CG	2.53	0.43
8:H:68:ARG:HG2	8:H:68:ARG:NH1	2.34	0.43
9:I:47:GLU:N	9:I:48:PRO:CD	2.81	0.43
10:J:10:ASP:OD1	10:J:12:LYS:N	2.48	0.43
13:M:104:THR:O	13:M:105:ASN:C	2.61	0.43
14:N:12:THR:N	14:N:13:PRO:CD	2.82	0.43
15:O:28:VAL:HG12	15:O:84:LEU:CD1	2.48	0.43
1:A:33:A:H2'	1:A:34:C:C6	2.54	0.42
1:A:934:C:C4	1:A:1345:U:C5	3.07	0.42
1:A:1001:A:H61	1:A:1002:G:H1	1.67	0.42
1:A:1223:C:P	19:S:77:ARG:NH1	2.92	0.42
1:A:1441:G:H4'	1:A:1442:G:C5	2.54	0.42
2:B:163:LYS:HD3	2:B:163:LYS:O	2.18	0.42
2:B:183:ASP:CG	2:B:184:THR:N	2.76	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:17:LYS:CE	4:D:32:MET:HB2	2.49	0.42
4:D:63:LEU:C	4:D:63:LEU:HD13	2.43	0.42
4:D:186:ARG:NH1	4:D:187:LEU:HB2	2.34	0.42
15:O:63:ARG:HB2	15:O:63:ARG:HH11	1.83	0.42
20:T:43:GLU:N	20:T:92:LEU:HD12	2.34	0.42
1:A:251:G:H4'	1:A:252:U:O5'	2.18	0.42
1:A:730:G:H3'	1:A:731:G:C5'	2.49	0.42
1:A:862:C:O2'	1:A:863:U:H5'	2.18	0.42
1:A:1337:G:H5''	1:A:1338:G:OP1	2.19	0.42
1:A:1394:A:C6	1:A:1501:C:H4'	2.54	0.42
1:A:1513:A:H2'	1:A:1514:C:C6	2.54	0.42
3:C:11:LEU:O	3:C:15:ARG:O	2.36	0.42
7:G:64:ALA:HB3	7:G:123:LEU:HD23	2.01	0.42
8:H:13:ILE:O	8:H:17:THR:HG23	2.19	0.42
10:J:21:ILE:HG23	10:J:83:LEU:HD22	2.02	0.42
15:O:26:VAL:O	15:O:29:ALA:HB3	2.19	0.42
16:P:28:ARG:NH1	16:P:29:ASP:OD1	2.51	0.42
16:P:40:ASP:HB3	16:P:48:TRP:HB2	2.01	0.42
18:R:31:GLU:CD	18:R:31:GLU:N	2.66	0.42
18:R:32:THR:HG23	18:R:68:GLU:H	1.84	0.42
1:A:443:C:O2'	1:A:444:C:H5'	2.20	0.42
1:A:620:C:C6	4:D:134:LEU:HD13	2.53	0.42
1:A:1126:U:C6	1:A:1280:A:N7	2.87	0.42
3:C:205:GLU:O	3:C:207:ILE:N	2.52	0.42
4:D:28:PRO:O	4:D:29:LYS:CG	2.61	0.42
4:D:149:GLU:C	4:D:151:SER:H	2.28	0.42
4:D:154:LEU:HB2	4:D:157:ILE:HG12	2.01	0.42
15:O:30:LEU:HD12	15:O:30:LEU:N	2.34	0.42
18:R:4:LYS:O	18:R:5:ALA:CB	2.67	0.42
1:A:162:A:C2'	1:A:163:C:H5'	2.48	0.42
1:A:190:U:H3	20:T:98:SER:HB2	1.84	0.42
1:A:457:C:H2'	1:A:458:C:H6	1.84	0.42
1:A:649:G:H5'	1:A:649:G:C8	2.52	0.42
1:A:1019:C:H2'	1:A:1020:U:O4'	2.19	0.42
1:A:1176:A:H2'	1:A:1177:G:C8	2.54	0.42
1:A:1244:C:C2'	1:A:1245:A:C5'	2.82	0.42
1:A:1477:C:H2'	1:A:1478:C:C6	2.54	0.42
2:B:108:ARG:HH12	2:B:112:LEU:HG	1.80	0.42
4:D:172:TRP:HB2	4:D:186:ARG:O	2.19	0.42
5:E:133:GLU:O	5:E:137:GLN:HG3	2.19	0.42
7:G:145:GLU:C	7:G:147:ASN:N	2.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:4:ASP:OD1	8:H:85:ARG:NH1	2.52	0.42
9:I:12:ALA:CB	9:I:66:GLY:O	2.68	0.42
14:N:7:GLU:O	14:N:9:ALA:N	2.52	0.42
15:O:63:ARG:HB2	15:O:63:ARG:NH1	2.34	0.42
19:S:40:VAL:H	19:S:43:MET:HE3	1.84	0.42
1:A:162:A:H2'	1:A:163:C:H5'	2.02	0.42
1:A:328:C:H4'	1:A:329:A:H5''	2.00	0.42
1:A:765:G:N1	1:A:812:C:H2'	2.32	0.42
1:A:1419:G:H1	1:A:1481:U:H3	1.67	0.42
2:B:47:ARG:NH1	2:B:193:TYR:HD1	2.18	0.42
2:B:110:GLU:HA	2:B:113:GLU:OE1	2.20	0.42
4:D:169:VAL:HG22	4:D:170:GLY:H	1.85	0.42
6:F:35:ALA:HA	6:F:67:MET:HB3	2.01	0.42
9:I:27:VAL:HG21	9:I:32:PHE:HD1	1.84	0.42
9:I:126:LYS:CD	9:I:126:LYS:N	2.81	0.42
11:K:12:HIS:CD2	11:K:12:HIS:O	2.73	0.42
13:M:10:ARG:C	13:M:12:LYS:H	2.28	0.42
17:Q:75:LEU:HD23	17:Q:76:VAL:H	1.84	0.42
19:S:21:LEU:HD22	19:S:27:LYS:HD2	2.01	0.42
19:S:35:ARG:HB2	19:S:71:GLY:CA	2.50	0.42
19:S:79:TYR:CG	19:S:80:ARG:N	2.88	0.42
1:A:58:C:O2'	1:A:59:A:H5'	2.20	0.42
1:A:189(K):U:H2'	1:A:189(L):G:C8	2.55	0.42
1:A:437:U:O2'	4:D:122:HIS:CD2	2.73	0.42
1:A:707:C:H2'	1:A:708:C:C6	2.55	0.42
1:A:976:G:H4'	1:A:977:A:OP1	2.19	0.42
1:A:1087:G:H2'	1:A:1088:G:C8	2.54	0.42
1:A:1168:A:O2'	1:A:1169:A:P	2.77	0.42
1:A:1178:G:H22	1:A:1180:A:H3'	1.82	0.42
1:A:1308:U:OP1	13:M:96:PRO:HA	2.20	0.42
1:A:1540:U:HO2'	1:A:1541:U:H6	1.65	0.42
2:B:85:PRO:HG3	2:B:149:LEU:HG	2.02	0.42
3:C:51:LEU:H	3:C:51:LEU:HD23	1.85	0.42
3:C:187:LEU:HD11	3:C:194:VAL:HG11	2.01	0.42
3:C:190:THR:HB	3:C:193:GLY:O	2.20	0.42
7:G:49:ILE:HG23	7:G:124:MET:HE3	2.00	0.42
7:G:113:ARG:HG2	7:G:113:ARG:NH1	2.31	0.42
8:H:46:LYS:N	8:H:64:LYS:HG3	2.35	0.42
9:I:45:ALA:HB1	9:I:76:ILE:HG22	2.02	0.42
12:L:7:VAL:HG22	17:Q:28:HIS:CD2	2.54	0.42
12:L:51:VAL:HG13	12:L:63:THR:HG23	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:28:ARG:HH22	14:N:40:ARG:HH12	1.67	0.42
16:P:52:ASP:OD1	16:P:52:ASP:O	2.37	0.42
19:S:43:MET:O	19:S:44:VAL:C	2.63	0.42
1:A:103:C:P	20:T:10:ARG:HH11	2.42	0.42
1:A:281:G:H4'	1:A:282:A:OP1	2.18	0.42
1:A:537:G:OP1	12:L:109:ARG:NH2	2.49	0.42
1:A:1182:G:O2'	1:A:1183:A:OP2	2.33	0.42
1:A:1189:C:H5'	1:A:1189:C:C6	2.43	0.42
1:A:1234:C:O2'	1:A:1235:U:H5'	2.19	0.42
1:A:1270:C:O2'	1:A:1271:G:H5'	2.20	0.42
1:A:1495:U:H2'	1:A:1496:C:C6	2.54	0.42
2:B:17:ARG:NH1	2:B:185:ASP:HB3	2.34	0.42
2:B:225:GLU:HB3	2:B:226:PRO:CD	2.50	0.42
4:D:145:ILE:N	4:D:145:ILE:CD1	2.80	0.42
8:H:10:LEU:HD22	8:H:83:ILE:HD11	2.01	0.42
8:H:51:VAL:HG12	8:H:52:ASP:N	2.35	0.42
10:J:25:ALA:C	10:J:27:ARG:N	2.77	0.42
11:K:4:VAL:HG23	11:K:67:MET:HG2	2.01	0.42
11:K:111:PRO:HG2	11:K:116:ARG:HG2	2.01	0.42
12:L:81:ILE:HG23	12:L:94:TYR:HB3	2.02	0.42
14:N:28:ARG:HG2	14:N:39:CYS:CB	2.50	0.42
15:O:44:VAL:O	15:O:45:HIS:C	2.59	0.42
18:R:32:THR:C	18:R:34:LYS:N	2.78	0.42
19:S:16:GLU:HG3	19:S:16:GLU:O	2.18	0.42
19:S:41:PRO:C	19:S:43:MET:N	2.74	0.42
20:T:23:LYS:O	20:T:27:LYS:HG3	2.20	0.42
20:T:77:LEU:O	20:T:81:VAL:HG23	2.20	0.42
1:A:41:G:H2'	1:A:42:G:H8	1.85	0.42
1:A:265:G:H2'	1:A:267:C:H5	1.84	0.42
1:A:620:C:C1'	4:D:134:LEU:HD13	2.50	0.42
1:A:857:C:H2'	1:A:858:G:O4'	2.20	0.42
1:A:913:A:H2'	1:A:914:A:O4'	2.19	0.42
1:A:961:U:H2'	1:A:962:C:H5'	2.01	0.42
1:A:1082:G:C2'	1:A:1083:U:H5'	2.50	0.42
1:A:1123:A:O2'	10:J:36:ILE:HD13	2.18	0.42
1:A:1221:G:O2'	1:A:1222:G:H5'	2.19	0.42
1:A:1256:A:H2'	3:C:26:LYS:NZ	2.35	0.42
1:A:1292:U:P	7:G:40:ARG:NH2	2.89	0.42
1:A:1405:G:O4'	1:A:1519:A:H4'	2.19	0.42
2:B:133:LYS:O	2:B:137:GLU:HG2	2.19	0.42
2:B:161:PRO:CD	2:B:182:ALA:HA	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:34:GLU:C	3:C:36:GLN:N	2.77	0.42
9:I:78:LEU:HD22	9:I:82:ARG:CD	2.50	0.42
18:R:54:THR:O	18:R:55:ILE:C	2.61	0.42
21:V:5:ASP:O	21:V:11:GLY:HA3	2.18	0.42
1:A:189(E):U:O2	1:A:189(E):U:H2'	2.20	0.42
1:A:828:A:H2'	1:A:829:G:O4'	2.20	0.42
1:A:1064:G:H1'	1:A:1190:G:H21	1.85	0.42
1:A:1300:G:HO2'	1:A:1301:U:H6	1.65	0.42
1:A:1328:C:O2'	1:A:1329:A:H5'	2.19	0.42
2:B:69:LYS:C	2:B:71:ALA:H	2.26	0.42
5:E:78:VAL:HG22	5:E:137:GLN:HE21	1.83	0.42
6:F:45:LEU:HD22	6:F:45:LEU:H	1.85	0.42
9:I:126:LYS:C	9:I:127:ARG:O	2.61	0.42
10:J:53:LYS:HG3	10:J:54:HIS:N	2.35	0.42
13:M:64:LYS:HG3	13:M:68:GLU:OE2	2.20	0.42
13:M:92:ARG:HE	13:M:92:ARG:HB2	1.62	0.42
15:O:31:LEU:O	15:O:35:ILE:HG12	2.19	0.42
17:Q:5:LEU:HB2	17:Q:58:ILE:HG22	2.01	0.42
20:T:69:ALA:O	20:T:73:ARG:HG3	2.20	0.42
1:A:91:C:H2'	1:A:92:C:H6	1.85	0.42
1:A:309:G:H1'	1:A:608:A:C2	2.54	0.42
1:A:572:A:N3	1:A:917:G:H1'	2.35	0.42
1:A:952:U:O4	13:M:103:ARG:HD3	2.20	0.42
1:A:977:A:O2'	1:A:978:A:H5'	2.18	0.42
2:B:48:THR:HG21	2:B:195:ILE:HD11	2.01	0.42
3:C:7:ILE:HD12	3:C:15:ARG:NE	2.35	0.42
3:C:16:ASP:HB3	3:C:20:ARG:HH12	1.84	0.42
3:C:149:LYS:HE2	3:C:151:ILE:HD11	2.01	0.42
3:C:178:ARG:HG2	3:C:206:VAL:HA	2.00	0.42
3:C:178:ARG:HD3	3:C:206:VAL:HG22	2.02	0.42
7:G:19:ASP:OD1	7:G:21:LEU:HB3	2.20	0.42
9:I:22:ASN:ND2	9:I:22:ASN:C	2.76	0.42
9:I:76:ILE:O	9:I:80:ILE:HG12	2.20	0.42
9:I:96:LYS:HB2	9:I:97:PRO:HD3	2.01	0.42
17:Q:52:LEU:C	17:Q:54:ASP:H	2.28	0.42
1:A:255:G:O6	1:A:266:G:O6	2.38	0.41
1:A:274:A:H4'	1:A:275:G:OP1	2.20	0.41
1:A:372:C:O2'	1:A:373:A:OP2	2.35	0.41
1:A:629:G:H2'	1:A:630:G:O4'	2.20	0.41
1:A:958:A:C6	1:A:959:A:N1	2.88	0.41
1:A:967:C:H4'	9:I:127:ARG:NE	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1303:C:N4	1:A:1304:G:C6	2.88	0.41
2:B:77:MET:HE2	2:B:229:SER:HA	2.01	0.41
2:B:80:GLU:C	2:B:82:ALA:H	2.27	0.41
2:B:161:PRO:HG3	2:B:182:ALA:CB	2.50	0.41
3:C:59:ALA:HB3	3:C:62:ASN:HD22	1.85	0.41
4:D:63:LEU:HB2	4:D:197:VAL:HG11	2.01	0.41
5:E:8:LEU:HD13	5:E:8:LEU:O	2.20	0.41
6:F:25:ILE:HD12	6:F:25:ILE:N	2.09	0.41
7:G:27:ASN:HA	7:G:30:MET:HE2	2.02	0.41
11:K:60:LYS:HA	11:K:63:MET:HE3	2.02	0.41
11:K:81:ARG:CD	18:R:73:LYS:HE2	2.50	0.41
12:L:52:ALA:HB2	12:L:66:ILE:HD11	2.01	0.41
12:L:82:ARG:HG3	12:L:82:ARG:NH1	2.32	0.41
13:M:95:LEU:C	13:M:109:ARG:HH11	2.28	0.41
14:N:16:LYS:C	14:N:18:ARG:H	2.26	0.41
16:P:67:THR:HG22	16:P:68:ASP:N	2.35	0.41
19:S:21:LEU:CD1	19:S:30:ILE:HD11	2.50	0.41
1:A:665:A:N3	1:A:732:C:H2'	2.35	0.41
1:A:977:A:H8	1:A:982:U:O4	2.03	0.41
1:A:1145:C:H4'	1:A:1146:A:O5'	2.20	0.41
2:B:15:ARG:HH11	2:B:17:ARG:CG	2.33	0.41
4:D:110:ALA:HB3	4:D:116:ALA:HB2	2.01	0.41
5:E:94:THR:HG22	5:E:97:ILE:HD13	2.02	0.41
5:E:145:GLU:O	5:E:149:LYS:HG3	2.21	0.41
6:F:4:TYR:HD1	6:F:92:LYS:HA	1.85	0.41
9:I:39:LEU:O	9:I:40:VAL:C	2.64	0.41
10:J:13:THR:O	10:J:15:ASP:N	2.53	0.41
10:J:51:PRO:O	10:J:52:PHE:C	2.63	0.41
10:J:85:THR:N	10:J:86:LEU:HD12	2.35	0.41
12:L:82:ARG:HD3	12:L:97:VAL:HG22	2.02	0.41
13:M:74:ALA:O	13:M:78:LYS:HB2	2.20	0.41
15:O:86:ILE:CG2	15:O:87:ARG:N	2.64	0.41
17:Q:39:LYS:HG3	17:Q:40:LYS:N	2.34	0.41
1:A:563:A:H2'	1:A:567:G:C8	2.55	0.41
1:A:998:G:H2'	1:A:999:C:H5''	2.03	0.41
1:A:1020:U:O2'	1:A:1021:G:H5'	2.20	0.41
1:A:1128:C:O2'	1:A:1130:A:C8	2.68	0.41
1:A:1470:G:O2'	1:A:1471:G:H5'	2.21	0.41
2:B:10:HIS:HB2	2:B:11:PHE:H	1.52	0.41
2:B:52:ILE:HD11	2:B:179:ILE:HG21	2.02	0.41
2:B:53:GLU:CB	2:B:215:LEU:HD11	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:91:TRP:HZ3	2:B:170:GLU:OE2	2.03	0.41
2:B:95:MET:C	2:B:96:LEU:HD12	2.45	0.41
6:F:13:ASN:O	6:F:14:LEU:HD23	2.20	0.41
10:J:23:GLU:C	10:J:25:ALA:N	2.75	0.41
13:M:5:GLY:O	13:M:7:GLU:HG2	2.20	0.41
20:T:2:ASN:C	20:T:3:LEU:HD23	2.45	0.41
1:A:116:A:H8	1:A:116:A:O5'	2.03	0.41
1:A:456:C:H2'	1:A:457:C:C6	2.55	0.41
1:A:686:U:O4	1:A:703:G:H1'	2.20	0.41
1:A:769:G:H4'	1:A:1513:A:H4'	2.02	0.41
1:A:1009:G:O2'	1:A:1010:G:H5'	2.20	0.41
1:A:1044:A:H2'	1:A:1045:C:C5'	2.50	0.41
1:A:1145:C:O2'	1:A:1146:A:P	2.79	0.41
1:A:1217:C:H2'	1:A:1218:C:O4'	2.21	0.41
2:B:210:SER:OG	2:B:211:ARG:N	2.53	0.41
5:E:88:LYS:O	5:E:114:ILE:HD13	2.21	0.41
7:G:49:ILE:O	7:G:53:THR:HB	2.20	0.41
7:G:50:GLN:O	7:G:53:THR:O	2.38	0.41
13:M:5:GLY:O	13:M:6:VAL:C	2.63	0.41
15:O:1:PRO:C	15:O:2:ILE:HD12	2.44	0.41
17:Q:77:GLU:O	17:Q:77:GLU:HG3	2.20	0.41
1:A:473:G:C2'	1:A:474:G:H5'	2.51	0.41
1:A:731:G:H5'	1:A:766:A:H4'	2.03	0.41
1:A:1123:A:O3'	10:J:34:GLY:HA3	2.20	0.41
1:A:1221:G:O3'	19:S:76:THR:HG21	2.21	0.41
1:A:1474:G:C2'	1:A:1475:G:C5'	2.94	0.41
1:A:1494:G:OP1	26:A:2733:3TS:NAC	2.51	0.41
26:A:2733:3TS:H4'	26:A:2733:3TS:OAX	2.21	0.41
2:B:158:VAL:HG11	2:B:161:PRO:HA	2.02	0.41
3:C:78:ARG:C	3:C:80:GLY:H	2.29	0.41
3:C:119:VAL:O	3:C:123:ILE:HG13	2.21	0.41
7:G:22:VAL:HG12	7:G:26:ILE:CD1	2.51	0.41
15:O:38:LEU:HD13	15:O:38:LEU:O	2.20	0.41
1:A:491:G:O2'	1:A:492:G:H5'	2.19	0.41
1:A:642:A:C6	1:A:643:C:C4	3.08	0.41
1:A:663:A:H5'	1:A:836:G:OP1	2.19	0.41
1:A:1113:C:O5'	1:A:1113:C:H6	2.03	0.41
2:B:76:ARG:O	2:B:80:GLU:HG3	2.21	0.41
4:D:130:ARG:HG3	4:D:130:ARG:NH1	2.35	0.41
7:G:92:PRO:HA	7:G:95:GLN:HE21	1.84	0.41
13:M:32:ALA:HA	13:M:58:TYR:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:83:ILE:CG2	19:S:65:MET:HB3	2.51	0.41
14:N:4:ALA:O	14:N:7:GLU:CG	2.69	0.41
16:P:1:MET:HE2	16:P:1:MET:HB3	1.69	0.41
18:R:68:GLU:HA	18:R:68:GLU:OE1	2.21	0.41
1:A:801:U:O2'	1:A:802:A:H5'	2.21	0.41
1:A:832:C:O2'	1:A:833:U:H5'	2.21	0.41
1:A:933:G:OP2	7:G:2:ARG:HB3	2.20	0.41
1:A:953:G:C1'	13:M:124:ARG:HA	2.48	0.41
3:C:10:ARG:NH1	3:C:176:THR:O	2.54	0.41
4:D:186:ARG:HH22	4:D:187:LEU:CG	2.33	0.41
5:E:72:ILE:HD12	5:E:138:LEU:CD1	2.51	0.41
7:G:43:TYR:O	7:G:46:CYS:N	2.54	0.41
8:H:12:ARG:NH1	8:H:27:PRO:HD3	2.36	0.41
9:I:80:ILE:O	9:I:84:LEU:HB2	2.21	0.41
10:J:6:LEU:O	10:J:67:ASN:HA	2.21	0.41
11:K:38:ILE:HD11	11:K:54:ALA:CA	2.51	0.41
13:M:47:LEU:HB3	13:M:52:VAL:HG23	2.01	0.41
18:R:1:PRO:HG2	18:R:2:SER:H	1.86	0.41
19:S:62:THR:H	19:S:65:MET:CG	2.34	0.41
1:A:168:G:O2'	1:A:169:C:H5'	2.21	0.41
1:A:811:C:O2'	1:A:901:A:N1	2.48	0.41
1:A:1409:C:O2'	1:A:1410:G:H5'	2.21	0.41
1:A:1491:G:H5''	12:L:42:LYS:HB3	2.01	0.41
2:B:81:ARG:O	2:B:82:ALA:CB	2.67	0.41
3:C:153:SER:HB3	3:C:196:GLY:H	1.84	0.41
8:H:114:THR:C	8:H:116:LYS:N	2.79	0.41
9:I:3:TYR:CD1	9:I:3:TYR:N	2.89	0.41
9:I:41:ARG:O	9:I:42:ALA:C	2.64	0.41
13:M:109:ARG:HH11	13:M:109:ARG:CG	2.34	0.41
1:A:32:A:H2'	1:A:33:A:C8	2.56	0.41
1:A:191:G:O2'	1:A:192:U:H5'	2.21	0.41
1:A:685:G:C2	1:A:686:U:C4	3.09	0.41
1:A:724:G:O2'	1:A:725:G:H5'	2.21	0.41
1:A:812:C:OP1	1:A:903:G:H1'	2.21	0.41
1:A:1113:C:H4'	3:C:13:ILE:HD11	2.02	0.41
1:A:1226:C:N4	13:M:103:ARG:HG3	2.35	0.41
1:A:1307:U:H2'	1:A:1308:U:C6	2.56	0.41
1:A:1316:G:H4'	14:N:17:VAL:HG11	2.03	0.41
1:A:1479:C:O2	1:A:1479:C:C2'	2.69	0.41
1:A:1502:A:C2	1:A:1504:G:C2	3.09	0.41
2:B:19:ASN:HD22	2:B:20:PRO:N	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:54:ASP:OD1	2:B:58:ARG:NH2	2.54	0.41
4:D:34:ARG:N	4:D:34:ARG:CD	2.83	0.41
4:D:149:GLU:CD	4:D:149:GLU:N	2.76	0.41
6:F:4:TYR:CE2	6:F:72:VAL:HG21	2.56	0.41
6:F:33:TYR:HB2	6:F:75:LEU:HD23	2.03	0.41
6:F:92:LYS:HE3	6:F:92:LYS:HB2	1.86	0.41
7:G:78:ARG:HH11	7:G:78:ARG:CB	2.11	0.41
10:J:78:LYS:O	10:J:78:LYS:HG3	2.21	0.41
11:K:116:ARG:C	11:K:118:ALA:N	2.79	0.41
13:M:18:LEU:O	13:M:21:ILE:HG13	2.21	0.41
15:O:69:LEU:HD23	15:O:69:LEU:HA	1.90	0.41
16:P:8:ARG:HG2	16:P:8:ARG:HH11	1.86	0.41
16:P:19:ILE:HG22	16:P:36:ILE:HG13	2.03	0.41
18:R:6:LYS:O	18:R:9:ALA:HB3	2.19	0.41
18:R:24:VAL:O	18:R:27:ARG:HB2	2.21	0.41
20:T:9:HIS:CE1	20:T:13:LEU:HD11	2.56	0.41
20:T:46:LEU:O	20:T:47:LYS:C	2.62	0.41
1:A:502:G:H2'	1:A:503:C:C6	2.56	0.41
1:A:559:A:P	5:E:122:ARG:HH22	2.44	0.41
1:A:1088:G:H8	1:A:1088:G:O5'	2.04	0.41
1:A:1160:G:O2'	1:A:1161:C:H5'	2.21	0.41
1:A:1320:C:N3	19:S:35:ARG:HG3	2.36	0.41
1:A:1475:G:H8	1:A:1475:G:H5'	1.85	0.41
3:C:133:ILE:HG21	3:C:166:TRP:O	2.21	0.41
6:F:38:GLU:O	6:F:39:LYS:CB	2.69	0.41
7:G:16:VAL:HG12	7:G:17:TYR:CD1	2.55	0.41
18:R:40:ARG:HB3	18:R:40:ARG:CZ	2.51	0.41
1:A:399:G:H2'	1:A:400:C:C6	2.57	0.40
1:A:437:U:O2'	4:D:122:HIS:HD2	2.04	0.40
1:A:836:G:C6	1:A:851:G:C6	3.09	0.40
1:A:1286:A:C8	1:A:1286:A:C3'	3.05	0.40
1:A:1300:G:C2'	1:A:1301:U:OP2	2.69	0.40
1:A:1366:C:O2'	1:A:1367:C:H5'	2.21	0.40
1:A:1469:G:O2'	1:A:1470:G:H5'	2.20	0.40
2:B:116:PHE:CZ	2:B:133:LYS:HG2	2.56	0.40
4:D:144:GLU:C	4:D:145:ILE:HD12	2.46	0.40
5:E:69:ASN:C	5:E:69:ASN:HD22	2.28	0.40
6:F:10:LEU:HD11	6:F:59:TYR:HD2	1.85	0.40
9:I:113:TYR:CE1	10:J:57:SER:O	2.74	0.40
10:J:29:GLY:CA	10:J:76:ASN:ND2	2.84	0.40
12:L:69:GLU:OE1	12:L:69:GLU:HA	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:17:PHE:CD1	15:O:17:PHE:C	2.98	0.40
16:P:67:THR:CG2	16:P:68:ASP:N	2.84	0.40
17:Q:14:MET:HB2	17:Q:17:THR:HB	2.03	0.40
17:Q:21:LEU:HD13	17:Q:40:LYS:HG2	2.02	0.40
17:Q:62:ARG:O	17:Q:63:PRO:C	2.64	0.40
1:A:84:U:H2'	1:A:88:A:O4'	2.21	0.40
1:A:182:U:O4	1:A:183:G:N3	2.53	0.40
1:A:279:A:H4'	1:A:281:G:C8	2.56	0.40
1:A:909:A:H2'	1:A:910:C:O4'	2.21	0.40
1:A:976:G:N7	1:A:1358:U:N3	2.69	0.40
1:A:1053:G:H4'	1:A:1054:C:H5'	2.02	0.40
1:A:1272:G:O2'	1:A:1273:G:H5'	2.21	0.40
1:A:1309:G:C2'	1:A:1310:G:H5''	2.51	0.40
2:B:6:GLU:OE1	2:B:9:VAL:HG21	2.21	0.40
2:B:191:VAL:CB	2:B:194:ILE:HG13	2.51	0.40
3:C:25:LYS:H	3:C:25:LYS:HZ2	1.62	0.40
3:C:106:GLN:O	3:C:107:ASN:HB3	2.20	0.40
4:D:5:GLY:O	4:D:6:PRO:C	2.64	0.40
1:A:229:U:O2'	1:A:230:G:H5'	2.22	0.40
1:A:1124:G:O2'	1:A:1145:C:N4	2.54	0.40
1:A:1182:G:C4'	1:A:1183:A:H5'	2.40	0.40
2:B:114:ALA:C	2:B:116:PHE:H	2.29	0.40
4:D:30:CYS:C	4:D:32:MET:N	2.79	0.40
8:H:86:ILE:HG12	8:H:135:CYS:HA	2.02	0.40
8:H:90:GLY:O	8:H:91:ARG:CB	2.69	0.40
9:I:113:TYR:C	9:I:115:LYS:H	2.30	0.40
18:R:43:LEU:HD11	18:R:51:LEU:HD22	2.02	0.40
20:T:84:LEU:C	20:T:86:GLU:N	2.79	0.40
1:A:16:A:N1	1:A:919:A:H2	2.18	0.40
1:A:403:C:OP1	4:D:135:PRO:HD2	2.21	0.40
1:A:764:C:H2'	1:A:765:G:O4'	2.22	0.40
1:A:952:U:O2'	1:A:953:G:H5'	2.21	0.40
1:A:998:G:H2'	1:A:999:C:C5'	2.51	0.40
5:E:75:GLU:HA	5:E:87:LEU:O	2.20	0.40
6:F:94:GLN:HB3	18:R:17:ARG:NH1	2.36	0.40
7:G:64:ALA:HB1	7:G:126:ALA:HB3	2.03	0.40
11:K:17:ASN:ND2	11:K:45:LYS:CD	2.83	0.40
11:K:81:ARG:HD3	18:R:73:LYS:HE2	2.03	0.40
14:N:7:GLU:OE1	14:N:8:LYS:N	2.54	0.40
15:O:35:ILE:HD11	15:O:58:MET:CB	2.50	0.40
15:O:35:ILE:HD11	15:O:58:MET:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:37:ALA:HB2	20:T:81:VAL:HG13	2.03	0.40
20:T:87:ALA:O	20:T:88:ALA:CB	2.68	0.40
1:A:186:C:H2'	1:A:187:C:C6	2.57	0.40
1:A:485:G:O2'	1:A:486:U:C6	2.73	0.40
1:A:953:G:H1'	13:M:124:ARG:CA	2.49	0.40
1:A:1128:C:O2'	1:A:1129:C:OP1	2.40	0.40
1:A:1135:U:O2	1:A:1135:U:C2'	2.67	0.40
2:B:91:TRP:HZ2	2:B:96:LEU:CD1	2.33	0.40
3:C:94:THR:HG23	3:C:94:THR:O	2.22	0.40
4:D:14:GLU:O	4:D:16:VAL:HG23	2.21	0.40
7:G:49:ILE:CG2	7:G:60:VAL:HG21	2.52	0.40
7:G:119:ILE:N	7:G:119:ILE:CD1	2.85	0.40
7:G:142:ARG:O	7:G:146:ALA:HB2	2.21	0.40
11:K:63:MET:C	11:K:65:TYR:N	2.79	0.40
11:K:72:VAL:HB	11:K:98:ILE:HA	2.04	0.40
13:M:66:GLU:CG	13:M:67:GLY:H	2.19	0.40
16:P:28:ARG:HG2	16:P:28:ARG:NH1	2.34	0.40
19:S:41:PRO:HA	19:S:44:VAL:HG23	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	233/256 (91%)	168 (72%)	40 (17%)	25 (11%)	0	2
3	C	205/239 (86%)	139 (68%)	48 (23%)	18 (9%)	0	3
4	D	206/208 (99%)	167 (81%)	29 (14%)	10 (5%)	1	10
5	E	149/161 (92%)	141 (95%)	5 (3%)	3 (2%)	6	28
6	F	99/101 (98%)	83 (84%)	15 (15%)	1 (1%)	12	45
7	G	153/155 (99%)	115 (75%)	31 (20%)	7 (5%)	2	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	H	136/138 (99%)	120 (88%)	15 (11%)	1 (1%)	18	53
9	I	125/128 (98%)	95 (76%)	14 (11%)	16 (13%)	0	1
10	J	97/104 (93%)	67 (69%)	14 (14%)	16 (16%)	0	0
11	K	117/129 (91%)	91 (78%)	19 (16%)	7 (6%)	1	7
12	L	123/132 (93%)	98 (80%)	17 (14%)	8 (6%)	1	5
13	M	123/126 (98%)	88 (72%)	20 (16%)	15 (12%)	0	1
14	N	58/60 (97%)	40 (69%)	13 (22%)	5 (9%)	0	3
15	O	86/88 (98%)	72 (84%)	13 (15%)	1 (1%)	10	40
16	P	82/88 (93%)	73 (89%)	7 (8%)	2 (2%)	4	24
17	Q	102/104 (98%)	86 (84%)	10 (10%)	6 (6%)	1	7
18	R	71/88 (81%)	62 (87%)	7 (10%)	2 (3%)	4	21
19	S	79/92 (86%)	53 (67%)	20 (25%)	6 (8%)	1	4
20	T	97/106 (92%)	74 (76%)	15 (16%)	8 (8%)	0	3
21	V	23/26 (88%)	19 (83%)	3 (13%)	1 (4%)	2	12
All	All	2364/2529 (94%)	1851 (78%)	355 (15%)	158 (7%)	1	5

All (158) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	12	GLY
2	B	18	TRP
2	B	117	ALA
3	C	14	THR
3	C	15	ARG
3	C	100	LEU
3	C	153	SER
4	D	28	PRO
4	D	35	ARG
4	D	174	SER
7	G	6	ALA
7	G	32	ASP
8	H	91	ARG
9	I	10	LYS
9	I	22	ASN
9	I	30	GLN
9	I	42	ALA
9	I	57	ARG

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Mol	Chain	Res	Type
9	I	117	LYS
9	I	126	LYS
10	J	32	VAL
10	J	52	PHE
10	J	88	LEU
12	L	23	LEU
12	L	76	HIS
13	M	3	ILE
13	M	22	TYR
13	M	66	GLU
14	N	21	THR
16	P	83	GLU
17	Q	79	GLY
17	Q	80	ARG
19	S	5	LYS
19	S	8	VAL
2	B	3	GLU
2	B	5	LEU
2	B	9	VAL
2	B	11	PHE
2	B	14	GLU
2	B	82	ALA
2	B	223	VAL
3	C	75	VAL
3	C	87	ARG
3	C	145	ALA
3	C	155	ARG
3	C	206	VAL
4	D	29	LYS
4	D	89	GLY
5	E	149	LYS
6	F	39	LYS
7	G	66	GLU
9	I	54	ALA
9	I	118	ALA
10	J	28	SER
10	J	70	VAL
11	K	118	ALA
12	L	24	LYS
12	L	25	GLY
13	M	5	GLY
13	M	23	GLY

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Mol	Chain	Res	Type
13	M	35	LYS
13	M	105	ASN
13	M	123	PRO
15	O	86	ILE
17	Q	11	SER
18	R	72	ARG
19	S	42	GLU
19	S	80	ARG
20	T	89	GLY
20	T	92	LEU
20	T	95	GLY
21	V	3	LYS
2	B	17	ARG
2	B	70	GLN
2	B	71	ALA
3	C	46	LEU
3	C	180	ASN
4	D	30	CYS
9	I	41	ARG
10	J	37	PRO
10	J	53	LYS
10	J	58	ARG
11	K	2	ARG
11	K	3	GLN
11	K	79	ALA
13	M	4	ALA
13	M	37	GLY
14	N	8	LYS
17	Q	52	LEU
17	Q	103	LYS
19	S	4	LEU
20	T	87	ALA
20	T	91	PRO
2	B	4	LEU
2	B	15	ARG
2	B	57	MET
2	B	77	MET
2	B	123	GLU
3	C	21	TRP
3	C	60	ALA
3	C	80	GLY
5	E	18	GLY

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Mol	Chain	Res	Type
7	G	65	VAL
9	I	23	GLY
9	I	43	VAL
10	J	34	GLY
10	J	38	LEU
10	J	55	LYS
10	J	71	ASP
11	K	80	GLY
11	K	108	GLY
13	M	31	GLU
16	P	27	LYS
18	R	5	ALA
19	S	23	ALA
20	T	4	SER
2	B	2	LYS
2	B	124	ARG
2	B	149	LEU
3	C	3	LYS
3	C	99	ALA
4	D	4	ILE
4	D	8	CYS
4	D	196	PRO
7	G	61	PHE
7	G	148	ARG
9	I	40	VAL
10	J	25	ALA
10	J	39	PRO
10	J	75	PRO
12	L	26	ALA
12	L	47	ALA
12	L	117	GLY
13	M	11	ASN
13	M	67	GLY
14	N	55	VAL
20	T	90	ALA
3	C	107	ASN
7	G	89	GLU
9	I	99	GLY
10	J	14	LEU
11	K	25	PRO
12	L	75	GLU
13	M	121	LYS

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Mol	Chain	Res	Type
14	N	22	ARG
20	T	2	ASN
2	B	177	PRO
3	C	102	VAL
13	M	6	VAL
2	B	221	GLY
2	B	226	PRO
4	D	87	VAL
9	I	108	VAL
5	E	150	GLY
9	I	52	VAL
17	Q	63	PRO
2	B	159	VAL
14	N	17	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%)	185 (92%)	17 (8%)	10	37
3	C	160/188 (85%)	147 (92%)	13 (8%)	11	38
4	D	180/180 (100%)	170 (94%)	10 (6%)	19	52
5	E	115/122 (94%)	102 (89%)	13 (11%)	5	24
6	F	90/90 (100%)	87 (97%)	3 (3%)	33	67
7	G	126/126 (100%)	119 (94%)	7 (6%)	19	52
8	H	119/119 (100%)	113 (95%)	6 (5%)	22	56
9	I	98/99 (99%)	90 (92%)	8 (8%)	10	37
10	J	88/91 (97%)	81 (92%)	7 (8%)	11	38
11	K	90/99 (91%)	82 (91%)	8 (9%)	9	34
12	L	104/109 (95%)	96 (92%)	8 (8%)	12	40
13	M	100/101 (99%)	86 (86%)	14 (14%)	3	16
14	N	49/49 (100%)	45 (92%)	4 (8%)	10	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	O	78/79 (99%)	73 (94%)	5 (6%)	16	48
16	P	72/74 (97%)	65 (90%)	7 (10%)	8	30
17	Q	96/96 (100%)	89 (93%)	7 (7%)	13	42
18	R	64/77 (83%)	62 (97%)	2 (3%)	35	68
19	S	71/79 (90%)	65 (92%)	6 (8%)	10	36
20	T	76/82 (93%)	66 (87%)	10 (13%)	4	18
21	V	19/21 (90%)	19 (100%)	0	100	100
All	All	1997/2101 (95%)	1842 (92%)	155 (8%)	11	39

All (155) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	3	GLU
2	B	10	HIS
2	B	17	ARG
2	B	19	ASN
2	B	76	ARG
2	B	86	TYR
2	B	92	LEU
2	B	138	ARG
2	B	162	THR
2	B	164	GLU
2	B	172	ARG
2	B	179	ILE
2	B	181	LEU
2	B	194	ILE
2	B	198	ASN
2	B	209	LEU
2	B	218	GLN
3	C	2	ASN
3	C	4	ILE
3	C	25	LYS
3	C	33	LEU
3	C	63	VAL
3	C	103	GLN
3	C	106	GLN
3	C	126	ARG
3	C	138	GLN
3	C	155	ARG
3	C	189	ARG

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Mol	Chain	Res	Type
3	C	191	THR
3	C	195	LEU
4	D	7	VAL
4	D	8	CYS
4	D	28	PRO
4	D	35	ARG
4	D	126	THR
4	D	145	ILE
4	D	155	GLU
4	D	161	LEU
4	D	195	LEU
4	D	198	ASN
5	E	8	LEU
5	E	12	THR
5	E	20	ARG
5	E	30	VAL
5	E	37	VAL
5	E	39	LEU
5	E	62	MET
5	E	76	ILE
5	E	97	ILE
5	E	114	ILE
5	E	117	LYS
5	E	127	ILE
5	E	140	THR
6	F	10	LEU
6	F	25	ILE
6	F	45	LEU
7	G	7	GLU
7	G	10	GLN
7	G	15	LEU
7	G	34	LYS
7	G	112	GLU
7	G	123	LEU
7	G	139	ASP
8	H	2	LEU
8	H	26	VAL
8	H	63	LEU
8	H	84	ARG
8	H	85	ARG
8	H	133	LEU
9	I	13	VAL

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Mol	Chain	Res	Type
9	I	15	ARG
9	I	24	LYS
9	I	28	ASN
9	I	37	GLN
9	I	55	LEU
9	I	78	LEU
9	I	98	LEU
10	J	4	ILE
10	J	39	PRO
10	J	43	ARG
10	J	63	LEU
10	J	71	ASP
10	J	81	GLU
10	J	96	ILE
11	K	19	ILE
11	K	25	PRO
11	K	44	ARG
11	K	70	VAL
11	K	82	GLU
11	K	83	GLN
11	K	99	VAL
11	K	107	ASN
12	L	3	ILE
12	L	23	LEU
12	L	38	THR
12	L	42	LYS
12	L	49	ARG
12	L	51	VAL
12	L	93	ARG
12	L	122	LYS
13	M	13	ARG
13	M	16	VAL
13	M	42	THR
13	M	55	LEU
13	M	80	LEU
13	M	83	ILE
13	M	95	LEU
13	M	101	ARG
13	M	105	ASN
13	M	109	ARG
13	M	114	LYS
13	M	116	VAL

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Mol	Chain	Res	Type
13	M	123	PRO
13	M	124	ARG
14	N	7	GLU
14	N	21	THR
14	N	30	ARG
14	N	43	LEU
15	O	2	ILE
15	O	5	GLU
15	O	33	LEU
15	O	69	LEU
15	O	80	LEU
16	P	1	MET
16	P	2	VAL
16	P	4	ILE
16	P	19	ILE
16	P	42	ARG
16	P	52	ASP
16	P	72	ARG
17	Q	24	ARG
17	Q	33	LYS
17	Q	37	ARG
17	Q	58	ILE
17	Q	73	LEU
17	Q	75	LEU
17	Q	91	ARG
18	R	13	GLU
18	R	23	GLU
19	S	5	LYS
19	S	12	ASP
19	S	19	LEU
19	S	35	ARG
19	S	42	GLU
19	S	61	ILE
20	T	2	ASN
20	T	3	LEU
20	T	6	LEU
20	T	18	ARG
20	T	35	GLN
20	T	50	ARG
20	T	61	LYS
20	T	66	HIS
20	T	68	ASN

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Mol	Chain	Res	Type
20	T	86	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	10	HIS
2	B	19	ASN
2	B	72	GLN
2	B	104	GLN
2	B	129	GLN
2	B	198	ASN
2	B	206	GLN
3	C	2	ASN
3	C	5	HIS
3	C	27	GLN
3	C	30	HIS
3	C	62	ASN
3	C	101	ASN
3	C	103	GLN
3	C	106	GLN
3	C	107	ASN
3	C	109	ASN
3	C	122	GLN
3	C	138	GLN
3	C	175	HIS
4	D	41	GLN
4	D	61	GLN
4	D	73	GLN
4	D	115	GLN
4	D	122	HIS
4	D	159	GLN
4	D	160	ASN
4	D	198	ASN
5	E	69	ASN
5	E	74	HIS
5	E	137	GLN
6	F	7	ASN
6	F	18	GLN
6	F	27	GLN
6	F	32	ASN
6	F	64	GLN
6	F	94	GLN

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Mol	Chain	Res	Type
6	F	100	ASN
7	G	10	GLN
7	G	36	ASN
7	G	55	GLN
7	G	63	GLN
7	G	67	ASN
7	G	83	ASN
7	G	95	GLN
7	G	105	GLN
9	I	22	ASN
9	I	72	GLN
10	J	54	HIS
10	J	60	HIS
10	J	67	ASN
10	J	76	ASN
11	K	12	HIS
11	K	52	GLN
11	K	83	GLN
12	L	45	ASN
12	L	71	HIS
13	M	11	ASN
13	M	39	ASN
13	M	61	ASN
15	O	12	GLN
15	O	36	ASN
16	P	16	HIS
16	P	76	GLN
17	Q	15	GLN
19	S	22	ASN
19	S	52	ASN
19	S	56	HIS
20	T	2	ASN
20	T	9	HIS
20	T	11	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1510/1521 (99%)	272 (18%)	58 (3%)
22	W	3/6 (50%)	0	0
23	Z	14/16 (87%)	2 (14%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	1527/1543 (98%)	274 (17%)	58 (3%)

All (274) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	G
1	A	8	A
1	A	9	G
1	A	32	A
1	A	39	G
1	A	47	C
1	A	48	C
1	A	51	A
1	A	52	G
1	A	60	A
1	A	61	G
1	A	65	U
1	A	69	G
1	A	105	G
1	A	121	C
1	A	131	C
1	A	144	G
1	A	146	G
1	A	147	G
1	A	156	G
1	A	157	G
1	A	173	U
1	A	174	C
1	A	189(E)	U
1	A	189(F)	U
1	A	189(G)	G
1	A	189(H)	G
1	A	195	A
1	A	196	A
1	A	197	A
1	A	202	U
1	A	203	U
1	A	204	U
1	A	216	G
1	A	224	C
1	A	244	U
1	A	247	G

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Mol	Chain	Res	Type
1	A	251	G
1	A	257	G
1	A	258	G
1	A	266	G
1	A	267	C
1	A	272	C
1	A	281	G
1	A	282	A
1	A	289	G
1	A	292	G
1	A	293	G
1	A	305	G
1	A	306	G
1	A	321	A
1	A	328	C
1	A	329	A
1	A	332	G
1	A	345	C
1	A	351	G
1	A	352	C
1	A	353	A
1	A	354	G
1	A	357	G
1	A	367	U
1	A	369	C
1	A	373	A
1	A	381	C
1	A	388	G
1	A	389	A
1	A	397	A
1	A	406	G
1	A	413	G
1	A	414	A
1	A	421	U
1	A	422	C
1	A	423	G
1	A	426	G
1	A	429	U
1	A	430	A
1	A	453	A
1	A	461	A
1	A	481	G

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Mol	Chain	Res	Type
1	A	484	G
1	A	485	G
1	A	486	U
1	A	487	A
1	A	488	C
1	A	496	A
1	A	498	U
1	A	511	C
1	A	517	G
1	A	518	C
1	A	531	U
1	A	532	A
1	A	545	C
1	A	547	A
1	A	548	G
1	A	561	U
1	A	562	C
1	A	564	C
1	A	572	A
1	A	573	A
1	A	576	G
1	A	577	G
1	A	591	U
1	A	596	C
1	A	607	A
1	A	625	G
1	A	631	G
1	A	632	A
1	A	649	G
1	A	653	A
1	A	654	G
1	A	665	A
1	A	687	A
1	A	688	G
1	A	721	G
1	A	723	U
1	A	731	G
1	A	734	G
1	A	751	U
1	A	755	G
1	A	777	A
1	A	793	U

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Mol	Chain	Res	Type
1	A	794	A
1	A	813	U
1	A	817	C
1	A	819	A
1	A	836	G
1	A	840	C
1	A	848	C
1	A	859	A
1	A	865	A
1	A	870	U
1	A	872	A
1	A	873	A
1	A	874	G
1	A	885	G
1	A	896	C
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	951	G
1	A	960	U
1	A	968	A
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	982	U
1	A	983	A
1	A	992	U
1	A	993	G
1	A	996	A
1	A	998	G
1	A	999	C
1	A	1001(A)	G
1	A	1003	G
1	A	1004	A
1	A	1007	C

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Mol	Chain	Res	Type
1	A	1009	G
1	A	1012	U
1	A	1013	G
1	A	1025	U
1	A	1026	G
1	A	1030	C
1	A	1045	C
1	A	1048	G
1	A	1049	U
1	A	1053	G
1	A	1054	C
1	A	1055	A
1	A	1065	U
1	A	1068	G
1	A	1081	G
1	A	1085	U
1	A	1086	U
1	A	1094	G
1	A	1095	U
1	A	1099	G
1	A	1101	A
1	A	1102	A
1	A	1106	G
1	A	1125	U
1	A	1126	U
1	A	1127	G
1	A	1128	C
1	A	1129	C
1	A	1130	A
1	A	1131	G
1	A	1135	U
1	A	1136	U
1	A	1137	C
1	A	1138	G
1	A	1139	G
1	A	1141	C
1	A	1144	G
1	A	1146	A
1	A	1159	U
1	A	1169	A
1	A	1179	A
1	A	1183	A

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Mol	Chain	Res	Type
1	A	1184	G
1	A	1189	C
1	A	1190	G
1	A	1196	U
1	A	1197	G
1	A	1202	G
1	A	1212	U
1	A	1213	A
1	A	1214	C
1	A	1215	G
1	A	1227	A
1	A	1238	A
1	A	1240	U
1	A	1241	G
1	A	1245	A
1	A	1250	A
1	A	1253	G
1	A	1256	A
1	A	1257	U
1	A	1260	C
1	A	1272	G
1	A	1277	C
1	A	1279	A
1	A	1280	A
1	A	1282	C
1	A	1287	A
1	A	1297	C
1	A	1299	A
1	A	1300	G
1	A	1301	U
1	A	1302	U
1	A	1310	G
1	A	1320	C
1	A	1324	A
1	A	1330	U
1	A	1331	G
1	A	1335	C
1	A	1336	C
1	A	1338	G
1	A	1346	A
1	A	1347	G
1	A	1363(A)	A

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Mol	Chain	Res	Type
1	A	1365	G
1	A	1401	G
1	A	1442	G
1	A	1442(B)	A
1	A	1443	G
1	A	1452	C
1	A	1456	G
1	A	1475	G
1	A	1479	C
1	A	1480	G
1	A	1481	U
1	A	1486	G
1	A	1492	A
1	A	1497	G
1	A	1503	A
1	A	1504	G
1	A	1506	U
1	A	1517	G
1	A	1520	G
1	A	1529	G
1	A	1530	G
1	A	1531	A
1	A	1533	C
1	A	1540	U
1	A	1541	U
23	Z	30	G
23	Z	34	G

All (58) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	7	G
1	A	47	C
1	A	51	A
1	A	173	U
1	A	189(E)	U
1	A	189(G)	G
1	A	196	A
1	A	203	U
1	A	250	A
1	A	281	G
1	A	292	G

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Mol	Chain	Res	Type
1	A	305	G
1	A	353	A
1	A	366	C
1	A	372	C
1	A	388	G
1	A	422	C
1	A	429	U
1	A	452	A
1	A	485	G
1	A	495	A
1	A	517	G
1	A	547	A
1	A	572	A
1	A	575	G
1	A	624	C
1	A	631	G
1	A	653	A
1	A	687	A
1	A	733	A
1	A	793	U
1	A	812	C
1	A	819	A
1	A	872	A
1	A	873	A
1	A	884	U
1	A	913	A
1	A	968	A
1	A	974	A
1	A	975	A
1	A	982	U
1	A	1048	G
1	A	1085	U
1	A	1128	C
1	A	1135	U
1	A	1145	C
1	A	1182	G
1	A	1201	A
1	A	1214	C
1	A	1240	U
1	A	1330	U
1	A	1335	C
1	A	1345	U

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Mol	Chain	Res	Type
1	A	1400	C
1	A	1442(A)	G
1	A	1447	A
1	A	1452	C
1	A	1479	C

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 239 ligands modelled in this entry, 238 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
26	3TS	A	2733	24	53,54,54	1.47	10 (18%)	74,79,79	1.11	4 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	3TS	A	2733	24	-	10/23/99/99	0/5/5/5

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	2733	3TS	CAU-CBE	-3.86	1.41	1.50
26	A	2733	3TS	CAO-CBD	3.50	1.44	1.38
26	A	2733	3TS	CAQ-CAO	3.34	1.44	1.38
26	A	2733	3TS	CAN-CBD	2.73	1.43	1.38
26	A	2733	3TS	CAP-CBE	2.62	1.44	1.38
26	A	2733	3TS	CAP-CAN	2.51	1.42	1.38
26	A	2733	3TS	CBX-CBV	2.47	1.57	1.52
26	A	2733	3TS	CAQ-CBE	2.46	1.43	1.38
26	A	2733	3TS	CBK-CBX	2.42	1.58	1.52
26	A	2733	3TS	OAX-CBR	2.18	1.47	1.41

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	2733	3TS	O1'-C1'-O4'	-3.97	107.31	111.37
26	A	2733	3TS	O4-CAU-CBE	3.23	117.31	109.91
26	A	2733	3TS	OAX-CBO-CAR	2.56	110.98	106.07
26	A	2733	3TS	CBX-CBV-CBG	-2.08	107.46	111.31

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
26	A	2733	3TS	NAA-CAR-CBO-OAX
26	A	2733	3TS	NAA-CAR-CBO-CBL
26	A	2733	3TS	CBV-CBX-O1'-C1'
26	A	2733	3TS	CBX-CBV-O1-C1
26	A	2733	3TS	CBK-CBX-O1'-C1'
26	A	2733	3TS	OAX-CBR-O3'-C3'
26	A	2733	3TS	O4'-C1'-O1'-CBX
26	A	2733	3TS	C2'-C1'-O1'-CBX
26	A	2733	3TS	CBG-CBV-O1-C1
26	A	2733	3TS	C4-C5-C6-O6

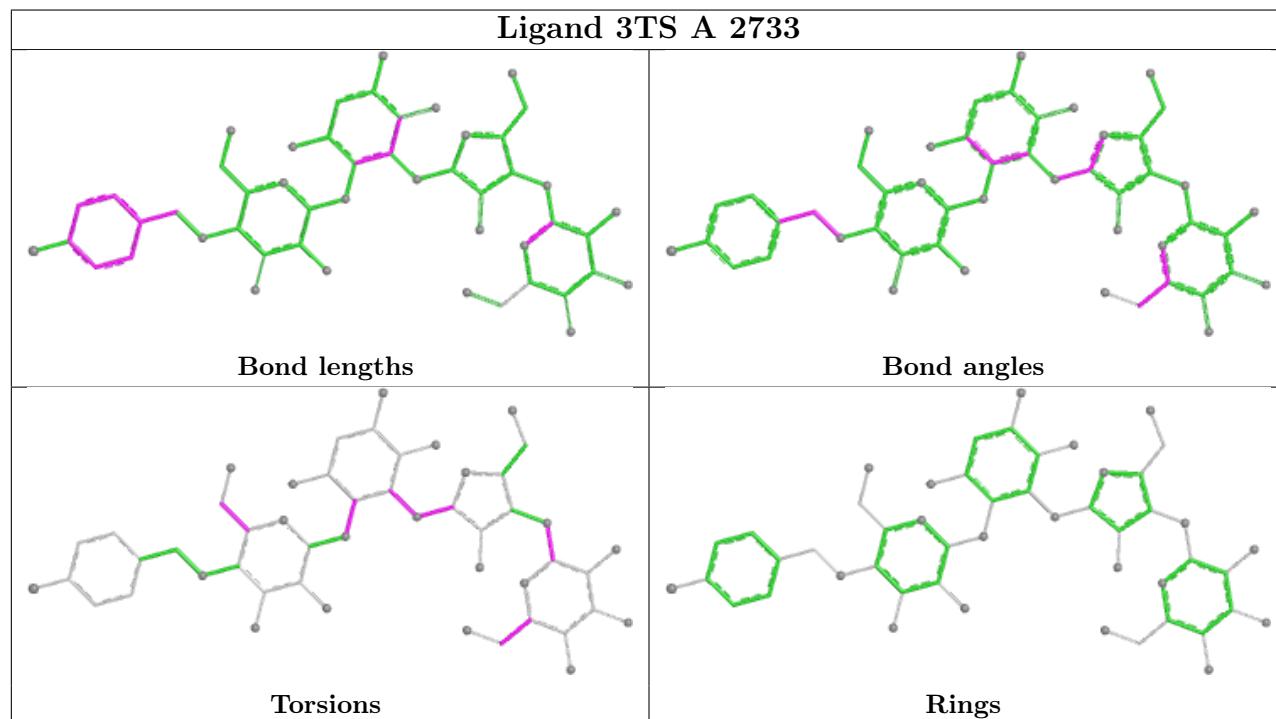
There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	A	2733	3TS	6	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1512/1521 (99%)	0.24	65 (4%) 40 21	45, 72, 141, 193	0
2	B	235/256 (91%)	0.80	27 (11%) 9 6	57, 105, 164, 195	0
3	C	207/239 (86%)	0.79	16 (7%) 19 10	57, 93, 132, 162	0
4	D	208/208 (100%)	0.56	18 (8%) 16 8	54, 81, 136, 191	0
5	E	151/161 (93%)	0.08	5 (3%) 49 28	43, 63, 99, 176	0
6	F	101/101 (100%)	0.59	1 (0%) 79 59	72, 101, 132, 163	0
7	G	155/155 (100%)	0.70	16 (10%) 12 6	60, 95, 152, 191	0
8	H	138/138 (100%)	-0.18	1 (0%) 84 66	38, 60, 89, 144	0
9	I	127/128 (99%)	0.97	18 (14%) 6 4	55, 100, 134, 161	0
10	J	99/104 (95%)	1.68	31 (31%) 1 1	45, 125, 180, 195	0
11	K	119/129 (92%)	0.54	12 (10%) 12 7	44, 77, 127, 174	0
12	L	125/132 (94%)	0.31	3 (2%) 59 36	39, 69, 113, 181	0
13	M	125/126 (99%)	0.96	18 (14%) 6 3	58, 87, 151, 196	0
14	N	60/60 (100%)	1.12	12 (20%) 3 2	58, 83, 110, 157	0
15	O	88/88 (100%)	0.26	1 (1%) 78 57	51, 79, 117, 174	0
16	P	84/88 (95%)	0.09	2 (2%) 59 36	49, 63, 98, 180	0
17	Q	104/104 (100%)	0.48	11 (10%) 11 6	42, 70, 129, 200	0
18	R	73/88 (82%)	0.32	2 (2%) 56 33	57, 86, 163, 193	0
19	S	81/92 (88%)	1.24	13 (16%) 5 3	73, 104, 145, 175	0
20	T	99/106 (93%)	0.55	10 (10%) 12 7	45, 73, 111, 129	0
21	V	25/26 (96%)	0.94	5 (20%) 3 2	56, 72, 113, 137	0
22	W	4/6 (66%)	0.92	1 (25%) 2 1	85, 86, 87, 102	0
23	Z	15/16 (93%)	0.99	1 (6%) 24 12	78, 118, 179, 180	0
All	All	3935/4072 (96%)	0.47	289 (7%) 21 11	38, 79, 146, 200	0

All (289) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	M	123	PRO	11.6
13	M	122	ALA	10.7
19	S	2	ARG	8.8
17	Q	104	ALA	7.6
11	K	79	ALA	7.1
13	M	119	LYS	7.0
19	S	81	GLY	6.9
4	D	1	GLY	6.9
13	M	6	VAL	6.9
10	J	73	ILE	6.8
1	A	1003	G	6.7
13	M	124	ARG	6.6
13	M	8	ILE	6.4
13	M	125	LYS	6.3
5	E	150	GLY	6.2
19	S	1	PRO	5.8
17	Q	103	LYS	5.8
13	M	7	GLU	5.7
8	H	1	MET	5.7
2	B	70	GLN	5.5
1	A	630	G	5.4
4	D	22	GLY	5.3
1	A	1533	C	5.2
1	A	1129	C	5.2
19	S	4	LEU	4.9
10	J	32	VAL	4.9
1	A	1539	C	4.9
20	T	93	ILE	4.9
1	A	1126	U	4.9
17	Q	102	GLY	4.8
14	N	1	ALA	4.6
17	Q	12	ASP	4.6
2	B	83	GLY	4.6
4	D	2	ARG	4.5
1	A	1125	U	4.5
1	A	631	G	4.4
2	B	10	HIS	4.4
7	G	155	TRP	4.3
1	A	1013	G	4.3
1	A	202	U	4.3
9	I	127	ARG	4.2
20	T	5	ALA	4.2

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Mol	Chain	Res	Type	RSRZ
2	B	127	LYS	4.2
1	A	1540	U	4.2
4	D	8	CYS	4.2
4	D	3	TYR	4.2
12	L	24	LYS	4.1
7	G	88	MET	4.1
1	A	1281	U	4.0
19	S	3	SER	4.0
19	S	36	ARG	4.0
1	A	1124	G	4.0
10	J	34	GLY	4.0
17	Q	101	GLY	4.0
23	Z	28	G	4.0
1	A	977	A	3.9
7	G	4	ARG	3.9
1	A	992	U	3.9
13	M	121	LYS	3.8
12	L	61	GLU	3.8
10	J	3	ARG	3.8
14	N	56	ARG	3.7
19	S	52	ASN	3.7
10	J	91	GLY	3.7
10	J	33	SER	3.6
5	E	1	ASP	3.6
10	J	70	VAL	3.6
13	M	120	LYS	3.6
2	B	90	ARG	3.6
11	K	26	ASP	3.6
1	A	991	U	3.5
9	I	126	LYS	3.5
11	K	117	LYS	3.5
13	M	10	ARG	3.5
9	I	6	THR	3.5
14	N	12	THR	3.5
13	M	84	GLY	3.5
4	D	30	CYS	3.4
10	J	68	ARG	3.4
11	K	2	ARG	3.4
9	I	1	GLU	3.4
4	D	186	ARG	3.4
1	A	993	G	3.4
11	K	42	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
7	G	114	ARG	3.3
10	J	71	ASP	3.3
10	J	88	LEU	3.3
21	V	25	LYS	3.3
11	K	41	LYS	3.3
1	A	5	U	3.3
10	J	35	PRO	3.3
9	I	125	SER	3.2
9	I	118	ALA	3.2
1	A	1030(B)	C	3.2
3	C	153	SER	3.2
14	N	31	SER	3.1
9	I	114	GLY	3.1
1	A	1256	A	3.1
9	I	124	TYR	3.1
21	V	6	ARG	3.1
10	J	2	ILE	3.1
1	A	1278	U	3.1
1	A	1001	A	3.1
4	D	28	PRO	3.1
9	I	55	LEU	3.0
1	A	1143	G	3.0
1	A	1190	G	3.0
16	P	83	GLU	3.0
9	I	101	LEU	3.0
7	G	145	GLU	3.0
20	T	3	LEU	3.0
2	B	200	ASP	3.0
10	J	72	ILE	3.0
1	A	1002	G	2.9
19	S	5	LYS	2.9
17	Q	95	GLN	2.9
10	J	40	THR	2.9
10	J	83	LEU	2.9
17	Q	100	ARG	2.9
1	A	1135	U	2.9
10	J	69	LEU	2.9
14	N	10	LYS	2.9
10	J	98	THR	2.9
1	A	1032	G	2.9
13	M	9	PRO	2.9
1	A	204	U	2.9

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Mol	Chain	Res	Type	RSRZ
5	E	151	GLU	2.9
2	B	223	VAL	2.9
1	A	1035	A	2.9
3	C	161	GLN	2.8
9	I	65	ARG	2.8
2	B	4	LEU	2.8
13	M	5	GLY	2.8
1	A	723	U	2.8
1	A	1212	U	2.8
3	C	70	ALA	2.8
21	V	24	ARG	2.8
10	J	99	VAL	2.8
1	A	840	C	2.8
10	J	57	SER	2.8
1	A	1004	A	2.8
7	G	76	SER	2.8
10	J	58	ARG	2.7
10	J	55	LYS	2.7
2	B	5	LEU	2.7
10	J	85	THR	2.7
4	D	34	ARG	2.7
11	K	1	LYS	2.7
1	A	1277	C	2.7
7	G	1	ALA	2.7
14	N	29	ALA	2.7
1	A	1134	G	2.7
10	J	75	PRO	2.7
2	B	217	ILE	2.7
14	N	34	ARG	2.7
2	B	9	VAL	2.7
10	J	36	ILE	2.7
20	T	96	GLY	2.7
1	A	306	G	2.7
4	D	36	PRO	2.6
4	D	48	ARG	2.6
5	E	46	GLU	2.6
3	C	105	VAL	2.6
15	O	1	PRO	2.6
2	B	197	GLY	2.6
3	C	20	ARG	2.6
1	A	1031	G	2.6
9	I	63	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	412	A	2.6
2	B	150	LYS	2.6
3	C	64	ALA	2.6
10	J	1	LYS	2.6
22	W	4	A	2.6
7	G	15	LEU	2.6
1	A	203	U	2.5
1	A	1541	U	2.5
4	D	29	LYS	2.5
3	C	86	LEU	2.5
17	Q	98	SER	2.5
20	T	67	LYS	2.5
3	C	65	VAL	2.5
1	A	1127	G	2.5
9	I	15	ARG	2.5
12	L	25	GLY	2.5
4	D	118	GLN	2.5
6	F	88	VAL	2.5
1	A	1144	G	2.5
20	T	61	LYS	2.5
3	C	1	GLY	2.5
1	A	1130	A	2.4
4	D	168	LYS	2.4
13	M	26	LYS	2.4
1	A	1034	G	2.4
2	B	116	PHE	2.4
13	M	93	ARG	2.4
21	V	9	ARG	2.4
14	N	21	THR	2.4
2	B	134	HIS	2.4
1	A	1054	C	2.4
4	D	32	MET	2.4
1	A	1183	A	2.4
7	G	79	VAL	2.4
9	I	13	VAL	2.4
13	M	105	ASN	2.3
19	S	31	LYS	2.3
3	C	106	GLN	2.3
7	G	25	PHE	2.3
1	A	1018	C	2.3
17	Q	99	LYS	2.3
21	V	10	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
10	J	8	GLY	2.3
19	S	33	TRP	2.3
10	J	84	MET	2.3
1	A	161	A	2.3
14	N	30	ARG	2.3
2	B	202	ILE	2.3
18	R	61	LEU	2.3
2	B	224	VAL	2.3
10	J	95	GLU	2.3
9	I	56	GLY	2.3
19	S	9	PHE	2.3
5	E	149	LYS	2.3
14	N	14	LYS	2.3
20	T	79	ARG	2.3
1	A	1001(A)	G	2.2
1	A	1260	C	2.2
1	A	1282	C	2.2
9	I	8	ARG	2.2
2	B	91	TRP	2.2
1	A	1418	A	2.2
11	K	107	ASN	2.2
10	J	87	ASP	2.2
2	B	117	ALA	2.2
13	M	117	ALA	2.2
11	K	4	VAL	2.2
11	K	119	SER	2.2
1	A	1146	A	2.2
18	R	13	GLU	2.2
19	S	26	GLU	2.2
7	G	81	GLY	2.2
2	B	126	LYS	2.2
16	P	50	LYS	2.2
2	B	130	VAL	2.2
3	C	27	GLN	2.2
4	D	4	ILE	2.2
2	B	232	LEU	2.2
4	D	20	LEU	2.2
4	D	155	GLU	2.2
7	G	72	MET	2.2
3	C	71	LYS	2.2
1	A	143	A	2.2
1	A	1017	G	2.2

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Mol	Chain	Res	Type	RSRZ
11	K	15	TYR	2.1
1	A	1037	C	2.1
19	S	6	LYS	2.1
2	B	125	PRO	2.1
9	I	26	THR	2.1
2	B	194	ILE	2.1
3	C	93	LEU	2.1
11	K	44	ARG	2.1
1	A	470	C	2.1
1	A	1006	C	2.1
20	T	92	LEU	2.1
1	A	1182	G	2.1
1	A	999	C	2.1
7	G	149	ALA	2.1
2	B	87	VAL	2.1
2	B	16	LYS	2.1
3	C	101	ASN	2.1
20	T	66	HIS	2.1
1	A	1043	C	2.1
7	G	136	LYS	2.0
14	N	3	LYS	2.0
14	N	2	ARG	2.0
1	A	532	A	2.0
1	A	1531	A	2.0
2	B	146	PHE	2.0
3	C	206	VAL	2.0
7	G	74	VAL	2.0
1	A	1036	G	2.0
10	J	67	ASN	2.0
3	C	68	HIS	2.0
9	I	60	ALA	2.0
10	J	37	PRO	2.0
17	Q	25	GLN	2.0
1	A	1279	A	2.0
7	G	75	ARG	2.0
17	Q	67	ARG	2.0
20	T	97	LEU	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
24	MG	A	2586	1/1	0.07	0.23	122,122,122,122	0
24	MG	A	2697	1/1	0.45	0.26	94,94,94,94	0
24	MG	A	2637	1/1	0.48	0.61	80,80,80,80	0
24	MG	A	2609	1/1	0.55	0.41	94,94,94,94	0
24	MG	A	2714	1/1	0.55	0.48	81,81,81,81	0
24	MG	A	2607	1/1	0.56	0.38	83,83,83,83	0
24	MG	A	2571	1/1	0.59	0.59	90,90,90,90	0
24	MG	A	2621	1/1	0.64	0.19	75,75,75,75	0
24	MG	A	2703	1/1	0.65	0.29	76,76,76,76	0
24	MG	A	2614	1/1	0.65	0.38	85,85,85,85	0
24	MG	A	2713	1/1	0.67	0.49	90,90,90,90	0
24	MG	A	2552	1/1	0.67	0.25	75,75,75,75	0
24	MG	A	2666	1/1	0.69	0.10	106,106,106,106	0
24	MG	A	3822	1/1	0.69	0.57	83,83,83,83	0
24	MG	A	2690	1/1	0.70	0.33	73,73,73,73	0
24	MG	A	3910	1/1	0.70	0.53	83,83,83,83	0
24	MG	A	2708	1/1	0.71	0.17	64,64,64,64	0
24	MG	A	2727	1/1	0.71	0.35	77,77,77,77	0
25	K	A	2680	1/1	0.71	0.24	113,113,113,113	0
25	K	A	2672	1/1	0.72	0.36	107,107,107,107	0
24	MG	C	1207	1/1	0.72	0.21	66,66,66,66	0
24	MG	A	2555	1/1	0.73	0.34	77,77,77,77	0
24	MG	A	2656	1/1	0.73	0.36	69,69,69,69	0
24	MG	A	2605	1/1	0.73	0.25	55,55,55,55	0
24	MG	A	2573	1/1	0.74	0.24	75,75,75,75	0
24	MG	A	2722	1/1	0.74	0.52	76,76,76,76	0
24	MG	A	2546	1/1	0.74	0.50	94,94,94,94	0
24	MG	A	2702	1/1	0.74	0.18	65,65,65,65	0
24	MG	A	3963	1/1	0.75	0.55	92,92,92,92	0
24	MG	A	3911	1/1	0.75	0.55	83,83,83,83	0
24	MG	A	2575	1/1	0.76	0.40	76,76,76,76	0
24	MG	A	2576	1/1	0.76	0.18	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	K	A	2671	1/1	0.76	0.35	135,135,135,135	0
24	MG	A	3743	1/1	0.76	0.69	98,98,98,98	0
25	K	A	2673	1/1	0.76	0.23	112,112,112,112	0
24	MG	A	3941	1/1	0.76	0.58	84,84,84,84	0
24	MG	G	1156	1/1	0.77	0.29	80,80,80,80	0
24	MG	A	2593	1/1	0.77	0.55	77,77,77,77	0
24	MG	A	2557	1/1	0.77	0.23	67,67,67,67	0
24	MG	A	2661	1/1	0.77	0.23	69,69,69,69	0
24	MG	A	2723	1/1	0.77	0.15	65,65,65,65	0
25	K	A	2683	1/1	0.77	0.13	103,103,103,103	0
24	MG	A	2660	1/1	0.78	0.15	71,71,71,71	0
24	MG	A	2718	1/1	0.78	0.66	85,85,85,85	0
24	MG	A	2636	1/1	0.78	0.30	76,76,76,76	0
24	MG	A	2597	1/1	0.78	0.17	50,50,50,50	0
25	K	A	2675	1/1	0.78	0.19	100,100,100,100	0
24	MG	A	2689	1/1	0.78	0.37	65,65,65,65	0
24	MG	A	2630	1/1	0.78	0.28	76,76,76,76	0
24	MG	A	2628	1/1	0.79	0.17	49,49,49,49	0
24	MG	A	2562	1/1	0.79	0.67	66,66,66,66	0
24	MG	A	2549	1/1	0.80	0.13	61,61,61,61	0
24	MG	A	2612	1/1	0.80	0.26	55,55,55,55	0
24	MG	A	2712	1/1	0.80	0.33	80,80,80,80	0
24	MG	A	2730	1/1	0.80	0.52	84,84,84,84	0
24	MG	A	3923	1/1	0.80	0.80	86,86,86,86	0
24	MG	A	2729	1/1	0.81	0.40	70,70,70,70	0
24	MG	A	2696	1/1	0.81	0.30	76,76,76,76	0
24	MG	A	2732	1/1	0.81	0.43	82,82,82,82	0
24	MG	A	2560	1/1	0.81	0.55	87,87,87,87	0
24	MG	A	2572	1/1	0.81	0.44	164,164,164,164	0
24	MG	A	2547	1/1	0.81	0.66	81,81,81,81	0
24	MG	A	2634	1/1	0.82	0.27	63,63,63,63	0
24	MG	A	2717	1/1	0.82	0.22	66,66,66,66	0
24	MG	A	2595	1/1	0.82	0.35	61,61,61,61	0
24	MG	A	2693	1/1	0.82	0.17	61,61,61,61	0
24	MG	A	2583	1/1	0.82	0.24	49,49,49,49	0
25	K	A	2682	1/1	0.82	0.13	106,106,106,106	0
24	MG	A	2653	1/1	0.82	0.30	76,76,76,76	0
24	MG	A	2598	1/1	0.83	0.27	46,46,46,46	0
24	MG	A	2626	1/1	0.83	0.28	74,74,74,74	0
24	MG	A	2589	1/1	0.83	0.28	88,88,88,88	0
24	MG	A	2565	1/1	0.83	0.36	63,63,63,63	0
24	MG	A	2631	1/1	0.83	0.15	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	MG	A	2620	1/1	0.83	0.23	63,63,63,63	0
25	K	E	1151	1/1	0.83	0.15	101,101,101,101	0
24	MG	A	2619	1/1	0.84	0.36	65,65,65,65	0
24	MG	A	2715	1/1	0.84	0.20	70,70,70,70	0
24	MG	A	2588	1/1	0.84	0.35	74,74,74,74	0
24	MG	A	2551	1/1	0.84	0.13	39,39,39,39	0
25	K	A	2678	1/1	0.84	0.19	97,97,97,97	0
24	MG	A	3954	1/1	0.84	0.61	75,75,75,75	0
24	MG	A	3740	1/1	0.84	0.38	83,83,83,83	0
24	MG	A	2600	1/1	0.84	0.29	76,76,76,76	0
24	MG	A	2596	1/1	0.84	0.29	53,53,53,53	0
24	MG	A	2721	1/1	0.85	0.23	82,82,82,82	0
24	MG	A	2606	1/1	0.85	0.66	77,77,77,77	0
24	MG	A	3909	1/1	0.85	0.52	77,77,77,77	0
24	MG	A	2642	1/1	0.85	0.35	68,68,68,68	0
24	MG	A	2698	1/1	0.85	0.28	76,76,76,76	0
25	K	A	2669	1/1	0.86	0.11	99,99,99,99	0
24	MG	A	2561	1/1	0.86	0.56	74,74,74,74	0
24	MG	A	2577	1/1	0.86	0.28	55,55,55,55	0
24	MG	A	2652	1/1	0.86	0.10	56,56,56,56	0
24	MG	A	2569	1/1	0.86	0.29	61,61,61,61	0
25	K	A	2677	1/1	0.86	0.18	109,109,109,109	0
24	MG	A	2655	1/1	0.86	0.17	73,73,73,73	0
24	MG	A	2608	1/1	0.86	0.31	52,52,52,52	0
24	MG	A	2709	1/1	0.86	0.21	73,73,73,73	0
24	MG	A	2695	1/1	0.86	0.17	54,54,54,54	0
24	MG	L	1127	1/1	0.86	0.31	81,81,81,81	0
24	MG	A	2728	1/1	0.87	0.13	77,77,77,77	0
24	MG	A	2704	1/1	0.87	0.15	62,62,62,62	0
24	MG	A	2706	1/1	0.87	0.26	69,69,69,69	0
24	MG	A	2688	1/1	0.87	0.32	58,58,58,58	0
25	K	A	2676	1/1	0.87	0.18	96,96,96,96	0
24	MG	A	2622	1/1	0.87	0.16	60,60,60,60	0
24	MG	A	2564	1/1	0.87	0.24	51,51,51,51	0
24	MG	A	2545	1/1	0.87	0.17	78,78,78,78	0
24	MG	A	2726	1/1	0.87	0.16	53,53,53,53	0
24	MG	T	1100	1/1	0.87	0.19	70,70,70,70	0
24	MG	A	2567	1/1	0.87	0.31	69,69,69,69	0
26	3TS	A	2733	50/50	0.87	0.17	61,68,89,90	0
24	MG	A	2603	1/1	0.88	0.40	90,90,90,90	0
24	MG	A	2590	1/1	0.88	0.19	43,43,43,43	0
24	MG	A	3749	1/1	0.88	0.35	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	MG	A	2700	1/1	0.88	0.46	73,73,73,73	0
24	MG	A	2615	1/1	0.88	0.21	47,47,47,47	0
24	MG	A	2684	1/1	0.88	0.16	46,46,46,46	0
24	MG	A	2617	1/1	0.88	0.32	58,58,58,58	0
24	MG	A	2731	1/1	0.89	0.14	80,80,80,80	0
24	MG	A	2553	1/1	0.89	0.33	108,108,108,108	0
24	MG	A	2711	1/1	0.89	0.46	81,81,81,81	0
24	MG	A	2629	1/1	0.89	0.16	77,77,77,77	0
24	MG	A	2563	1/1	0.89	0.30	53,53,53,53	0
24	MG	A	2694	1/1	0.89	0.41	71,71,71,71	0
24	MG	A	2610	1/1	0.89	0.21	53,53,53,53	0
25	K	A	2679	1/1	0.89	0.14	104,104,104,104	0
24	MG	N	1062	1/1	0.89	0.23	65,65,65,65	0
24	MG	P	1084	1/1	0.89	0.29	63,63,63,63	0
24	MG	A	2632	1/1	0.89	0.21	65,65,65,65	0
24	MG	T	1101	1/1	0.89	0.17	49,49,49,49	0
24	MG	A	2559	1/1	0.89	0.36	51,51,51,51	0
24	MG	A	3748	1/1	0.90	0.51	61,61,61,61	0
24	MG	A	2582	1/1	0.90	0.18	52,52,52,52	0
24	MG	A	3780	1/1	0.90	0.32	84,84,84,84	0
24	MG	A	3813	1/1	0.90	0.32	55,55,55,55	0
24	MG	L	1126	1/1	0.90	0.14	59,59,59,59	0
24	MG	A	2568	1/1	0.90	0.32	54,54,54,54	0
24	MG	A	3907	1/1	0.90	0.34	64,64,64,64	0
24	MG	A	2556	1/1	0.90	0.21	82,82,82,82	0
24	MG	A	2641	1/1	0.90	0.09	45,45,45,45	0
24	MG	A	3735	1/1	0.90	0.57	72,72,72,72	0
25	K	A	3892	1/1	0.90	0.09	103,103,103,103	0
24	MG	A	2710	1/1	0.90	0.18	58,58,58,58	0
24	MG	A	2633	1/1	0.90	0.14	72,72,72,72	0
24	MG	A	2667	1/1	0.91	0.11	56,56,56,56	0
24	MG	A	3828	1/1	0.91	0.16	68,68,68,68	0
24	MG	A	2579	1/1	0.91	0.35	53,53,53,53	0
25	K	A	2670	1/1	0.91	0.12	105,105,105,105	0
24	MG	A	2699	1/1	0.91	0.10	74,74,74,74	0
24	MG	A	2685	1/1	0.91	0.47	63,63,63,63	0
24	MG	A	2585	1/1	0.91	0.52	61,61,61,61	0
25	K	A	2674	1/1	0.91	0.07	101,101,101,101	0
24	MG	A	2625	1/1	0.91	0.10	48,48,48,48	0
24	MG	A	3928	1/1	0.91	0.50	64,64,64,64	0
24	MG	A	2640	1/1	0.91	0.22	52,52,52,52	0
24	MG	A	2720	1/1	0.91	0.13	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	MG	A	2613	1/1	0.91	0.40	61,61,61,61	0
24	MG	A	2602	1/1	0.91	0.22	46,46,46,46	0
25	K	A	2681	1/1	0.91	0.12	107,107,107,107	0
24	MG	A	2663	1/1	0.91	0.12	54,54,54,54	0
24	MG	A	3750	1/1	0.91	0.31	68,68,68,68	0
24	MG	A	2725	1/1	0.91	0.17	68,68,68,68	0
24	MG	A	3789	1/1	0.91	0.46	73,73,73,73	0
24	MG	A	2646	1/1	0.91	0.24	59,59,59,59	0
24	MG	A	2701	1/1	0.92	0.66	78,78,78,78	0
24	MG	A	3774	1/1	0.92	0.56	69,69,69,69	0
24	MG	A	2668	1/1	0.92	0.17	117,117,117,117	0
24	MG	A	2650	1/1	0.92	0.10	58,58,58,58	0
24	MG	A	3795	1/1	0.92	0.80	77,77,77,77	0
24	MG	A	3810	1/1	0.92	0.31	53,53,53,53	0
24	MG	A	2651	1/1	0.92	0.25	50,50,50,50	0
24	MG	A	2724	1/1	0.92	0.15	64,64,64,64	0
24	MG	A	2705	1/1	0.92	0.09	52,52,52,52	0
24	MG	A	2635	1/1	0.92	0.11	37,37,37,37	0
24	MG	A	2707	1/1	0.92	0.15	48,48,48,48	0
24	MG	A	2550	1/1	0.92	0.12	63,63,63,63	0
24	MG	A	2654	1/1	0.92	0.33	59,59,59,59	0
24	MG	A	2591	1/1	0.92	0.30	39,39,39,39	0
24	MG	A	2638	1/1	0.92	0.14	57,57,57,57	0
24	MG	A	2587	1/1	0.92	0.09	52,52,52,52	0
24	MG	A	2616	1/1	0.92	0.10	49,49,49,49	0
24	MG	A	2662	1/1	0.92	0.19	52,52,52,52	0
24	MG	A	3967	1/1	0.92	0.37	83,83,83,83	0
24	MG	A	2594	1/1	0.92	0.33	64,64,64,64	0
24	MG	E	2148	1/1	0.92	0.20	66,66,66,66	0
24	MG	A	2599	1/1	0.92	0.20	58,58,58,58	0
24	MG	A	2647	1/1	0.92	0.08	39,39,39,39	0
24	MG	A	2566	1/1	0.93	0.33	56,56,56,56	0
24	MG	A	2664	1/1	0.93	0.28	64,64,64,64	0
24	MG	A	3757	1/1	0.93	0.47	51,51,51,51	0
24	MG	A	2665	1/1	0.93	0.19	63,63,63,63	0
24	MG	A	2580	1/1	0.93	0.46	79,79,79,79	0
24	MG	A	2548	1/1	0.93	0.10	48,48,48,48	0
24	MG	A	2644	1/1	0.93	0.10	46,46,46,46	0
24	MG	E	1152	1/1	0.93	0.34	66,66,66,66	0
24	MG	A	2570	1/1	0.93	0.09	49,49,49,49	0
24	MG	A	2657	1/1	0.93	0.17	57,57,57,57	0
24	MG	H	1139	1/1	0.93	0.07	48,48,48,48	0

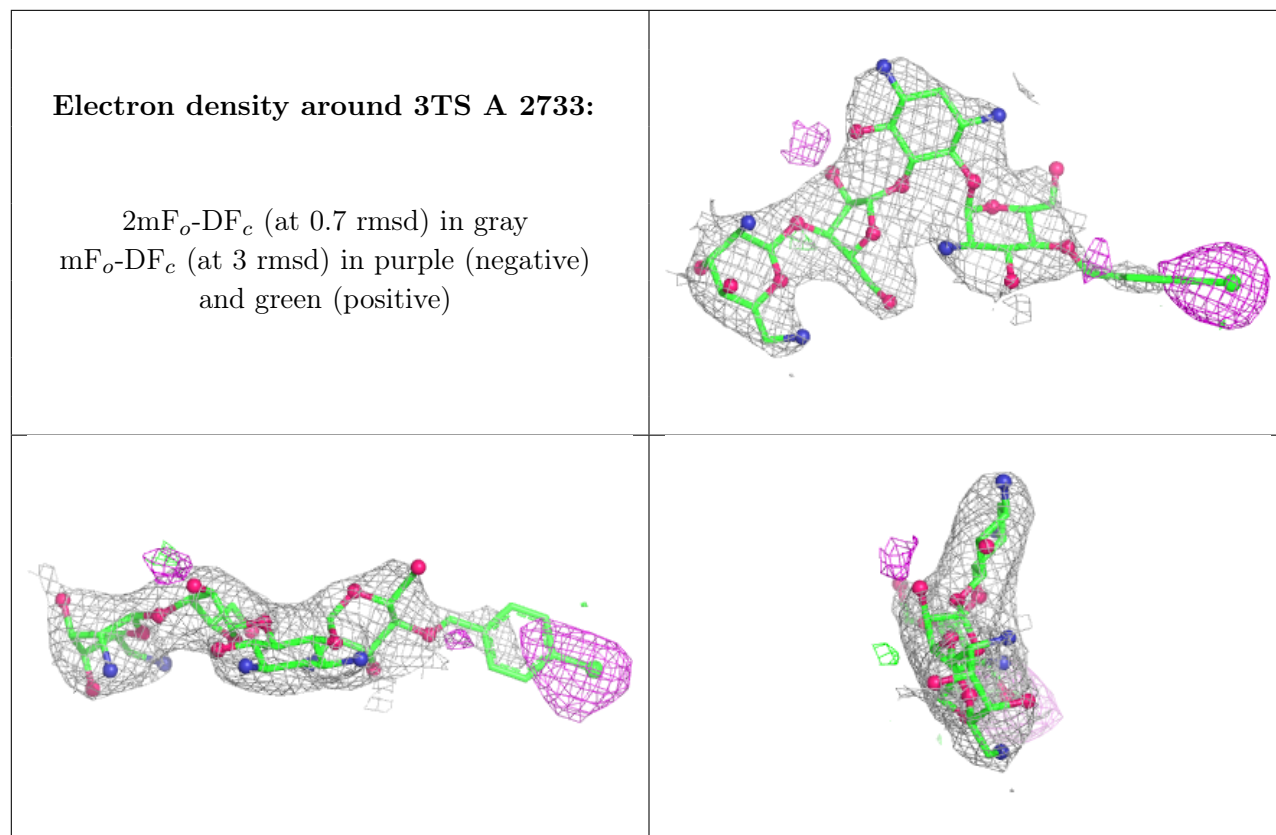
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	MG	A	2687	1/1	0.93	0.26	12,12,12,12	0
24	MG	A	2601	1/1	0.93	0.34	51,51,51,51	0
24	MG	A	2578	1/1	0.93	0.27	52,52,52,52	0
24	MG	A	2639	1/1	0.93	0.14	62,62,62,62	0
24	MG	Q	2217	1/1	0.93	0.17	62,62,62,62	0
24	MG	A	2691	1/1	0.93	0.25	55,55,55,55	0
24	MG	A	2692	1/1	0.93	0.59	71,71,71,71	0
24	MG	A	2719	1/1	0.94	0.47	74,74,74,74	0
24	MG	A	2618	1/1	0.94	0.09	53,53,53,53	0
24	MG	A	2649	1/1	0.94	0.16	34,34,34,34	0
24	MG	A	2658	1/1	0.94	0.08	58,58,58,58	0
24	MG	A	2716	1/1	0.94	0.17	67,67,67,67	0
24	MG	A	2592	1/1	0.94	0.25	47,47,47,47	0
24	MG	A	2584	1/1	0.94	0.17	60,60,60,60	0
24	MG	A	3759	1/1	0.94	0.41	66,66,66,66	0
24	MG	A	2686	1/1	0.95	0.50	65,65,65,65	0
24	MG	A	2645	1/1	0.95	0.05	23,23,23,23	0
24	MG	D	1210	1/1	0.95	0.07	60,60,60,60	0
24	MG	A	2604	1/1	0.95	0.15	37,37,37,37	0
24	MG	A	3933	1/1	0.95	0.42	73,73,73,73	0
24	MG	A	2623	1/1	0.95	0.08	44,44,44,44	0
24	MG	A	2648	1/1	0.95	0.12	49,49,49,49	0
24	MG	A	2624	1/1	0.95	0.10	39,39,39,39	0
24	MG	M	1126	1/1	0.96	0.05	61,61,61,61	0
24	MG	A	3753	1/1	0.96	0.42	46,46,46,46	0
24	MG	A	2611	1/1	0.96	0.11	55,55,55,55	0
24	MG	A	3804	1/1	0.96	0.46	66,66,66,66	0
24	MG	A	2627	1/1	0.96	0.08	51,51,51,51	0
24	MG	A	2574	1/1	0.96	0.39	50,50,50,50	0
24	MG	A	2554	1/1	0.96	0.46	67,67,67,67	0
24	MG	A	3927	1/1	0.96	0.11	59,59,59,59	0
24	MG	A	2581	1/1	0.97	0.19	44,44,44,44	0
24	MG	A	3734	1/1	0.98	0.45	49,49,49,49	0
24	MG	L	1125	1/1	0.98	0.07	63,63,63,63	0
24	MG	A	2558	1/1	0.98	0.06	50,50,50,50	0
24	MG	A	2659	1/1	0.98	0.15	28,28,28,28	0
27	ZN	D	1209	1/1	0.98	0.12	106,106,106,106	0
27	ZN	N	1061	1/1	0.98	0.04	131,131,131,131	0
24	MG	A	2643	1/1	0.99	0.13	43,43,43,43	0

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

orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.