



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:12 PM GMT

PDB ID : 3T1Y
Title : Structure of the *Thermus thermophilus* 30S ribosomal subunit complexed with a human anti-codon stem loop (HASL) of transfer RNA Lysine 3 (TRNALYS3) bound to an mRNA with an AAG-codon in the A-site and paromomycin
Authors : Murphy, F.V.; Vendeix, F.A.P.; Cantara, W.; Leszczynska, G.; Gustilo, E.M.; Sproat, B.; Malkiewicz, A.A.P.; Agris, P.F.
Deposited on : 2011-07-22
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

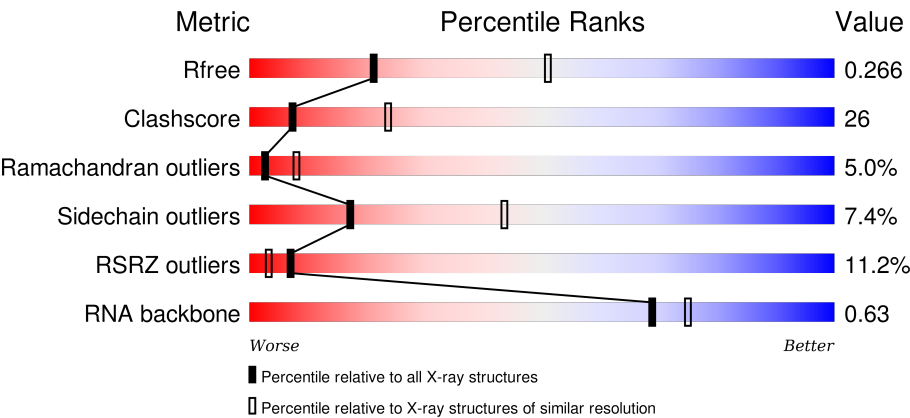
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)
RNA backbone	2183	1091 (3.20-2.40)

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

Mol	Chain	Length	Quality of chain
1	A	1513	<div><div>9%</div><div><div></div><div>42%</div><div>35%</div><div>18%</div><div>5%</div></div></div>
2	B	256	<div><div>19%</div><div><div></div><div>34%</div><div>50%</div><div>8%</div><div>9%</div></div></div>
3	C	239	<div><div>12%</div><div><div></div><div>33%</div><div>46%</div><div>6%</div><div>14%</div></div></div>
4	D	209	<div><div>9%</div><div><div></div><div>49%</div><div>44%</div><div>7%</div></div></div>

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	MG	A	1605	-	-	-	X
24	MG	A	1637	-	-	-	X
24	MG	A	1648	-	-	-	X
24	MG	A	1650	-	-	-	X
24	MG	A	1654	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	MG	A	1658	-	-	-	X
24	MG	A	1663	-	-	-	X
24	MG	A	1667	-	-	-	X
24	MG	A	1670	-	-	-	X
24	MG	A	1679	-	-	-	X
24	MG	A	1680	-	-	-	X
24	MG	A	1683	-	-	-	X
24	MG	A	1692	-	-	-	X
24	MG	A	1725	-	-	-	X
24	MG	A	1728	-	-	-	X
24	MG	A	1738	-	-	-	X
24	MG	A	1739	-	-	-	X
24	MG	A	1752	-	-	-	X
24	MG	A	1756	-	-	-	X
24	MG	A	1758	-	-	-	X
24	MG	A	1759	-	-	-	X
24	MG	A	1760	-	-	-	X
24	MG	A	1762	-	-	-	X
24	MG	A	1764	-	-	-	X
24	MG	A	1784	-	-	-	X
26	PAR	A	1786	-	-	-	X

2 Entry composition

There are 26 unique types of molecules in this entry. The entry contains 52289 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

There are 5 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	127	Total	C	N	O	S	0	0	0
			1011	639	198	174				

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	98	Total	C	N	O	S	0	0	0
			792	498	156	137	1			

- Molecule 11 is a protein called 30S ribosomal protein S11.

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

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	124	Total	C	N	O	S	0	0	0
			970	611	195	163	1			

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

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

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

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

- Molecule 15 is a protein called 30S ribosomal protein S15.

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

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	P	83	Total	C	N	O	S	0	0	0
			700	443	139	117	1			

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	104	Total	C	N	O	S	0	0	0
			857	547	161	147	2			

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	W	3	Total	C	N	O	P	0	0	0
			68	30	15	20	3			

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

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

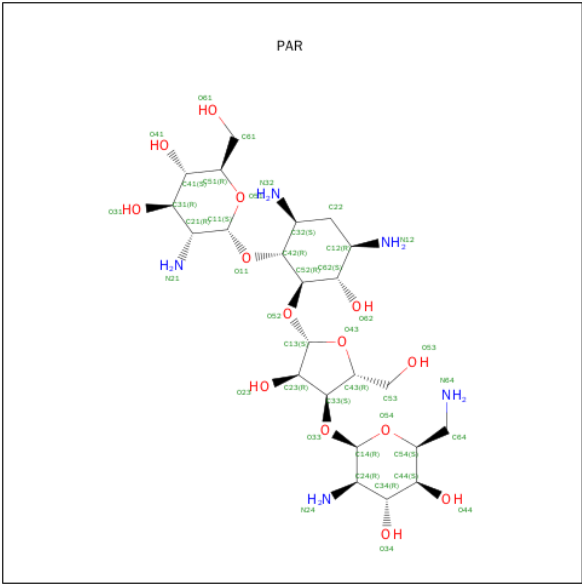
- Molecule 24 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	B	1	Total	Mg	0	0
			1	1		
24	A	185	Total	Mg	0	0
			185	185		

- Molecule 25 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 26 is PAROMOMYCIN (three-letter code: PAR) (formula: C₂₃H₄₅N₅O₁₄).

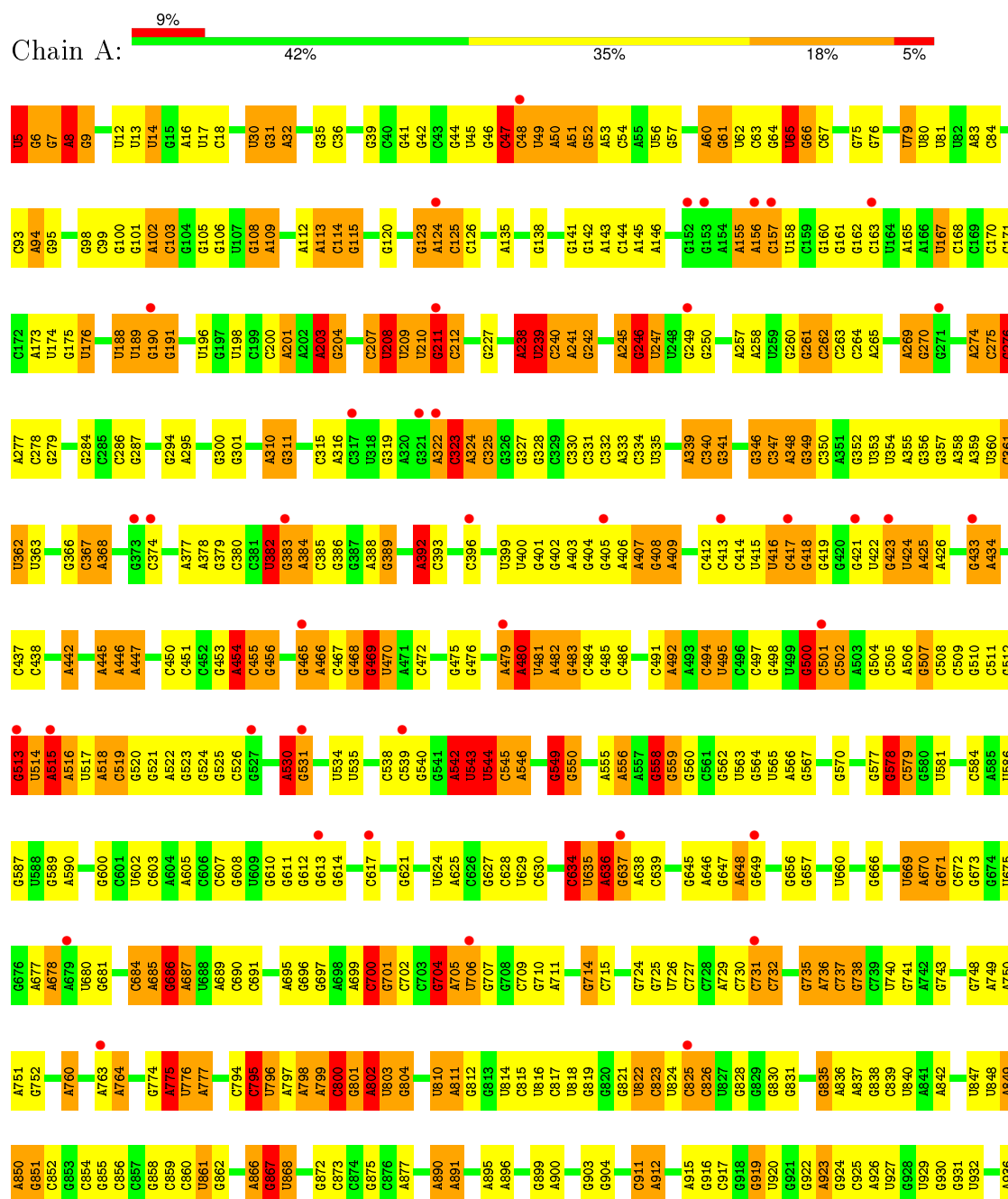


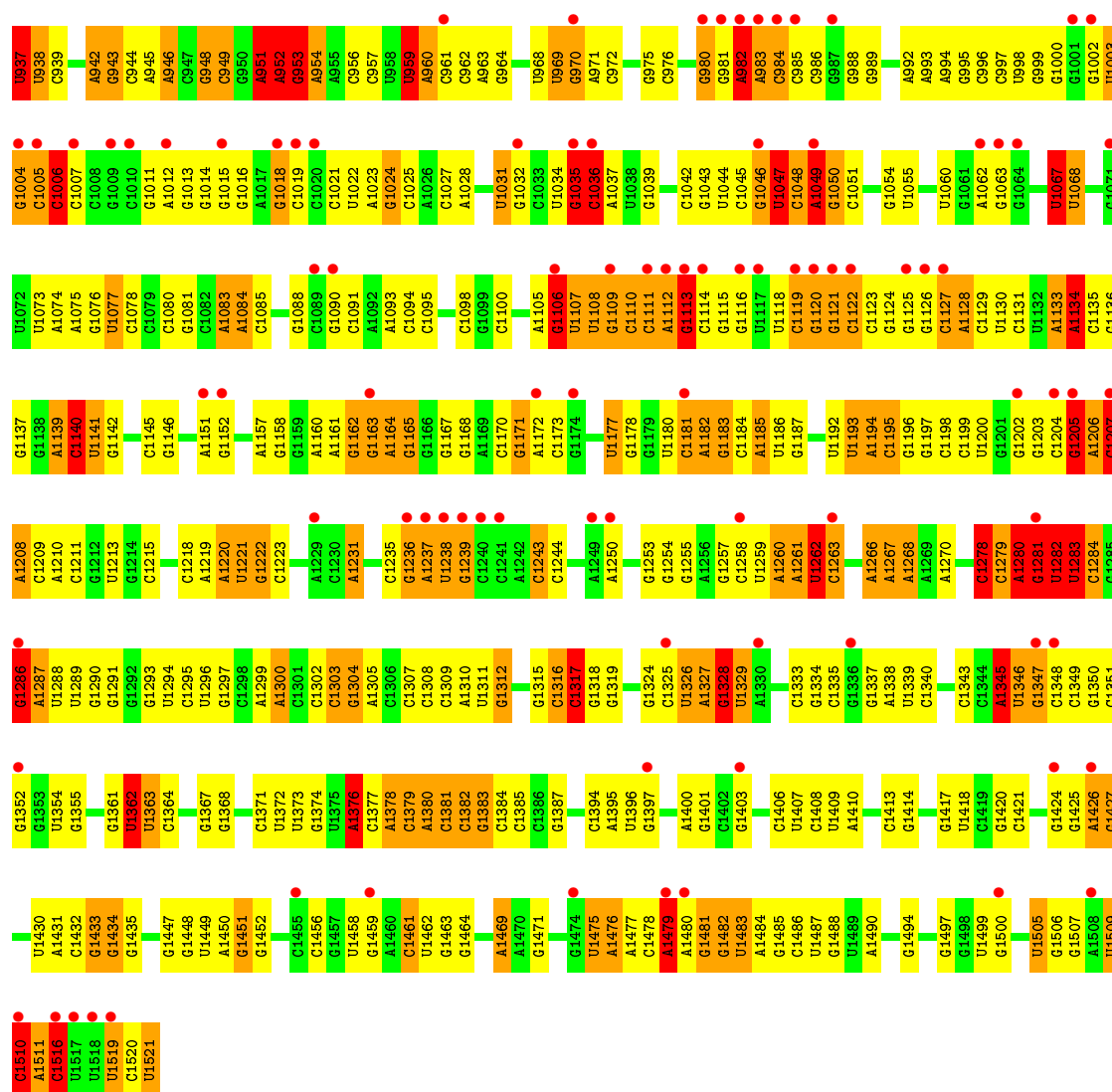
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	A	1	Total	C	N	O	0	0
			42	23	5	14		

3 Residue-property plots

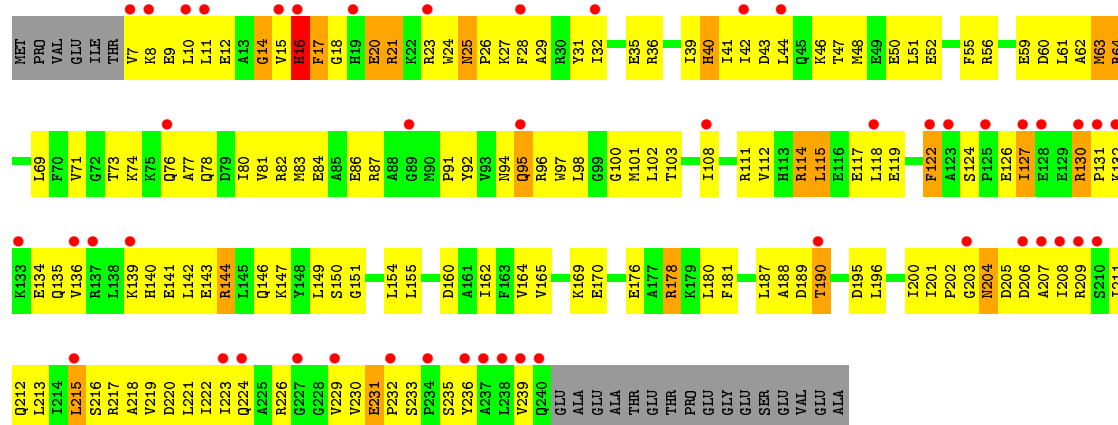
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

• Molecule 1: 16S rRNA

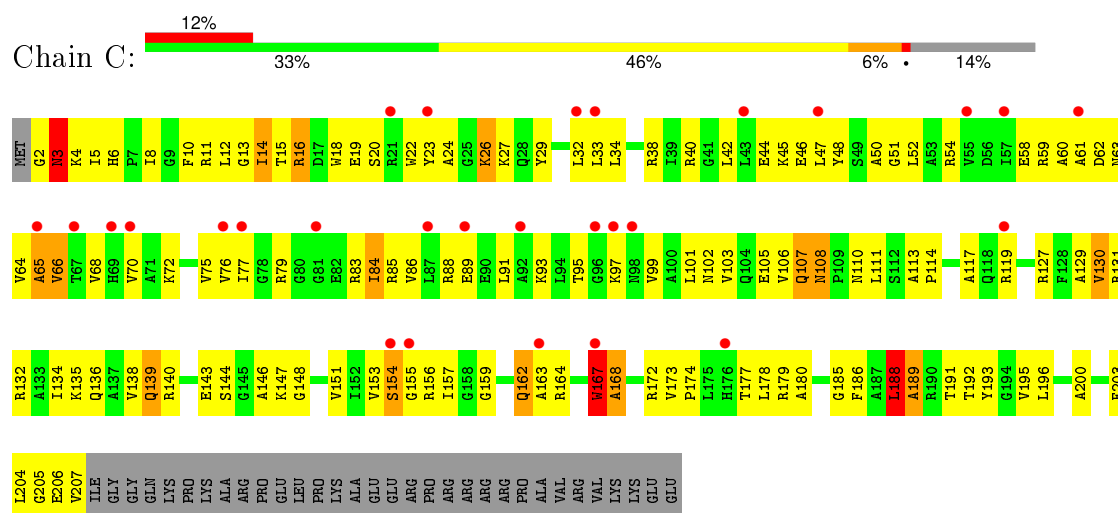




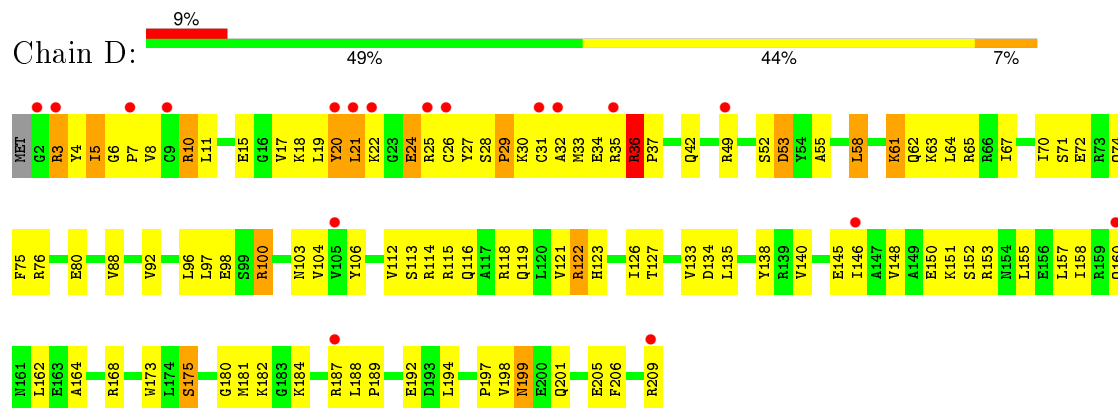
• Molecule 2: 30S ribosomal protein S2



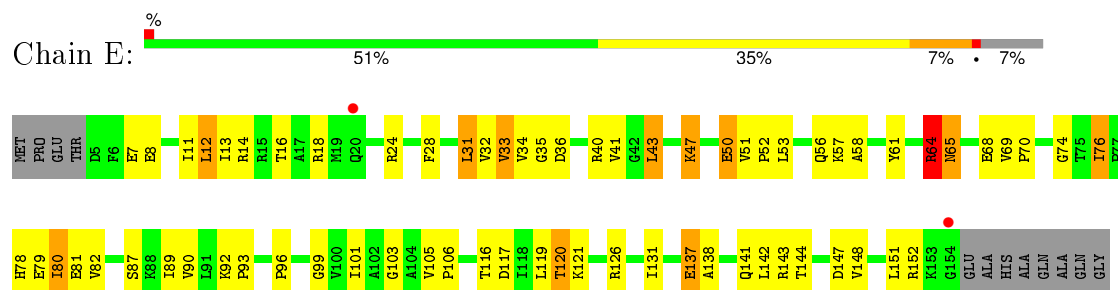
• Molecule 3: 30S ribosomal protein S3



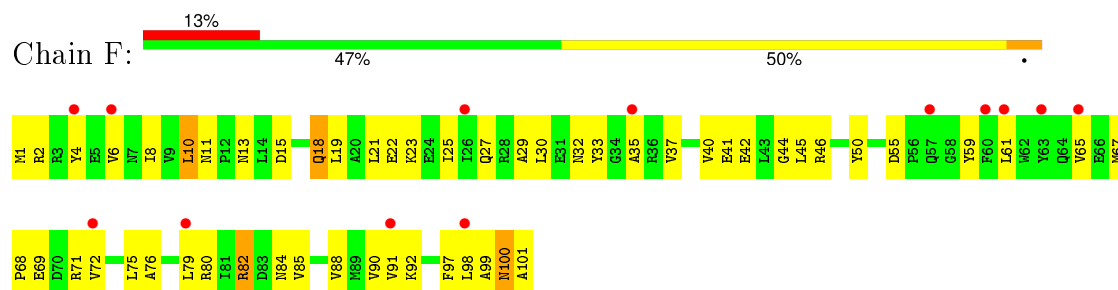
• Molecule 4: 30S ribosomal protein S4



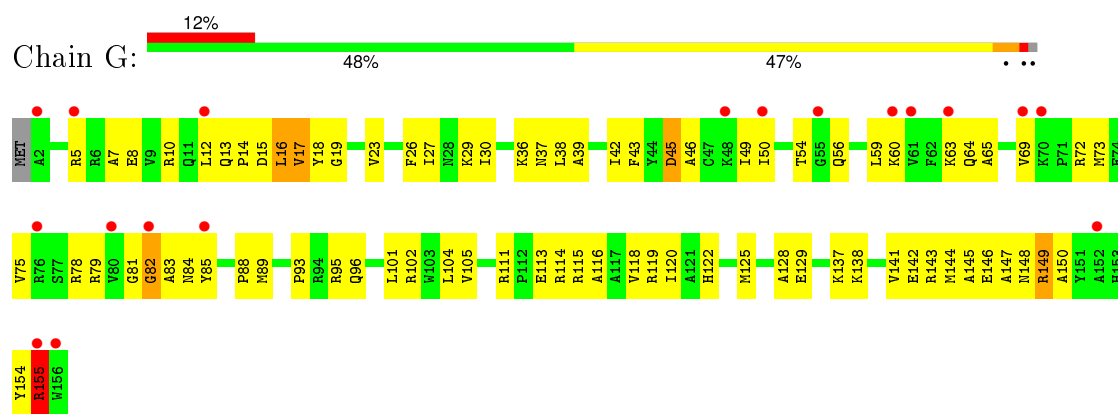
• Molecule 5: 30S ribosomal protein S5



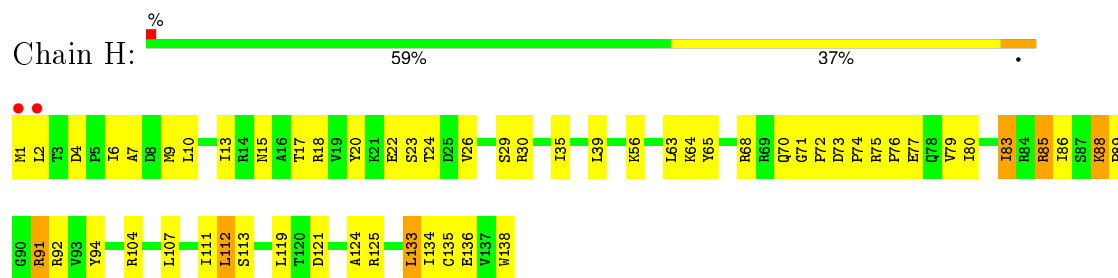
• Molecule 6: 30S ribosomal protein S6



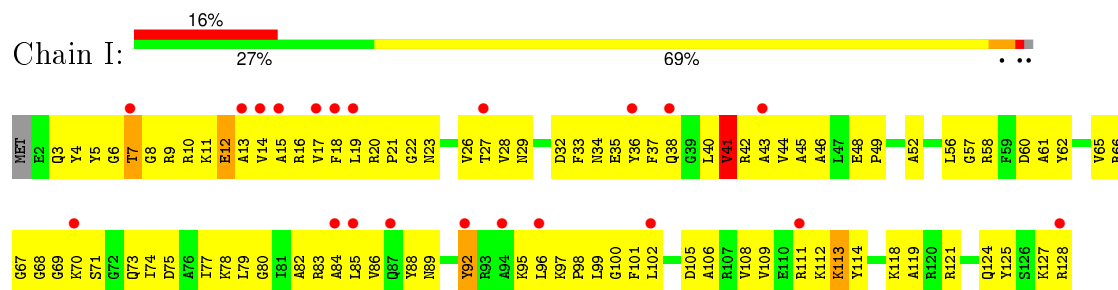
• Molecule 7: 30S ribosomal protein S7



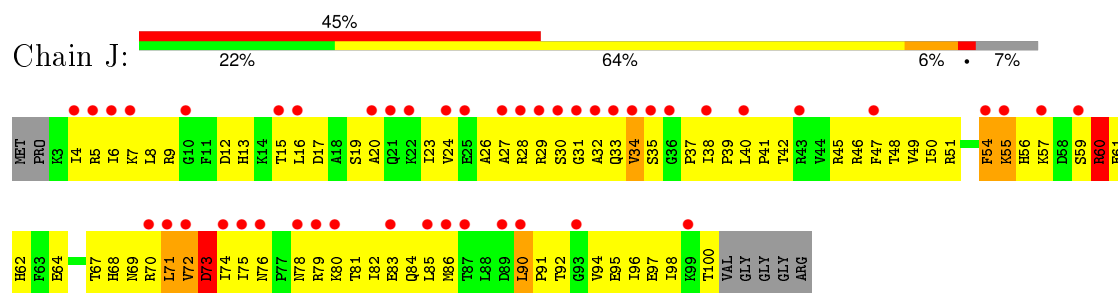
• Molecule 8: 30S ribosomal protein S8



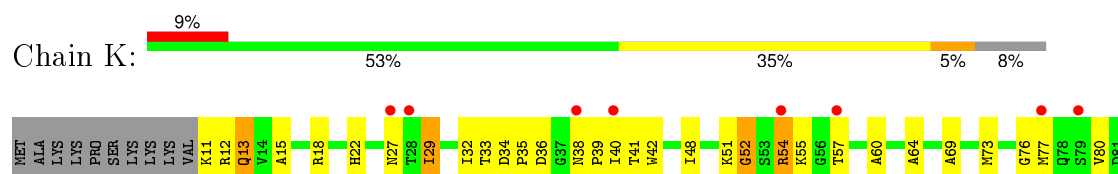
• Molecule 9: 30S ribosomal protein S9

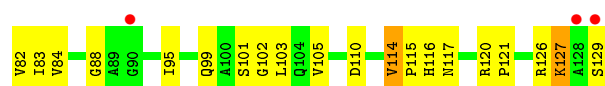


• Molecule 10: 30S ribosomal protein S10

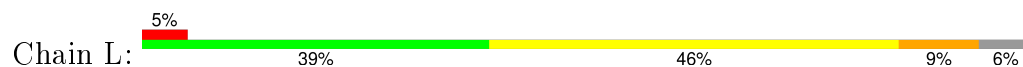


• Molecule 11: 30S ribosomal protein S11

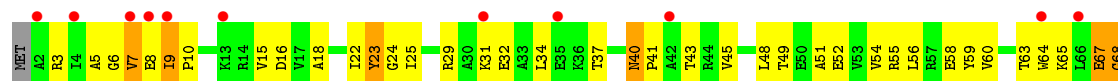




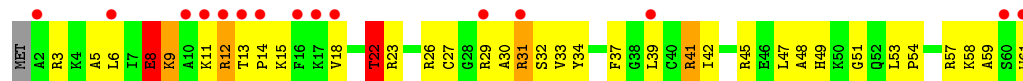
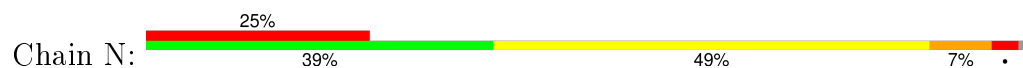
- Molecule 12: 30S ribosomal protein S12



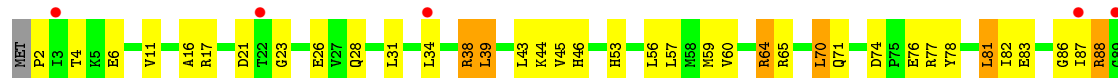
- Molecule 13: 30S ribosomal protein S13



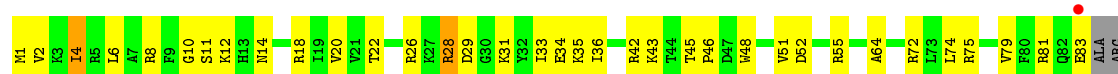
- Molecule 14: 30S ribosomal protein S14 type Z



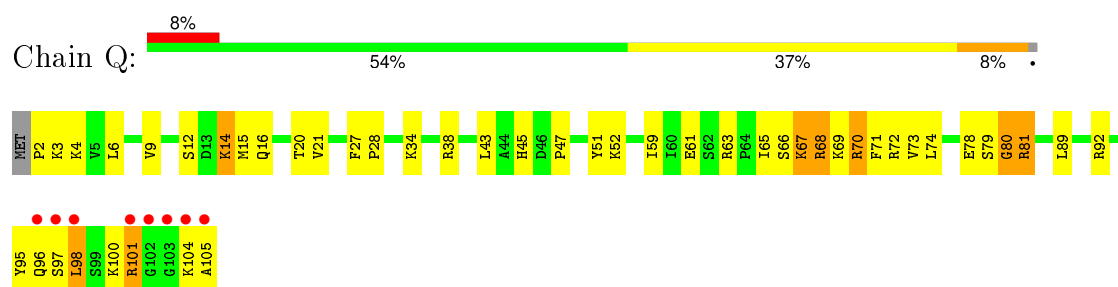
- Molecule 15: 30S ribosomal protein S15



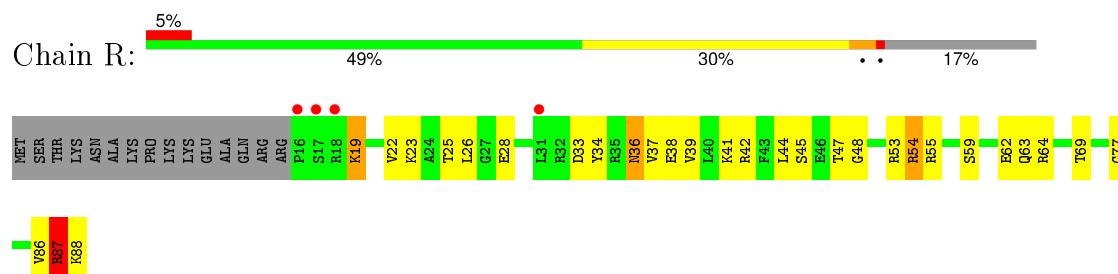
- Molecule 16: 30S ribosomal protein S16



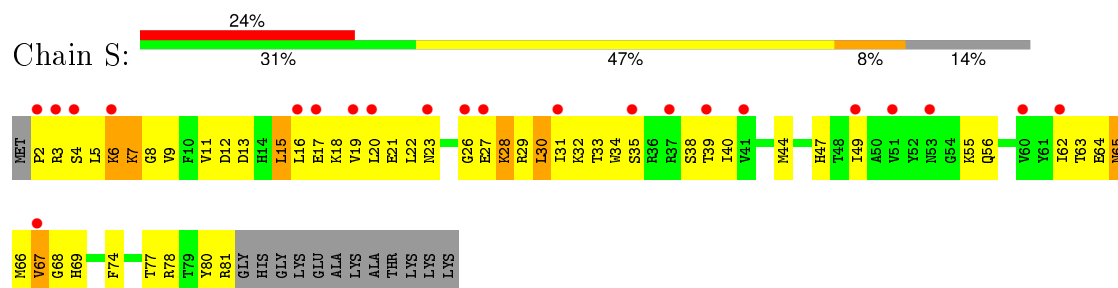
- Molecule 17: 30S ribosomal protein S17



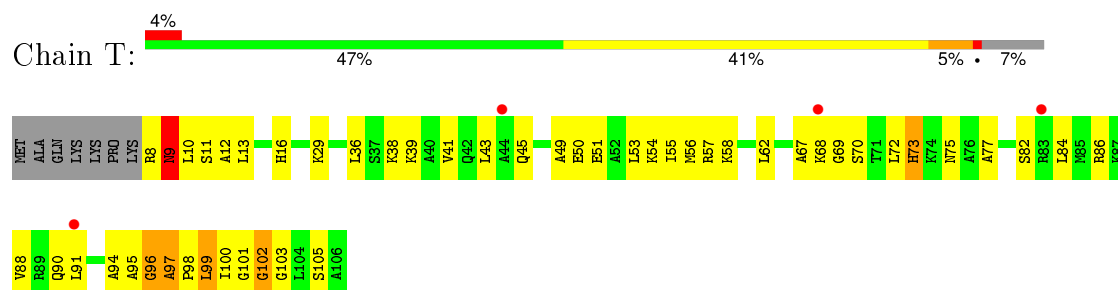
- Molecule 18: 30S ribosomal protein S18



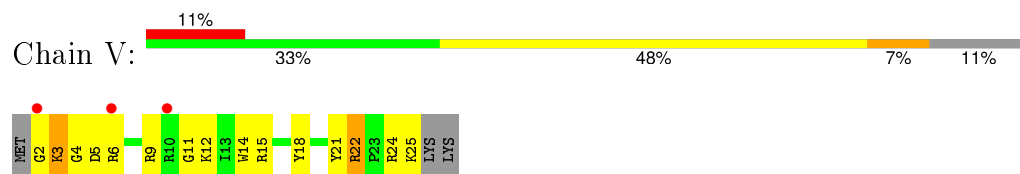
- Molecule 19: 30S ribosomal protein S19



- Molecule 20: 30S ribosomal protein S20



- Molecule 21: 30S ribosomal protein Thx



- Molecule 22: mRNA A-site fragment





● Molecule 23: tRNA ASL human Lys3



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	400.97Å 400.97Å 174.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.89 – 2.80 283.53 – 2.78	Depositor EDS
% Data completeness (in resolution range)	99.2 (29.89-2.80) 99.0 (283.53-2.78)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 2.77Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.245 , 0.268 0.244 , 0.266	Depositor DCC
R_{free} test set	16829 reflections (4.93%)	DCC
Wilson B-factor (Å ²)	59.3	Xtriage
Anisotropy	0.205	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 72.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 350474 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	52289	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.38% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 12A, MG, ZN, 70U, PAR, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.58	5/36395 (0.0%)	0.86	98/56801 (0.2%)
2	B	0.37	0/1935	0.60	0/2609
3	C	0.39	0/1636	0.62	0/2205
4	D	0.39	0/1733	0.59	0/2318
5	E	0.45	0/1162	0.73	1/1564 (0.1%)
6	F	0.36	0/856	0.58	0/1154
7	G	0.38	0/1276	0.56	0/1709
8	H	0.44	0/1136	0.73	1/1527 (0.1%)
9	I	0.38	0/1029	0.63	0/1378
10	J	0.39	0/805	0.62	0/1082
11	K	0.44	0/900	0.65	0/1213
12	L	0.49	0/986	0.76	0/1320
13	M	0.39	0/1008	0.64	0/1347
14	N	0.43	0/501	0.64	0/664
15	O	0.38	0/745	0.61	0/992
16	P	0.42	0/716	0.75	1/963 (0.1%)
17	Q	0.44	0/870	0.73	1/1159 (0.1%)
18	R	0.39	0/603	0.61	0/799
19	S	0.34	0/661	0.60	0/890
20	T	0.44	0/764	0.69	0/1006
21	V	0.46	0/212	0.59	0/277
22	W	1.26	1/76 (1.3%)	0.95	0/115
23	X	0.91	1/184 (0.5%)	0.91	0/277
All	All	0.53	7/56189 (0.0%)	0.80	102/83369 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	42

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1511	A	N9-C4	7.67	1.42	1.37
22	W	1	A	OP3-P	-7.53	1.52	1.61
1	A	634	C	O3'-P	7.47	1.70	1.61
23	X	30	G	OP3-P	-6.68	1.53	1.61
1	A	5	U	OP3-P	-6.51	1.53	1.61
1	A	1511	A	O3'-P	6.24	1.68	1.61
1	A	1510	C	C5'-C4'	5.64	1.58	1.51

All (102) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	634	C	P-O3'-C3'	-15.04	101.65	119.70
1	A	801	G	C2'-C3'-O3'	8.53	128.26	109.50
1	A	937	U	N1-C1'-C2'	8.47	125.02	114.00
1	A	558	G	N9-C1'-C2'	8.39	124.91	114.00
1	A	513	G	N9-C1'-C2'	8.32	124.82	114.00
1	A	636	A	P-O3'-C3'	8.26	129.61	119.70
1	A	686	G	C2'-C3'-O3'	8.19	127.52	109.50
1	A	1036	C	N1-C1'-C2'	-8.15	103.03	112.00
1	A	500	G	C2'-C3'-O3'	7.64	126.32	109.50
1	A	276	G	C2'-C3'-O3'	7.61	126.25	109.50
1	A	578	G	C2'-C3'-O3'	7.56	126.13	109.50
1	A	735	G	N9-C1'-C2'	7.51	123.76	114.00
1	A	238	A	N9-C1'-C2'	7.41	123.63	114.00
1	A	65	U	C2'-C3'-O3'	7.34	125.65	109.50
1	A	1516	C	O4'-C4'-C3'	-7.30	96.70	104.00
1	A	1047	U	C2'-C3'-O3'	7.20	125.33	109.50
1	A	1452	G	O5'-P-OP2	-7.08	99.32	105.70
1	A	1483	U	N1-C1'-C2'	7.08	123.21	114.00
1	A	469	G	N9-C1'-C2'	7.07	123.19	114.00
1	A	953	G	C4'-C3'-O3'	-7.07	94.56	109.40
1	A	542	A	C2'-C3'-O3'	7.04	124.98	109.50
1	A	1047	U	N1-C1'-C2'	7.03	123.14	114.00
1	A	1483	U	C2'-C3'-O3'	6.97	124.86	113.70
1	A	1006	C	N1-C1'-C2'	-6.95	104.35	112.00
1	A	1278	C	C2'-C3'-O3'	6.65	124.34	113.70
1	A	1479	A	N9-C1'-C2'	6.58	122.56	114.00
1	A	1451	G	OP2-P-O3'	6.58	119.68	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	982	A	N9-C1'-C2'	-6.53	104.81	112.00
1	A	861	U	C2'-C3'-O3'	6.50	124.10	113.70
1	A	578	G	N9-C1'-C2'	6.47	122.42	114.00
1	A	392	A	C5'-C4'-C3'	-6.34	105.86	116.00
5	E	64	ARG	N-CA-C	-6.30	93.99	111.00
1	A	1280	A	N9-C1'-C2'	6.21	122.07	114.00
1	A	246	G	N9-C1'-C2'	6.20	122.06	114.00
1	A	1300	A	N9-C1'-C2'	6.16	122.01	114.00
1	A	323	C	N1-C1'-C2'	6.11	121.94	114.00
1	A	239	U	C2'-C3'-O3'	6.09	123.44	113.70
1	A	700	C	N1-C1'-C2'	6.05	121.87	114.00
1	A	795	C	OP2-P-O3'	6.00	118.39	105.20
1	A	1141	U	C2'-C3'-O3'	5.99	123.29	113.70
1	A	802	A	N9-C1'-C2'	5.97	121.77	114.00
1	A	775	A	N9-C1'-C2'	5.93	121.70	114.00
1	A	47	C	C2'-C3'-O3'	5.92	123.17	113.70
1	A	1516	C	O5'-P-OP2	-5.89	100.39	105.70
1	A	1345	A	C2'-C3'-O3'	5.89	123.12	113.70
1	A	1511	A	O4'-C1'-N9	5.84	112.87	108.20
1	A	775	A	C2'-C3'-O3'	5.82	123.01	113.70
1	A	704	G	N9-C1'-C2'	5.81	121.55	114.00
1	A	238	A	C2'-C3'-O3'	5.79	122.96	113.70
1	A	1521	U	C4'-C3'-O3'	-5.77	97.29	109.40
1	A	982	A	C4'-C3'-O3'	5.73	124.47	113.00
1	A	14	U	C5'-C4'-C3'	-5.70	106.89	116.00
1	A	1282	U	C2'-C3'-O3'	5.67	122.77	113.70
1	A	445	A	C2'-C3'-O3'	5.66	122.75	113.70
1	A	1184	C	OP1-P-O3'	5.65	117.63	105.20
1	A	480	A	C2'-C3'-O3'	5.64	122.72	113.70
1	A	543	U	N1-C1'-C2'	5.61	121.29	114.00
1	A	704	G	C2'-C3'-O3'	5.61	122.68	113.70
1	A	1286	G	C2'-C3'-O3'	5.58	122.64	113.70
1	A	1134	A	C5'-C4'-O4'	-5.58	102.40	109.10
1	A	1141	U	N1-C1'-C2'	5.57	121.23	114.00
1	A	953	G	O4'-C1'-C2'	5.55	112.59	107.60
1	A	1362	U	C2'-C3'-O3'	5.52	122.53	113.70
1	A	542	A	N9-C1'-C2'	5.47	121.11	114.00
1	A	1278	C	N1-C1'-C2'	5.47	121.11	114.00
1	A	1505	U	C2'-C3'-O3'	5.45	122.42	113.70
1	A	47	C	N1-C1'-C2'	5.37	120.98	114.00
1	A	513	G	C2'-C3'-O3'	5.37	122.29	113.70
1	A	1312	G	N9-C1'-C2'	5.37	120.98	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1516	C	O4'-C1'-N1	5.36	112.49	108.20
1	A	797	A	C5'-C4'-C3'	-5.36	107.42	116.00
8	H	112	LEU	CA-CB-CG	5.36	127.62	115.30
1	A	951	A	N9-C1'-C2'	5.34	120.94	114.00
1	A	454	A	C2'-C3'-O3'	5.30	122.18	113.70
17	Q	67	LYS	N-CA-C	-5.28	96.74	111.00
1	A	1140	C	N1-C1'-C2'	5.28	120.86	114.00
1	A	867	G	N9-C1'-C2'	5.28	120.86	114.00
1	A	500	G	N9-C1'-C2'	5.27	120.85	114.00
1	A	8	A	O4'-C1'-N9	5.25	112.40	108.20
1	A	800	C	N1-C1'-C2'	5.21	120.78	114.00
1	A	382	U	C5'-C4'-C3'	-5.17	107.73	116.00
1	A	1049	A	N9-C1'-C2'	5.16	120.71	114.00
1	A	445	A	N9-C1'-C2'	5.16	120.71	114.00
1	A	1376	A	C5'-C4'-C3'	-5.16	107.75	116.00
1	A	953	G	O4'-C4'-C3'	5.15	110.22	106.10
1	A	1510	C	C3'-C2'-C1'	-5.15	97.38	101.50
1	A	558	G	C4'-C3'-C2'	5.13	107.73	102.60
1	A	208	U	OP2-P-O3'	5.12	116.47	105.20
16	P	4	ILE	N-CA-C	-5.08	97.28	111.00
1	A	959	U	N1-C1'-C2'	5.08	120.60	114.00
1	A	1511	A	OP1-P-O3'	5.08	116.37	105.20
1	A	1328	G	N9-C1'-C2'	5.07	120.59	114.00
1	A	63	C	C5'-C4'-C3'	-5.07	107.89	116.00
1	A	1317	C	C2'-C3'-O3'	5.05	121.79	113.70
1	A	1283	U	C2'-C3'-O3'	5.04	121.77	113.70
1	A	953	G	N9-C1'-C2'	5.03	120.54	114.00
1	A	800	C	C4'-C3'-C2'	5.03	107.63	102.60
1	A	530	A	N9-C1'-C2'	5.03	120.53	114.00
1	A	1106	G	N9-C1'-C2'	5.01	120.52	114.00
1	A	480	A	N9-C1'-C2'	5.01	120.51	114.00
1	A	1281	G	N9-C1'-C2'	5.01	120.51	114.00
1	A	1035	G	O4'-C1'-N9	5.01	112.20	108.20

There are no chirality outliers.

All (42) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1003	U	Sidechain
1	A	1006	C	Sidechain
1	A	1036	C	Sidechain
1	A	1047	U	Sidechain

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Mol	Chain	Res	Type	Group
1	A	1049	A	Sidechain
1	A	1067	U	Sidechain
1	A	1098	C	Sidechain
1	A	1113	G	Sidechain
1	A	1177	U	Sidechain
1	A	1205	G	Sidechain
1	A	1207	C	Sidechain
1	A	1262	U	Sidechain
1	A	1300	A	Sidechain
1	A	1387	G	Sidechain
1	A	1430	U	Sidechain
1	A	1434	G	Sidechain
1	A	1509	U	Sidechain
1	A	203	A	Sidechain
1	A	208	U	Sidechain
1	A	211	G	Sidechain
1	A	239	U	Sidechain
1	A	246	G	Sidechain
1	A	357	G	Sidechain
1	A	382	U	Sidechain
1	A	47	C	Sidechain
1	A	515	A	Sidechain
1	A	543	U	Sidechain
1	A	544	U	Sidechain
1	A	549	G	Sidechain
1	A	556	A	Sidechain
1	A	558	G	Sidechain
1	A	617	C	Sidechain
1	A	710	G	Sidechain
1	A	79	U	Sidechain
1	A	800	C	Sidechain
1	A	851	G	Sidechain
1	A	856	C	Sidechain
1	A	875	G	Sidechain
1	A	923	A	Sidechain
1	A	951	A	Sidechain
1	A	952	A	Sidechain
1	A	980	G	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32515	0	16410	1003	0
2	B	1900	0	1951	180	0
3	C	1612	0	1677	162	0
4	D	1703	0	1765	107	0
5	E	1146	0	1207	64	0
6	F	843	0	857	57	0
7	G	1257	0	1296	74	0
8	H	1116	0	1177	59	0
9	I	1011	0	1043	95	0
10	J	792	0	835	106	0
11	K	885	0	904	53	0
12	L	970	0	1057	100	0
13	M	997	0	1072	92	0
14	N	492	0	529	46	0
15	O	734	0	771	31	0
16	P	700	0	720	30	0
17	Q	857	0	930	46	0
18	R	597	0	668	40	0
19	S	647	0	673	64	0
20	T	762	0	859	57	0
21	V	208	0	221	12	0
22	W	68	0	34	12	0
23	X	247	0	130	18	0
24	A	185	0	0	0	0
24	B	1	0	0	0	0
25	D	1	0	0	0	0
25	N	1	0	0	0	0
26	A	42	0	45	4	0
All	All	52289	0	36831	2289	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 26.

All (2289) 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:50:A:H3'	1:A:50:A:P	1.73	1.29
1:A:1236:G:N2	1:A:1263:C:O2	1.78	1.16
1:A:1425:G:H5''	1:A:1426:A:C5'	1.74	1.15
1:A:1425:G:C5'	1:A:1426:A:H5'	1.76	1.15
1:A:669:U:H1'	11:K:42:TRP:HE1	1.09	1.14
19:S:33:THR:HG22	19:S:35:SER:H	1.09	1.13
1:A:1237:A:H2'	1:A:1238:U:C4'	1.79	1.11
1:A:1236:G:N2	1:A:1263:C:C2	2.18	1.11
1:A:1035:G:H4'	1:A:1036:C:H5'	1.25	1.11
10:J:8:LEU:HB2	10:J:70:ARG:HB2	1.34	1.09
12:L:47:LYS:HB3	12:L:48:PRO:HD2	1.34	1.07
12:L:41:ARG:HG2	12:L:42:THR:H	1.18	1.07
12:L:47:LYS:HB3	12:L:48:PRO:CD	1.82	1.06
1:A:1237:A:C2'	1:A:1238:U:H4'	1.85	1.05
1:A:48:C:O2'	1:A:49:U:OP1	1.74	1.05
12:L:41:ARG:HB3	12:L:41:ARG:HH11	1.19	1.04
12:L:41:ARG:HB3	12:L:41:ARG:NH1	1.73	1.04
1:A:802:A:H5'	1:A:802:A:H8	1.23	1.04
1:A:1133:A:O2'	1:A:1134:A:H5'	1.56	1.03
10:J:6:ILE:HG22	10:J:98:ILE:HG22	1.33	1.03
1:A:50:A:H3'	1:A:50:A:OP1	1.55	1.02
10:J:90:LEU:H	10:J:91:PRO:HD2	1.22	1.02
5:E:81:GLU:HG2	5:E:90:VAL:HG22	1.42	1.01
1:A:1036:C:C6	1:A:1036:C:H3'	1.97	0.99
3:C:119:ARG:HE	3:C:140:ARG:HH12	0.97	0.97
13:M:3:ARG:HA	13:M:8:GLU:O	1.65	0.97
2:B:80:ILE:HD12	2:B:80:ILE:H	1.27	0.96
1:A:1219:A:H5'	1:A:1317:C:H41	1.30	0.96
23:X:30:G:H2'	23:X:31:A:H8	1.32	0.94
1:A:367:C:H5''	1:A:368:A:OP1	1.67	0.94
1:A:50:A:P	1:A:50:A:C3'	2.55	0.94
1:A:647:G:H22	1:A:724:G:H1	1.11	0.94
26:A:1786:PAR:H11	26:A:1786:PAR:O52	1.63	0.94
1:A:821:G:H22	1:A:825:C:H42	1.13	0.94
1:A:1349:C:H5'	10:J:60:ARG:HH12	1.29	0.93
1:A:406:A:H62	1:A:408:G:H21	1.08	0.93
1:A:238:A:H4'	1:A:239:U:H5'	1.50	0.93
1:A:1133:A:HO2'	1:A:1134:A:H8	0.93	0.93
4:D:187:ARG:HD2	4:D:188:LEU:H	1.32	0.92
1:A:49:U:O3'	1:A:50:A:H3'	1.68	0.92
1:A:1083:A:H4'	1:A:1084:A:O5'	1.67	0.92
1:A:952:A:H4'	1:A:953:G:C5'	2.00	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1106:G:H4'	1:A:1107:U:OP1	1.69	0.91
19:S:62:ILE:HD12	19:S:66:MET:HG3	1.50	0.91
1:A:562:G:H5'	1:A:711:A:H1'	1.53	0.91
1:A:636:A:H5'	8:H:56:LYS:HE3	1.50	0.91
3:C:70:VAL:HG21	3:C:76:VAL:HG21	1.53	0.90
1:A:802:A:H5'	1:A:802:A:C8	2.06	0.90
1:A:1236:G:N2	1:A:1263:C:N3	2.15	0.90
1:A:1121:G:H5'	1:A:1122:C:OP1	1.71	0.90
9:I:8:GLY:HA2	9:I:79:LEU:HD12	1.53	0.90
14:N:12:ARG:HA	14:N:12:ARG:CZ	2.01	0.90
6:F:2:ARG:HE	6:F:69:GLU:HG2	1.37	0.90
7:G:50:ILE:O	7:G:54:THR:HG22	1.73	0.89
1:A:339:A:H4'	1:A:340:C:OP2	1.68	0.89
12:L:59:ARG:HD3	12:L:65:GLU:HG3	1.55	0.89
19:S:13:ASP:HA	19:S:16:LEU:HB3	1.55	0.89
1:A:1479:A:H2	1:A:1482:G:H1	1.16	0.88
3:C:14:ILE:H	3:C:14:ILE:HD13	1.36	0.88
1:A:246:G:H4'	1:A:247:U:O5'	1.71	0.88
13:M:65:LYS:HE3	13:M:69:GLU:HG2	1.55	0.88
17:Q:97:SER:HB3	17:Q:105:ALA:HB3	1.55	0.87
20:T:39:LYS:HD2	20:T:55:ILE:HD13	1.56	0.87
1:A:408:G:H2'	1:A:423:G:N2	1.88	0.87
12:L:42:THR:HG21	12:L:52:LEU:HD22	1.56	0.87
1:A:545:C:O2'	12:L:15:ARG:HB3	1.73	0.86
1:A:123:G:N3	1:A:189:U:H5'	1.90	0.86
1:A:485:G:OP1	12:L:118:SER:HB3	1.74	0.86
13:M:117:VAL:HG12	13:M:118:ALA:H	1.39	0.86
1:A:50:A:N6	1:A:356:G:H4'	1.89	0.86
9:I:15:ALA:HB2	9:I:65:VAL:HG13	1.55	0.86
5:E:80:ILE:HD12	5:E:138:ALA:HB1	1.55	0.86
11:K:54:ARG:O	11:K:57:THR:HG22	1.74	0.86
19:S:15:LEU:HD23	19:S:15:LEU:H	1.40	0.86
1:A:346:G:H4'	1:A:347:C:OP1	1.76	0.86
1:A:1004:G:H1	1:A:1018:G:H22	1.22	0.85
13:M:10:PRO:HB2	13:M:18:ALA:HB1	1.58	0.85
2:B:21:ARG:HD3	2:B:21:ARG:H	1.40	0.85
2:B:80:ILE:HD11	2:B:208:ILE:HG23	1.58	0.85
1:A:1266:A:H4'	1:A:1267:A:O5'	1.74	0.85
2:B:230:VAL:HG12	2:B:231:GLU:H	1.42	0.85
2:B:102:LEU:HD21	2:B:162:ILE:HD11	1.58	0.85
1:A:1516:C:H5	7:G:82:GLY:HA2	1.40	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:22:THR:HB	14:N:33:VAL:HG21	1.57	0.84
2:B:209:ARG:NH2	2:B:239:VAL:HG23	1.92	0.84
1:A:1303:C:H4'	1:A:1304:G:OP1	1.77	0.84
1:A:1406:C:H2'	1:A:1407:U:H5'	1.59	0.84
1:A:446:A:H5'	16:P:72:ARG:NH2	1.93	0.84
6:F:101:ALA:HB2	18:R:28:GLU:HA	1.58	0.84
3:C:64:VAL:HG21	3:C:95:THR:HG21	1.59	0.84
13:M:120:LYS:NZ	13:M:123:ALA:HB3	1.93	0.84
15:O:17:ARG:HH11	15:O:17:ARG:HG3	1.43	0.84
1:A:1243:C:H2'	1:A:1244:C:H5'	1.58	0.84
1:A:1133:A:H4'	1:A:1134:A:OP1	1.76	0.84
10:J:24:VAL:HG13	10:J:34:VAL:HG11	1.56	0.84
1:A:634:C:H5''	1:A:635:U:OP2	1.77	0.84
2:B:16:HIS:NE2	2:B:213:LEU:HD13	1.92	0.83
10:J:9:ARG:O	10:J:16:LEU:HD21	1.79	0.83
1:A:997:C:H2'	1:A:998:U:H5'	1.60	0.83
3:C:58:GLU:HB3	10:J:92:THR:HG21	1.60	0.83
1:A:49:U:H4'	1:A:50:A:OP2	1.78	0.83
12:L:59:ARG:NH1	12:L:65:GLU:HB3	1.94	0.83
1:A:849:A:H4'	1:A:850:A:OP1	1.76	0.83
2:B:95:GLN:O	2:B:96:ARG:HD2	1.79	0.83
5:E:64:ARG:HG2	5:E:64:ARG:HH11	1.43	0.82
8:H:86:ILE:HD11	8:H:136:GLU:HB2	1.61	0.82
1:A:936:A:H3'	1:A:937:U:H5''	1.59	0.82
2:B:55:PHE:HE1	2:B:218:ALA:HA	1.43	0.82
2:B:209:ARG:HH21	2:B:239:VAL:HG23	1.44	0.81
1:A:1005:C:H2'	1:A:1006:C:C5	2.14	0.81
1:A:916:G:H5''	7:G:102:ARG:HH22	1.44	0.81
1:A:106:G:H1'	1:A:349:G:H5'	1.62	0.81
2:B:132:LYS:O	2:B:136:VAL:HG23	1.80	0.81
19:S:11:VAL:HG13	19:S:38:SER:HB2	1.62	0.81
2:B:82:ARG:HB2	2:B:94:ASN:ND2	1.95	0.81
2:B:9:GLU:HG2	2:B:217:ARG:NH2	1.95	0.81
18:R:19:LYS:H	18:R:19:LYS:HD2	1.45	0.81
1:A:1221:U:OP1	7:G:116:ALA:HB2	1.80	0.81
11:K:48:ILE:HD11	11:K:64:ALA:HA	1.63	0.81
12:L:41:ARG:HG2	12:L:42:THR:N	1.95	0.81
1:A:1004:G:H1	1:A:1018:G:N2	1.79	0.81
1:A:666:G:H21	11:K:38:ASN:HD22	1.29	0.81
10:J:46:ARG:HG2	10:J:46:ARG:HH11	1.46	0.81
1:A:669:U:H1'	11:K:42:TRP:NE1	1.93	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:208:ILE:HD12	2:B:208:ILE:H	1.46	0.81
1:A:1192:U:H5'	1:A:1193:U:OP1	1.81	0.81
1:A:406:A:N6	1:A:408:G:H21	1.79	0.81
1:A:35:G:H2'	1:A:36:C:C6	2.15	0.80
3:C:119:ARG:NE	3:C:140:ARG:HH12	1.79	0.80
1:A:916:G:H5''	7:G:102:ARG:NH2	1.96	0.80
1:A:1521:U:O3'	22:W:1:A:OP3	1.99	0.80
1:A:1036:C:C3'	1:A:1036:C:C6	2.63	0.80
1:A:1121:G:N2	1:A:1125:G:H21	1.80	0.80
14:N:29:ARG:HH11	14:N:29:ARG:HG2	1.45	0.80
18:R:37:VAL:O	18:R:41:LYS:HG3	1.80	0.80
11:K:54:ARG:HH11	11:K:54:ARG:HB3	1.45	0.80
18:R:88:LYS:NZ	18:R:88:LYS:HB3	1.97	0.80
1:A:1237:A:H2'	1:A:1238:U:H4'	0.90	0.79
1:A:388:A:H2'	1:A:389:G:C5'	2.13	0.79
2:B:71:VAL:O	2:B:165:VAL:HG23	1.82	0.79
18:R:54:ARG:HD3	18:R:55:ARG:HG2	1.63	0.79
18:R:86:VAL:O	18:R:87:ARG:HB2	1.82	0.79
1:A:196:U:O2	20:T:105:SER:HB2	1.82	0.79
13:M:49:THR:HB	13:M:52:GLU:HG3	1.64	0.79
6:F:2:ARG:NE	6:F:69:GLU:HG2	1.97	0.79
1:A:424:U:H4'	1:A:425:A:O5'	1.80	0.79
1:A:1231:A:H4'	9:I:68:GLY:H	1.46	0.79
1:A:1261:A:O2'	1:A:1262:U:OP1	2.01	0.79
1:A:1479:A:H2	1:A:1482:G:N1	1.81	0.79
1:A:543:U:H4'	1:A:544:U:H5''	1.65	0.78
4:D:151:LYS:N	4:D:151:LYS:HD2	1.98	0.78
18:R:38:GLU:HA	18:R:41:LYS:HE2	1.64	0.78
1:A:637:G:C6	1:A:638:A:C5	2.71	0.78
1:A:50:A:OP1	1:A:50:A:C3'	2.31	0.78
1:A:201:A:H4'	20:T:68:LYS:HE2	1.65	0.78
2:B:87:ARG:HD2	2:B:233:SER:HB3	1.66	0.78
19:S:33:THR:HG22	19:S:35:SER:N	1.95	0.77
2:B:178:ARG:HG3	2:B:178:ARG:HH11	1.48	0.77
12:L:26:ALA:O	12:L:27:LEU:O	2.02	0.77
1:A:1139:A:H5'	1:A:1140:C:C6	2.19	0.77
1:A:203:A:H4'	1:A:204:G:O5'	1.83	0.77
1:A:60:A:H4'	1:A:61:G:O5'	1.84	0.77
5:E:12:LEU:HD23	5:E:31:LEU:HB2	1.66	0.77
2:B:51:LEU:HD13	2:B:201:ILE:HG23	1.66	0.77
13:M:59:TYR:O	13:M:63:THR:HG22	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1133:A:O2'	1:A:1134:A:H8	1.66	0.77
1:A:984:C:H42	1:A:1002:G:H21	1.31	0.77
2:B:114:ARG:HH11	2:B:118:LEU:HD11	1.48	0.76
1:A:952:A:H4'	1:A:953:G:H5''	1.66	0.76
1:A:1237:A:OP2	1:A:1260:A:N6	2.18	0.76
3:C:101:LEU:HD23	3:C:102:ASN:N	2.01	0.76
1:A:238:A:H4'	1:A:239:U:C5'	2.15	0.76
6:F:22:GLU:OE2	6:F:82:ARG:HD3	1.84	0.76
10:J:79:ARG:O	10:J:83:GLU:HG3	1.85	0.76
1:A:1035:G:H4'	1:A:1036:C:C5'	2.12	0.76
2:B:78:GLN:HE22	2:B:96:ARG:HH12	1.34	0.76
1:A:944:C:H4'	9:I:128:ARG:HG3	1.68	0.76
1:A:1035:G:H2'	1:A:1180:U:H5	1.48	0.76
1:A:1093:A:N1	3:C:177:THR:HG22	2.01	0.76
9:I:65:VAL:HG11	9:I:73:GLN:HB3	1.68	0.76
1:A:1068:U:H3	1:A:1081:G:H22	1.33	0.76
22:W:3:G:H22	23:X:34:70U:HN3	1.32	0.76
5:E:51:VAL:HB	5:E:52:PRO:HD3	1.68	0.76
1:A:388:A:H2'	1:A:389:G:H5'	1.69	0.75
3:C:52:LEU:H	3:C:52:LEU:HD23	1.50	0.75
4:D:162:LEU:HD22	4:D:181:MET:CE	2.16	0.75
1:A:407:A:N1	4:D:35:ARG:HB3	2.00	0.75
10:J:26:ALA:HB1	10:J:81:THR:HG23	1.68	0.75
1:A:238:A:C4'	1:A:239:U:H5'	2.16	0.75
12:L:25:PRO:C	12:L:27:LEU:H	1.88	0.75
20:T:45:GLN:HG2	20:T:91:LEU:HD22	1.69	0.75
3:C:64:VAL:HB	3:C:99:VAL:HG12	1.68	0.75
12:L:53:ARG:HG3	12:L:93:LEU:HD21	1.68	0.75
1:A:49:U:C4	1:A:359:A:C6	2.74	0.75
1:A:361:C:O2'	1:A:389:G:N2	2.20	0.75
1:A:986:C:H42	1:A:999:G:H1	1.32	0.75
2:B:211:ILE:O	2:B:215:LEU:HB2	1.87	0.75
17:Q:68:ARG:HG3	17:Q:68:ARG:HH11	1.51	0.75
12:L:74:GLY:O	12:L:102:ARG:NH2	2.15	0.75
1:A:49:U:O3'	1:A:50:A:C3'	2.35	0.74
3:C:12:LEU:HD21	14:N:51:GLY:HA2	1.67	0.74
8:H:4:ASP:OD2	8:H:7:ALA:HB2	1.87	0.74
5:E:79:GLU:HG3	5:E:93:PRO:HD2	1.69	0.74
5:E:152:ARG:HA	8:H:64:LYS:NZ	2.03	0.74
13:M:9:ILE:N	13:M:9:ILE:HD12	2.02	0.74
12:L:42:THR:HG21	12:L:52:LEU:CD2	2.17	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:15:LEU:HA	19:S:18:LYS:HB3	1.69	0.74
2:B:141:GLU:O	2:B:144:ARG:HG3	1.88	0.74
1:A:705:A:O2'	1:A:706:U:H3'	1.87	0.73
3:C:29:TYR:HE2	3:C:33:LEU:HD22	1.51	0.73
20:T:39:LYS:HD2	20:T:55:ILE:CD1	2.19	0.73
1:A:340:C:H4'	1:A:341:G:O5'	1.87	0.73
23:X:30:G:H2'	23:X:31:A:C8	2.20	0.73
3:C:3:ASN:N	3:C:3:ASN:HD22	1.84	0.73
5:E:64:ARG:O	5:E:65:ASN:HB3	1.86	0.73
1:A:1521:U:O3'	22:W:1:A:P	2.47	0.73
6:F:33:TYR:HA	6:F:71:ARG:HH21	1.53	0.73
1:A:241:A:H4'	1:A:242:G:OP1	1.88	0.73
1:A:211:G:H2'	1:A:212:C:C6	2.23	0.73
8:H:113:SER:HB2	8:H:134:ILE:HD11	1.71	0.73
20:T:10:LEU:HD12	20:T:12:ALA:HB2	1.71	0.73
19:S:12:ASP:H	19:S:38:SER:HB3	1.52	0.73
10:J:49:VAL:O	10:J:60:ARG:HA	1.87	0.73
13:M:49:THR:HG22	13:M:51:ALA:H	1.53	0.73
1:A:949:C:OP1	10:J:57:LYS:HD3	1.88	0.73
3:C:26:LYS:HD3	3:C:26:LYS:H	1.54	0.72
1:A:416:U:H5'	1:A:417:C:C5	2.23	0.72
1:A:530:A:H4'	1:A:531:G:O5'	1.88	0.72
13:M:15:VAL:HG23	13:M:43:THR:O	1.87	0.72
4:D:3:ARG:HE	4:D:3:ARG:HA	1.54	0.72
1:A:1110:C:H5''	9:I:16:ARG:HH22	1.52	0.72
18:R:33:ASP:OD2	18:R:36:ASN:HB2	1.90	0.72
7:G:138:LYS:HE2	7:G:142:GLU:OE1	1.90	0.72
2:B:80:ILE:CD1	2:B:80:ILE:H	1.98	0.72
1:A:821:G:N2	1:A:825:C:H42	1.88	0.72
19:S:47:HIS:O	19:S:62:ILE:HG22	1.89	0.72
7:G:15:ASP:OD2	7:G:18:TYR:N	2.20	0.72
1:A:689:A:H1'	11:K:29:ILE:HD11	1.70	0.72
1:A:985:C:H42	1:A:1000:G:H1	1.36	0.72
10:J:78:ASN:HB2	10:J:81:THR:HB	1.71	0.72
15:O:39:LEU:HD13	15:O:56:LEU:HB2	1.69	0.72
4:D:36:ARG:N	4:D:37:PRO:HD3	2.05	0.72
8:H:86:ILE:HG21	8:H:133:LEU:HD13	1.71	0.71
1:A:1116:G:H1	1:A:1122:C:H42	1.36	0.71
2:B:143:GLU:O	2:B:147:LYS:HG3	1.90	0.71
4:D:119:GLN:HG2	4:D:123:HIS:CD2	2.24	0.71
2:B:95:GLN:HG3	2:B:147:LYS:O	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:33:THR:HG22	19:S:34:TRP:N	2.06	0.71
2:B:16:HIS:CD2	2:B:213:LEU:HD13	2.25	0.71
6:F:99:ALA:C	6:F:101:ALA:H	1.93	0.71
20:T:67:ALA:HA	20:T:73:HIS:H	1.55	0.71
3:C:119:ARG:HE	3:C:140:ARG:NH1	1.82	0.71
5:E:137:GLU:O	5:E:141:GLN:HG3	1.90	0.71
21:V:6:ARG:HD2	21:V:15:ARG:HH12	1.55	0.71
2:B:35:GLU:HA	2:B:39:ILE:O	1.90	0.71
13:M:8:GLU:HG3	13:M:22:ILE:HG12	1.72	0.71
1:A:1349:C:C5'	10:J:60:ARG:HH12	2.02	0.71
1:A:1207:C:H4'	1:A:1208:A:OP1	1.90	0.71
1:A:1417:G:H2'	1:A:1418:U:C6	2.24	0.71
1:A:589:G:H2'	1:A:614:G:H1	1.54	0.71
2:B:235:SER:O	2:B:239:VAL:HG22	1.91	0.71
2:B:144:ARG:HA	2:B:147:LYS:HD2	1.73	0.71
1:A:637:G:C6	1:A:638:A:C4	2.79	0.70
13:M:34:LEU:HD13	13:M:41:PRO:HA	1.72	0.70
1:A:468:G:H4'	1:A:469:G:O5'	1.91	0.70
1:A:1036:C:C4	23:X:34:70U:H4'	2.26	0.70
3:C:45:LYS:HE3	3:C:46:GLU:OE2	1.90	0.70
18:R:88:LYS:HZ2	18:R:88:LYS:HB3	1.55	0.70
1:A:1288:U:H5'	13:M:109:THR:HG21	1.72	0.70
1:A:348:A:H8	1:A:348:A:H5'	1.56	0.70
14:N:27:CYS:SG	14:N:29:ARG:HB2	2.32	0.70
1:A:8:A:H4'	1:A:9:G:OP1	1.90	0.70
1:A:1185:A:H5'	1:A:1186:U:OP2	1.91	0.70
1:A:1113:G:C8	1:A:1113:G:H3'	2.27	0.70
5:E:7:GLU:O	5:E:34:VAL:HA	1.91	0.70
4:D:8:VAL:HG22	4:D:115:ARG:NH1	2.06	0.70
12:L:46:LYS:HE3	12:L:47:LYS:HG3	1.74	0.70
1:A:1349:C:H5'	10:J:60:ARG:NH1	2.04	0.70
2:B:142:LEU:HD21	2:B:146:GLN:OE1	1.92	0.70
10:J:27:ALA:HB1	10:J:31:GLY:H	1.55	0.70
16:P:51:VAL:O	16:P:52:ASP:HB3	1.91	0.70
4:D:24:GLU:O	4:D:26:CYS:N	2.24	0.70
20:T:56:MET:HE3	20:T:88:VAL:HG11	1.72	0.70
9:I:3:GLN:HG3	9:I:20:ARG:HG2	1.74	0.70
2:B:80:ILE:N	2:B:80:ILE:HD12	2.04	0.70
1:A:748:G:N2	1:A:795:C:HO2'	1.90	0.70
1:A:997:C:C2'	1:A:998:U:H5'	2.21	0.69
1:A:1521:U:HO3'	22:W:1:A:P	2.15	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:8:VAL:CG2	4:D:115:ARG:NH1	2.54	0.69
1:A:1170:C:P	10:J:51:ARG:HH22	2.16	0.69
7:G:122:HIS:HA	7:G:125:MET:HE3	1.74	0.69
1:A:951:A:OP1	14:N:31:ARG:HG2	1.91	0.69
1:A:701:G:H5'	11:K:117:ASN:ND2	2.08	0.69
12:L:70:ILE:HD13	12:L:77:LEU:HD12	1.73	0.69
17:Q:45:HIS:HB3	17:Q:72:ARG:HG2	1.75	0.69
12:L:33:ARG:HD3	12:L:62:SER:HB3	1.74	0.69
10:J:90:LEU:N	10:J:91:PRO:HD2	2.02	0.69
1:A:1287:A:N6	1:A:1312:G:H1'	2.07	0.69
2:B:55:PHE:CE1	2:B:218:ALA:HA	2.27	0.69
3:C:3:ASN:N	3:C:3:ASN:ND2	2.37	0.69
1:A:1110:C:O2'	1:A:1111:C:H5''	1.91	0.69
1:A:1207:C:H5''	13:M:103:THR:OG1	1.93	0.69
9:I:70:LYS:O	9:I:74:ILE:HG13	1.93	0.69
4:D:70:ILE:HD11	4:D:100:ARG:HD3	1.75	0.69
4:D:7:PRO:HB2	4:D:10:ARG:HG2	1.74	0.69
22:W:2:A:H5'	22:W:2:A:H8	1.58	0.69
2:B:78:GLN:NE2	2:B:96:ARG:HH12	1.90	0.69
4:D:36:ARG:H	4:D:37:PRO:HD3	1.57	0.69
20:T:49:ALA:HB3	20:T:99:LEU:HG	1.75	0.69
1:A:636:A:N3	1:A:636:A:H2'	2.06	0.68
1:A:1279:C:O2'	1:A:1280:A:OP2	2.12	0.68
1:A:1035:G:H2'	1:A:1180:U:C5	2.28	0.68
1:A:260:G:C2'	1:A:261:G:H5'	2.23	0.68
12:L:59:ARG:HH11	12:L:65:GLU:HB3	1.58	0.68
1:A:1406:C:C2'	1:A:1407:U:H5'	2.22	0.68
1:A:102:A:H4'	1:A:103:C:OP2	1.93	0.68
1:A:1206:A:H3'	1:A:1207:C:C6	2.28	0.68
4:D:8:VAL:HG22	4:D:115:ARG:HH12	1.57	0.68
6:F:29:ALA:HA	6:F:32:ASN:OD1	1.93	0.68
8:H:23:SER:HA	8:H:63:LEU:HD22	1.75	0.68
12:L:41:ARG:CB	12:L:41:ARG:NH1	2.54	0.68
1:A:610:G:O2'	1:A:611:G:H5'	1.92	0.68
9:I:127:LYS:HD2	9:I:127:LYS:H	1.59	0.68
7:G:111:ARG:HB3	7:G:113:GLU:OE2	1.93	0.68
26:A:1786:PAR:O62	26:A:1786:PAR:H13	1.95	0.68
6:F:2:ARG:HE	6:F:69:GLU:CG	2.07	0.68
2:B:80:ILE:HD11	2:B:208:ILE:CG2	2.24	0.67
12:L:75:HIS:HA	12:L:102:ARG:NH2	2.10	0.67
1:A:1114:C:H2'	1:A:1115:G:C8	2.29	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:62:ASP:O	3:C:97:LYS:HB3	1.95	0.67
1:A:1243:C:H2'	1:A:1244:C:C5'	2.24	0.67
1:A:1047:U:O2'	1:A:1048:C:OP2	2.10	0.67
10:J:6:ILE:HD11	10:J:72:VAL:HG11	1.76	0.67
2:B:212:GLN:HE22	2:B:235:SER:HB2	1.59	0.67
1:A:1350:G:O2'	1:A:1351:C:H5'	1.94	0.67
11:K:57:THR:HG23	11:K:60:ALA:H	1.58	0.67
7:G:125:MET:O	7:G:129:GLU:HG2	1.94	0.67
6:F:15:ASP:H	6:F:18:GLN:NE2	1.93	0.67
17:Q:59:ILE:HG22	17:Q:71:PHE:CD1	2.29	0.67
1:A:1005:C:H2'	1:A:1006:C:C6	2.30	0.67
10:J:4:ILE:O	10:J:73:ASP:HA	1.95	0.67
1:A:1516:C:C5	7:G:82:GLY:HA2	2.28	0.67
17:Q:69:LYS:C	17:Q:70:ARG:HD2	2.15	0.67
7:G:15:ASP:HB3	7:G:19:GLY:N	2.09	0.67
1:A:1119:C:H4'	1:A:1120:G:C2	2.29	0.67
1:A:670:A:H4'	1:A:671:G:O5'	1.95	0.67
1:A:170:C:OP1	20:T:29:LYS:NZ	2.27	0.67
6:F:15:ASP:H	6:F:18:GLN:HE22	1.42	0.67
9:I:10:ARG:HD3	9:I:105:ASP:HB3	1.77	0.67
1:A:1035:G:O2'	1:A:1036:C:OP2	2.06	0.67
4:D:187:ARG:HD2	4:D:188:LEU:N	2.09	0.67
1:A:416:U:H4'	1:A:417:C:OP2	1.94	0.67
1:A:433:G:H4'	1:A:434:A:OP1	1.93	0.67
19:S:77:THR:HG22	19:S:78:ARG:N	2.10	0.66
13:M:16:ASP:OD2	13:M:31:LYS:HE2	1.95	0.66
1:A:79:U:H3'	1:A:79:U:H6	1.60	0.66
19:S:62:ILE:CD1	19:S:66:MET:HG3	2.25	0.66
9:I:111:ARG:HG2	9:I:112:LYS:N	2.08	0.66
1:A:1077:U:H2'	1:A:1078:C:C6	2.30	0.66
1:A:1107:U:H3	10:J:5:ARG:HH21	1.43	0.66
1:A:120:G:HO2'	17:Q:2:PRO:N	1.94	0.66
1:A:830:G:O2'	1:A:831:G:H5'	1.96	0.66
13:M:15:VAL:HG21	13:M:48:LEU:HD21	1.78	0.66
1:A:358:A:H62	12:L:28:LYS:NZ	1.93	0.66
16:P:18:ARG:HG3	16:P:35:LYS:HE3	1.77	0.66
1:A:388:A:H2'	1:A:389:G:H5''	1.78	0.66
1:A:1047:U:H5''	1:A:1171:G:N2	2.11	0.66
1:A:507:G:H2'	1:A:508:C:C6	2.31	0.66
2:B:95:GLN:C	2:B:96:ARG:HD2	2.16	0.66
1:A:358:A:H62	12:L:28:LYS:HZ1	1.43	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:25:ASN:C	2:B:25:ASN:HD22	2.00	0.66
14:N:22:THR:CB	14:N:33:VAL:HG21	2.26	0.65
3:C:72:LYS:O	3:C:75:VAL:HG22	1.96	0.65
11:K:120:ARG:HH21	11:K:126:ARG:CZ	2.08	0.65
1:A:982:A:H5''	1:A:982:A:N3	2.10	0.65
1:A:760:A:H5''	1:A:760:A:H8	1.61	0.65
12:L:34:ARG:O	12:L:61:THR:HG23	1.96	0.65
1:A:1487:U:H2'	1:A:1488:G:C8	2.32	0.65
1:A:408:G:H2'	1:A:423:G:H22	1.62	0.65
1:A:803:U:H4'	1:A:804:G:OP2	1.97	0.65
1:A:79:U:H3'	1:A:79:U:C6	2.32	0.65
19:S:30:LEU:O	19:S:31:ILE:HD13	1.96	0.65
1:A:382:U:H5'	1:A:383:G:OP1	1.96	0.65
1:A:1039:G:H5''	3:C:154:SER:HB2	1.79	0.65
1:A:35:G:H2'	1:A:36:C:H6	1.62	0.65
1:A:948:G:H4'	1:A:949:C:OP2	1.95	0.65
11:K:22:HIS:HB3	11:K:29:ILE:HG23	1.79	0.65
3:C:60:ALA:O	3:C:62:ASP:N	2.29	0.65
1:A:1449:U:H2'	1:A:1450:A:H8	1.62	0.65
6:F:80:ARG:NH1	6:F:88:VAL:HB	2.11	0.65
1:A:242:G:OP2	17:Q:100:LYS:HE2	1.97	0.65
1:A:1260:A:H5''	1:A:1261:A:OP1	1.97	0.65
12:L:41:ARG:HH22	12:L:57:LYS:CE	2.09	0.65
1:A:822:U:H5'	1:A:823:C:H5	1.61	0.65
1:A:1123:C:H2'	1:A:1124:G:H5'	1.79	0.65
7:G:26:PHE:CE2	7:G:30:ILE:HD11	2.32	0.65
1:A:379:G:H2'	1:A:380:C:C6	2.32	0.65
10:J:7:LYS:HB3	10:J:97:GLU:HB3	1.78	0.65
9:I:106:ALA:O	9:I:108:VAL:HG23	1.97	0.65
21:V:5:ASP:O	21:V:11:GLY:HA3	1.97	0.65
2:B:103:THR:HG23	2:B:176:GLU:OE1	1.97	0.65
13:M:3:ARG:NH1	13:M:7:VAL:HG12	2.12	0.64
2:B:21:ARG:HD3	2:B:21:ARG:N	2.11	0.64
1:A:348:A:H5'	1:A:348:A:C8	2.32	0.64
1:A:660:U:H3	1:A:696:G:H22	1.44	0.64
4:D:164:ALA:O	4:D:168:ARG:HD3	1.98	0.64
1:A:238:A:C5'	1:A:239:U:H5'	2.27	0.64
9:I:40:LEU:O	9:I:42:ARG:N	2.30	0.64
1:A:1108:U:H2'	1:A:1109:G:H5'	1.79	0.64
20:T:53:LEU:HB2	20:T:100:ILE:CG2	2.28	0.64
4:D:187:ARG:CD	4:D:188:LEU:H	2.10	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:A:O2'	1:A:125:C:O5'	2.14	0.64
9:I:127:LYS:HE2	13:M:126:LYS:CE	2.28	0.64
1:A:982:A:N6	1:A:1019:C:H42	1.96	0.64
1:A:198:U:O4'	20:T:103:GLY:HA2	1.97	0.64
15:O:45:VAL:HG12	15:O:46:HIS:H	1.63	0.64
1:A:1381:C:H4'	1:A:1382:C:O5'	1.96	0.64
1:A:494:C:HO2'	1:A:495:U:C5'	2.10	0.64
1:A:1236:G:C2	1:A:1263:C:N3	2.65	0.64
2:B:223:ILE:HG13	2:B:224:GLN:N	2.10	0.64
1:A:442:A:OP2	1:A:469:G:N2	2.22	0.64
2:B:25:ASN:HD22	2:B:26:PRO:N	1.96	0.64
7:G:16:LEU:H	7:G:16:LEU:HD22	1.62	0.64
1:A:31:G:N1	1:A:48:C:H5''	2.13	0.64
1:A:825:C:H6	1:A:825:C:O5'	1.80	0.64
2:B:82:ARG:O	2:B:86:GLU:HG3	1.96	0.64
11:K:84:VAL:HG23	11:K:110:ASP:HA	1.79	0.64
3:C:70:VAL:O	3:C:106:VAL:HG23	1.96	0.64
1:A:1374:G:N2	1:A:1479:A:H8	1.96	0.64
1:A:542:A:H4'	1:A:543:U:H5''	1.80	0.64
1:A:1013:G:H2'	1:A:1014:G:H8	1.61	0.64
1:A:1333:C:H2'	1:A:1334:G:C8	2.32	0.64
2:B:80:ILE:CD1	2:B:208:ILE:HG23	2.26	0.64
10:J:61:GLU:OE1	14:N:45:ARG:NH1	2.31	0.64
1:A:1093:A:H61	3:C:177:THR:HG22	1.61	0.64
13:M:65:LYS:CE	13:M:69:GLU:HG2	2.27	0.64
2:B:230:VAL:HG12	2:B:231:GLU:N	2.11	0.64
1:A:93:C:H2'	1:A:94:A:C8	2.33	0.64
15:O:74:ASP:OD1	15:O:76:GLU:HB3	1.98	0.64
12:L:28:LYS:O	12:L:29:GLY:C	2.34	0.63
1:A:1421:C:OP1	20:T:38:LYS:HE2	1.98	0.63
7:G:114:ARG:HG2	7:G:114:ARG:HH11	1.63	0.63
1:A:402:G:H2'	1:A:403:A:C8	2.33	0.63
12:L:47:LYS:CB	12:L:48:PRO:CD	2.68	0.63
1:A:1124:G:H2'	1:A:1125:G:O4'	1.98	0.63
6:F:4:TYR:CZ	6:F:72:VAL:HG21	2.33	0.63
1:A:1006:C:H2'	1:A:1007:C:H5'	1.80	0.63
9:I:27:THR:HB	9:I:62:TYR:HD1	1.63	0.63
3:C:79:ARG:O	3:C:79:ARG:HG3	1.97	0.63
22:W:3:G:N2	23:X:34:70U:S2	2.71	0.63
1:A:1006:C:H6	1:A:1006:C:O5'	1.81	0.63
15:O:17:ARG:HG3	15:O:17:ARG:NH1	2.14	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:111:ILE:O	8:H:134:ILE:HB	1.98	0.63
3:C:14:ILE:HD13	3:C:14:ILE:N	2.10	0.63
15:O:70:LEU:HD12	15:O:78:TYR:CA	2.28	0.63
1:A:1337:G:H2'	1:A:1338:A:C8	2.33	0.63
1:A:406:A:H62	1:A:408:G:N2	1.90	0.63
1:A:209:U:H4'	1:A:210:U:OP1	1.98	0.63
1:A:1127:C:H5''	1:A:1128:A:OP1	1.97	0.63
6:F:44:GLY:HA2	6:F:59:TYR:CE1	2.34	0.63
19:S:33:THR:CG2	19:S:35:SER:H	1.98	0.63
18:R:36:ASN:ND2	18:R:38:GLU:HG2	2.13	0.63
17:Q:70:ARG:N	17:Q:70:ARG:HD2	2.14	0.63
1:A:79:U:H2'	1:A:81:U:OP2	1.98	0.63
9:I:46:ALA:HA	9:I:78:LYS:HB2	1.80	0.63
3:C:64:VAL:HG12	3:C:66:VAL:HG23	1.81	0.63
15:O:2:PRO:C	15:O:38:ARG:HH22	2.01	0.63
1:A:1262:U:H5'	1:A:1263:C:H5	1.64	0.63
4:D:162:LEU:HD22	4:D:181:MET:HE3	1.79	0.63
2:B:77:ALA:HB2	2:B:211:ILE:HD13	1.81	0.63
1:A:1509:U:H2'	1:A:1510:C:C5'	2.28	0.63
6:F:100:ASN:HB2	18:R:23:LYS:HZ2	1.63	0.63
1:A:823:C:H3'	1:A:823:C:OP2	1.99	0.62
12:L:59:ARG:HH11	12:L:65:GLU:CB	2.11	0.62
6:F:99:ALA:O	6:F:101:ALA:N	2.32	0.62
15:O:70:LEU:HD12	15:O:78:TYR:HA	1.80	0.62
12:L:41:ARG:HD2	12:L:42:THR:O	1.99	0.62
1:A:1203:G:OP1	19:S:77:THR:HG21	1.98	0.62
4:D:62:GLN:HE22	4:D:65:ARG:NH1	1.97	0.62
12:L:89:ARG:HH21	12:L:97:ARG:HH21	1.47	0.62
1:A:1259:U:H5''	1:A:1260:A:H5'	1.80	0.62
12:L:47:LYS:CB	12:L:48:PRO:HD2	2.22	0.62
12:L:41:ARG:HH22	12:L:57:LYS:NZ	1.96	0.62
5:E:57:LYS:HG2	5:E:61:TYR:CE2	2.34	0.62
16:P:28:ARG:HG3	16:P:29:ASP:OD2	1.99	0.62
1:A:1307:C:OP1	21:V:12:LYS:NZ	2.31	0.62
1:A:686:G:O2'	1:A:687:A:OP2	2.16	0.62
26:A:1786:PAR:O44	26:A:1786:PAR:N64	2.30	0.62
6:F:8:ILE:HD11	6:F:79:LEU:HD13	1.80	0.62
1:A:506:A:H61	12:L:92:ASP:HB2	1.62	0.62
3:C:179:ARG:O	3:C:179:ARG:HG2	1.96	0.62
1:A:1286:G:N2	1:A:1312:G:O2'	2.33	0.62
12:L:27:LEU:O	12:L:29:GLY:N	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1286:G:N2	1:A:1312:G:C2'	2.62	0.62
1:A:1110:C:C5'	9:I:16:ARG:HH22	2.12	0.62
12:L:46:LYS:CE	12:L:47:LYS:HG3	2.28	0.62
1:A:542:A:H4'	1:A:543:U:C5'	2.30	0.62
13:M:120:LYS:HZ1	13:M:123:ALA:HB3	1.64	0.62
15:O:26:GLU:OE1	15:O:77:ARG:HD2	1.99	0.62
1:A:1110:C:H5''	9:I:16:ARG:NH2	2.14	0.62
1:A:867:G:O2'	1:A:868:U:OP2	2.18	0.62
1:A:1171:G:OP1	3:C:4:LYS:HA	2.00	0.62
17:Q:63:ARG:O	17:Q:65:ILE:HD12	2.00	0.62
9:I:9:ARG:HG2	9:I:14:VAL:HG22	1.82	0.62
1:A:923:A:H2'	1:A:924:G:C8	2.34	0.62
1:A:774:G:H2'	1:A:775:A:H5'	1.82	0.62
6:F:21:LEU:O	6:F:25:ILE:HG13	2.00	0.62
4:D:36:ARG:HH11	4:D:36:ARG:HG2	1.65	0.62
14:N:8:GLU:O	14:N:11:LYS:HB2	2.00	0.62
3:C:154:SER:OG	3:C:155:GLY:N	2.33	0.62
1:A:997:C:H2'	1:A:998:U:C5'	2.30	0.62
1:A:726:U:H2'	1:A:727:C:C6	2.35	0.62
13:M:120:LYS:HZ2	13:M:123:ALA:HB3	1.63	0.61
2:B:178:ARG:NH1	2:B:178:ARG:HG3	2.13	0.61
7:G:137:LYS:O	7:G:141:VAL:HG23	2.00	0.61
12:L:59:ARG:HH11	12:L:65:GLU:CG	2.12	0.61
10:J:26:ALA:HA	10:J:84:GLN:HE22	1.65	0.61
20:T:57:ARG:HH22	20:T:100:ILE:HG12	1.65	0.61
4:D:28:SER:O	4:D:30:LYS:N	2.32	0.61
10:J:49:VAL:HG22	14:N:41:ARG:HB2	1.82	0.61
11:K:48:ILE:O	11:K:48:ILE:HG22	2.00	0.61
4:D:98:GLU:HG2	4:D:189:PRO:HG3	1.83	0.61
1:A:1121:G:H21	1:A:1125:G:H21	1.46	0.61
1:A:984:C:H3'	1:A:984:C:H6	1.65	0.61
1:A:705:A:H1'	1:A:706:U:H6	1.65	0.61
1:A:1267:A:C8	1:A:1268:A:H4'	2.36	0.61
3:C:3:ASN:ND2	3:C:3:ASN:H	1.97	0.61
1:A:260:G:H2'	1:A:261:G:H5'	1.82	0.61
8:H:91:ARG:HG3	12:L:7:ILE:HG13	1.83	0.61
3:C:139:GLN:HA	3:C:139:GLN:NE2	2.15	0.61
1:A:328:G:H4'	20:T:16:HIS:CE1	2.35	0.61
1:A:1209:C:H4'	13:M:116:THR:HA	1.82	0.61
18:R:53:ARG:HG2	18:R:63:GLN:OE1	2.00	0.61
2:B:17:PHE:HA	2:B:44:LEU:HD21	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:125:ARG:HH12	13:M:126:LYS:CG	2.13	0.61
2:B:169:LYS:HD3	2:B:169:LYS:O	2.00	0.61
2:B:41:ILE:HD12	2:B:41:ILE:N	2.15	0.61
1:A:1267:A:C2	21:V:18:TYR:OH	2.54	0.61
3:C:64:VAL:CB	3:C:99:VAL:HG12	2.30	0.61
7:G:79:ARG:NH1	7:G:83:ALA:HA	2.15	0.61
13:M:108:ARG:NH2	13:M:114:ARG:HA	2.16	0.61
1:A:1134:A:H2'	1:A:1135:C:O4'	2.01	0.60
1:A:367:C:C5'	1:A:368:A:OP1	2.45	0.60
1:A:1203:G:P	19:S:77:THR:HG21	2.41	0.60
4:D:104:VAL:HG21	4:D:140:VAL:HG21	1.83	0.60
13:M:22:ILE:HD12	13:M:25:ILE:HD12	1.83	0.60
2:B:226:ARG:HH11	2:B:226:ARG:HG2	1.66	0.60
1:A:1080:C:H2'	1:A:1081:G:C8	2.35	0.60
1:A:323:C:O2	1:A:323:C:H2'	2.02	0.60
5:E:105:VAL:HB	5:E:106:PRO:HD3	1.82	0.60
1:A:563:U:H2'	1:A:564:G:O4'	2.01	0.60
3:C:76:VAL:O	3:C:83:ARG:HG2	2.01	0.60
2:B:87:ARG:HD2	2:B:233:SER:CB	2.30	0.60
13:M:122:LYS:HG2	23:X:40:C:H5'	1.84	0.60
1:A:814:U:H2'	1:A:815:C:H6	1.66	0.60
10:J:6:ILE:HG22	10:J:98:ILE:CG2	2.20	0.60
1:A:1077:U:H5''	1:A:1091:C:O2	2.01	0.60
10:J:40:LEU:HD11	10:J:71:LEU:HD23	1.83	0.60
13:M:125:ARG:HH12	13:M:126:LYS:HG2	1.65	0.60
1:A:1118:U:H5''	1:A:1119:C:OP2	2.01	0.60
21:V:24:ARG:O	21:V:25:LYS:HB2	2.01	0.60
7:G:29:LYS:HE2	7:G:29:LYS:HA	1.84	0.60
1:A:636:A:C5'	8:H:56:LYS:HE3	2.27	0.60
1:A:242:G:OP2	17:Q:100:LYS:HB3	2.02	0.60
1:A:930:G:H5'	1:A:942:A:H61	1.67	0.60
3:C:135:LYS:NZ	5:E:50:GLU:HG2	2.17	0.60
10:J:75:ILE:O	10:J:76:ASN:HB2	2.02	0.60
3:C:58:GLU:H	3:C:65:ALA:HB3	1.67	0.60
1:A:388:A:C2'	1:A:389:G:H5''	2.31	0.60
1:A:1113:G:H8	1:A:1113:G:H3'	1.67	0.60
1:A:52:G:C5	1:A:355:A:C2	2.90	0.60
3:C:155:GLY:HA3	3:C:163:ALA:HB1	1.84	0.60
14:N:29:ARG:NH1	14:N:29:ARG:HG2	2.15	0.60
11:K:121:PRO:HG2	11:K:126:ARG:CG	2.32	0.60
16:P:81:ARG:NH1	16:P:83:GLU:HG3	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1406:C:H2'	1:A:1407:U:C5'	2.31	0.59
1:A:701:G:C5'	11:K:117:ASN:ND2	2.64	0.59
1:A:1509:U:H2'	1:A:1510:C:H5'	1.84	0.59
1:A:520:G:OP1	12:L:113:ARG:NH2	2.34	0.59
1:A:680:U:H2'	1:A:681:G:H5'	1.83	0.59
1:A:325:C:H5''	1:A:325:C:H6	1.66	0.59
3:C:12:LEU:HD21	14:N:51:GLY:CA	2.32	0.59
10:J:78:ASN:HB2	10:J:81:THR:CB	2.32	0.59
3:C:3:ASN:O	3:C:4:LYS:HB2	2.02	0.59
19:S:4:SER:O	19:S:5:LEU:HD23	2.02	0.59
4:D:31:CYS:C	4:D:33:MET:H	2.05	0.59
1:A:49:U:O4	1:A:359:A:C5	2.55	0.59
1:A:1425:G:H5''	1:A:1426:A:H5'	0.81	0.59
19:S:15:LEU:HD23	19:S:15:LEU:N	2.14	0.59
2:B:142:LEU:O	2:B:146:GLN:HG3	2.02	0.59
7:G:145:ALA:O	7:G:146:GLU:C	2.41	0.59
2:B:36:ARG:H	2:B:41:ILE:CD1	2.15	0.59
14:N:14:PRO:O	14:N:15:LYS:HB2	2.02	0.59
13:M:3:ARG:HG2	13:M:9:ILE:HG13	1.85	0.59
1:A:339:A:C4'	1:A:340:C:OP2	2.48	0.59
1:A:1426:A:H4'	1:A:1427:G:OP1	2.02	0.59
3:C:76:VAL:O	3:C:83:ARG:HB3	2.02	0.59
1:A:1373:U:H2'	1:A:1374:G:C8	2.37	0.59
12:L:60:LEU:HB2	12:L:64:TYR:O	2.02	0.59
1:A:501:C:O2'	12:L:50:SER:HB3	2.02	0.59
6:F:23:LYS:NZ	6:F:42:GLU:OE2	2.33	0.59
1:A:959:U:H4'	1:A:960:A:O5'	2.01	0.59
1:A:731:C:H5'	1:A:732:C:OP1	2.03	0.59
4:D:11:LEU:O	4:D:15:GLU:HG2	2.01	0.59
1:A:1237:A:H1'	1:A:1239:G:O4'	2.02	0.59
1:A:937:U:O2'	1:A:1204:C:H4'	2.02	0.59
12:L:24:VAL:O	12:L:24:VAL:HG23	2.02	0.59
12:L:27:LEU:C	12:L:29:GLY:N	2.53	0.59
6:F:82:ARG:HE	6:F:82:ARG:HA	1.66	0.59
1:A:645:G:H2'	1:A:646:A:C8	2.37	0.59
9:I:11:LYS:HG2	9:I:11:LYS:O	2.03	0.59
7:G:65:ALA:O	7:G:69:VAL:HG23	2.03	0.59
1:A:1231:A:H4'	9:I:68:GLY:N	2.17	0.59
1:A:1108:U:H2'	1:A:1109:G:C5'	2.33	0.59
3:C:132:ARG:O	3:C:136:GLN:HG3	2.01	0.59
19:S:49:ILE:HD12	19:S:49:ILE:N	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:146:ILE:HD12	4:D:146:ILE:N	2.17	0.59
1:A:1262:U:H4'	1:A:1263:C:OP2	2.03	0.59
1:A:402:G:H2'	1:A:403:A:H8	1.66	0.59
1:A:1035:G:C4'	1:A:1036:C:H5'	2.16	0.59
7:G:141:VAL:O	7:G:144:MET:HB2	2.03	0.59
1:A:274:A:H5''	1:A:275:C:H3'	1.82	0.59
1:A:1039:G:H5''	3:C:154:SER:CB	2.33	0.59
1:A:821:G:H22	1:A:825:C:N4	1.92	0.59
20:T:10:LEU:HD12	20:T:12:ALA:CB	2.33	0.59
1:A:1206:A:H5'	13:M:103:THR:OG1	2.03	0.59
1:A:260:G:O2'	1:A:261:G:H5'	2.02	0.59
10:J:80:LYS:HA	10:J:83:GLU:OE1	2.03	0.58
9:I:127:LYS:HE2	13:M:126:LYS:HE2	1.85	0.58
19:S:12:ASP:HB2	19:S:35:SER:OG	2.03	0.58
1:A:1243:C:H42	1:A:1254:G:H1	1.48	0.58
11:K:34:ASP:O	11:K:36:ASP:N	2.36	0.58
13:M:52:GLU:HG2	13:M:55:ARG:HH21	1.68	0.58
3:C:15:THR:O	3:C:16:ARG:HB2	2.03	0.58
15:O:56:LEU:HA	15:O:59:MET:HE2	1.84	0.58
1:A:701:G:H4'	11:K:117:ASN:HD21	1.68	0.58
4:D:63:LYS:HD2	4:D:198:VAL:HG12	1.86	0.58
6:F:91:VAL:HG12	6:F:92:LYS:N	2.18	0.58
3:C:189:ALA:O	3:C:191:THR:HG23	2.03	0.58
1:A:238:A:H5''	1:A:239:U:H5'	1.85	0.58
1:A:48:C:C2'	1:A:49:U:OP1	2.52	0.58
10:J:24:VAL:O	10:J:24:VAL:HG12	2.04	0.58
10:J:71:LEU:O	10:J:72:VAL:HB	2.03	0.58
1:A:562:G:C5'	1:A:711:A:H1'	2.32	0.58
2:B:102:LEU:HD21	2:B:162:ILE:CD1	2.32	0.58
1:A:1206:A:H5''	1:A:1207:C:C5	2.38	0.58
2:B:124:SER:O	2:B:127:ILE:HG13	2.03	0.58
3:C:19:GLU:O	3:C:40:ARG:NH2	2.36	0.58
1:A:1316:C:O2'	1:A:1317:C:OP2	2.18	0.58
1:A:406:A:C4	1:A:408:G:H1'	2.37	0.58
12:L:115:LYS:O	12:L:117:ARG:N	2.32	0.58
2:B:91:PRO:HG2	2:B:155:LEU:HD23	1.86	0.58
1:A:1237:A:H2'	1:A:1238:U:C5'	2.32	0.58
2:B:209:ARG:HH21	2:B:239:VAL:CG2	2.15	0.58
2:B:82:ARG:HB2	2:B:94:ASN:HD22	1.69	0.58
1:A:388:A:C2'	1:A:389:G:C5'	2.82	0.58
10:J:78:ASN:O	10:J:82:ILE:HG13	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:656:G:H2'	1:A:657:G:C8	2.38	0.58
14:N:12:ARG:O	14:N:13:THR:C	2.42	0.58
6:F:10:LEU:HD12	6:F:59:TYR:O	2.02	0.58
16:P:11:SER:OG	16:P:14:ASN:HB3	2.03	0.58
10:J:4:ILE:HG13	10:J:74:ILE:O	2.03	0.58
14:N:9:LYS:HG3	14:N:22:THR:O	2.04	0.58
3:C:148:GLY:HA3	3:C:172:ARG:O	2.03	0.58
8:H:10:LEU:HD12	8:H:85:ARG:HG2	1.84	0.58
4:D:32:ALA:O	4:D:36:ARG:HB3	2.02	0.58
3:C:139:GLN:HE21	3:C:139:GLN:CA	2.15	0.58
1:A:1105:A:H2	10:J:39:PRO:HG3	1.69	0.58
1:A:1351:C:H2'	1:A:1352:G:C8	2.39	0.58
1:A:446:A:HO2'	1:A:447:A:C5'	2.15	0.58
3:C:155:GLY:O	3:C:156:ARG:HB2	2.03	0.58
2:B:108:ILE:HG22	2:B:108:ILE:O	2.04	0.58
1:A:211:G:H2'	1:A:212:C:H6	1.68	0.58
11:K:101:SER:C	11:K:103:LEU:H	2.07	0.58
2:B:10:LEU:O	2:B:12:GLU:N	2.32	0.58
7:G:59:LEU:HG	7:G:63:LYS:HE2	1.85	0.58
12:L:40:VAL:O	12:L:40:VAL:HG12	2.03	0.58
1:A:542:A:OP1	5:E:126:ARG:NH2	2.37	0.57
1:A:413:C:H2'	1:A:414:C:C6	2.39	0.57
4:D:32:ALA:C	4:D:34:GLU:H	2.07	0.57
1:A:208:U:OP2	1:A:209:U:OP2	2.22	0.57
9:I:46:ALA:O	9:I:49:PRO:HD2	2.04	0.57
1:A:1054:G:H2'	1:A:1055:U:C6	2.39	0.57
10:J:20:ALA:HB1	10:J:37:PRO:HG3	1.86	0.57
10:J:6:ILE:CG2	10:J:98:ILE:HG22	2.22	0.57
3:C:6:HIS:HD2	3:C:8:ILE:H	1.51	0.57
1:A:981:G:H2'	1:A:982:A:O4'	2.04	0.57
1:A:504:G:OP1	12:L:73:GLU:O	2.22	0.57
1:A:1157:A:H2'	1:A:1158:G:C8	2.38	0.57
1:A:264:C:H2'	1:A:265:A:C8	2.38	0.57
2:B:114:ARG:NH1	2:B:118:LEU:HD21	2.20	0.57
1:A:1449:U:H2'	1:A:1450:A:C8	2.39	0.57
7:G:69:VAL:HG21	7:G:104:LEU:HD21	1.86	0.57
11:K:12:ARG:N	11:K:12:ARG:HD2	2.19	0.57
6:F:2:ARG:HH21	6:F:69:GLU:HG2	1.69	0.57
1:A:446:A:O2'	1:A:447:A:O5'	2.22	0.57
8:H:64:LYS:HG2	8:H:79:VAL:HG21	1.87	0.57
9:I:4:TYR:CD2	9:I:88:TYR:HA	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:34:LEU:O	3:C:38:ARG:HG2	2.04	0.57
1:A:350:C:O4'	1:A:383:G:O2'	2.20	0.57
19:S:28:LYS:HD3	19:S:29:ARG:N	2.18	0.57
17:Q:92:ARG:HH11	17:Q:92:ARG:HG3	1.70	0.57
3:C:8:ILE:HG23	3:C:16:ARG:HG2	1.87	0.57
1:A:1447:G:O2'	1:A:1448:G:H5'	2.04	0.57
1:A:1036:C:H6	1:A:1036:C:H5''	1.70	0.57
20:T:36:LEU:HD12	20:T:62:LEU:HD12	1.86	0.57
1:A:1221:U:O2'	1:A:1222:G:OP1	2.21	0.57
1:A:416:U:H5'	1:A:417:C:H5	1.69	0.57
5:E:92:LYS:HB3	5:E:119:LEU:HB2	1.85	0.57
7:G:113:GLU:HG2	7:G:119:ARG:HG2	1.87	0.57
7:G:46:ALA:O	7:G:50:ILE:HG13	2.04	0.57
1:A:484:C:H2'	1:A:485:G:C8	2.40	0.57
1:A:984:C:H3'	1:A:984:C:C6	2.39	0.57
20:T:53:LEU:HD13	20:T:102:GLY:H	1.70	0.57
1:A:269:A:O2'	1:A:270:G:H8	1.88	0.57
1:A:450:C:H2'	1:A:451:C:H6	1.70	0.57
4:D:151:LYS:H	4:D:151:LYS:HD2	1.68	0.57
6:F:22:GLU:OE2	6:F:25:ILE:HD12	2.05	0.57
2:B:81:VAL:HG22	2:B:215:LEU:HD11	1.85	0.57
1:A:748:G:H22	1:A:795:C:HO2'	1.50	0.57
1:A:774:G:C2'	1:A:775:A:H5'	2.34	0.57
7:G:155:ARG:NH1	7:G:155:ARG:HA	2.19	0.57
1:A:952:A:H8	1:A:952:A:H5'	1.68	0.57
1:A:589:G:H2'	1:A:614:G:N1	2.18	0.57
3:C:19:GLU:HA	3:C:54:ARG:HH21	1.69	0.57
10:J:90:LEU:H	10:J:91:PRO:CD	2.06	0.56
1:A:705:A:H1'	1:A:706:U:C6	2.40	0.56
1:A:198:U:C1'	20:T:103:GLY:HA2	2.35	0.56
1:A:1509:U:H2'	1:A:1510:C:O5'	2.04	0.56
11:K:27:ASN:OD1	11:K:55:LYS:HB3	2.05	0.56
6:F:37:VAL:HA	6:F:65:VAL:HG12	1.87	0.56
4:D:64:LEU:HD21	4:D:97:LEU:HD13	1.87	0.56
1:A:1258:C:HO2'	1:A:1260:A:H8	1.50	0.56
3:C:154:SER:O	3:C:164:ARG:O	2.22	0.56
1:A:1219:A:C5'	1:A:1317:C:H41	2.10	0.56
19:S:17:GLU:O	19:S:21:GLU:HG3	2.05	0.56
6:F:2:ARG:NH2	6:F:69:GLU:HG2	2.19	0.56
6:F:2:ARG:CZ	6:F:69:GLU:HG2	2.35	0.56
1:A:637:G:C5	1:A:638:A:C8	2.93	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:119:GLU:HG2	2:B:142:LEU:HD11	1.86	0.56
1:A:404:G:H5''	4:D:24:GLU:HB2	1.88	0.56
4:D:98:GLU:HA	4:D:103:ASN:ND2	2.21	0.56
13:M:88:ARG:HH11	19:S:3:ARG:NH2	2.02	0.56
19:S:27:GLU:O	19:S:28:LYS:HB2	2.05	0.56
1:A:685:A:H4'	1:A:686:G:OP2	2.05	0.56
19:S:33:THR:CG2	19:S:34:TRP:N	2.68	0.56
1:A:1218:C:H3'	1:A:1219:A:H5'	1.88	0.56
1:A:821:G:H2'	1:A:822:U:H5''	1.87	0.56
3:C:107:GLN:O	3:C:108:ASN:HB3	2.05	0.56
1:A:188:U:O2'	1:A:189:U:O5'	2.19	0.56
1:A:125:C:H2'	1:A:126:C:C6	2.41	0.56
1:A:347:C:H4'	1:A:349:G:OP1	2.04	0.56
8:H:10:LEU:HD22	8:H:83:ILE:HD11	1.87	0.56
1:A:931:G:H21	1:A:1208:A:H62	1.52	0.56
1:A:501:C:HO2'	12:L:50:SER:HB3	1.70	0.56
12:L:45:PRO:HD3	12:L:51:ALA:O	2.06	0.56
4:D:112:VAL:HG22	4:D:116:GLN:OE1	2.05	0.56
4:D:150:GLU:HA	4:D:153:ARG:HG3	1.87	0.56
7:G:23:VAL:O	7:G:27:ILE:HG13	2.05	0.56
2:B:140:HIS:O	2:B:143:GLU:HB2	2.05	0.56
16:P:4:ILE:HG13	16:P:64:ALA:HB1	1.88	0.56
1:A:602:U:O2	4:D:133:VAL:HA	2.05	0.56
9:I:58:ARG:HG2	9:I:58:ARG:HH11	1.70	0.56
1:A:49:U:C4	1:A:359:A:C5	2.93	0.56
2:B:36:ARG:H	2:B:41:ILE:HD11	1.69	0.56
1:A:678:A:OP1	11:K:52:GLY:HA3	2.05	0.56
1:A:1345:A:H1'	1:A:1347:G:N7	2.20	0.56
5:E:57:LYS:HG2	5:E:61:TYR:HE2	1.67	0.56
3:C:34:LEU:O	3:C:34:LEU:HD12	2.06	0.56
1:A:269:A:HO2'	1:A:270:G:H8	1.51	0.56
4:D:92:VAL:O	4:D:96:LEU:HD13	2.06	0.56
4:D:152:SER:HB3	4:D:155:LEU:HD12	1.88	0.56
1:A:1107:U:OP1	10:J:38:ILE:HD11	2.06	0.56
6:F:99:ALA:C	6:F:101:ALA:N	2.58	0.56
1:A:1253:G:C2'	1:A:1254:G:H5'	2.36	0.56
1:A:1253:G:H2'	1:A:1254:G:H5'	1.86	0.56
9:I:125:TYR:HE1	9:I:128:ARG:HB3	1.70	0.56
17:Q:68:ARG:HG3	17:Q:68:ARG:NH1	2.19	0.56
1:A:1206:A:H5''	1:A:1207:C:H5	1.71	0.56
9:I:11:LYS:O	9:I:12:GLU:CB	2.54	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:19:LEU:O	4:D:20:TYR:C	2.44	0.56
1:A:1215:C:H5'	1:A:1347:G:OP1	2.06	0.56
19:S:13:ASP:O	19:S:17:GLU:HG2	2.05	0.56
1:A:1113:G:H2'	1:A:1114:C:O4'	2.06	0.56
13:M:23:TYR:CB	13:M:67:GLU:HA	2.36	0.56
6:F:101:ALA:HB2	18:R:28:GLU:CA	2.32	0.56
1:A:1193:U:H3'	1:A:1193:U:C6	2.40	0.56
2:B:47:THR:HA	2:B:202:PRO:HG2	1.88	0.56
10:J:26:ALA:CB	10:J:81:THR:HG23	2.35	0.56
20:T:96:GLY:O	20:T:97:ALA:HB3	2.06	0.56
3:C:5:ILE:O	3:C:5:ILE:HD12	2.06	0.56
2:B:60:ASP:OD1	2:B:64:ARG:NH2	2.39	0.56
13:M:6:GLY:O	13:M:8:GLU:HG2	2.05	0.56
1:A:124:A:H1'	1:A:258:A:O2'	2.06	0.56
1:A:1042:C:C5	3:C:2:GLY:HA2	2.41	0.56
22:W:1:A:H2'	22:W:2:A:H5'	1.87	0.55
1:A:736:A:H4'	1:A:737:C:O5'	2.06	0.55
16:P:34:GLU:OE2	16:P:55:ARG:HD3	2.06	0.55
1:A:951:A:OP2	14:N:41:ARG:NH1	2.38	0.55
14:N:12:ARG:NH1	14:N:12:ARG:HA	2.21	0.55
21:V:6:ARG:CD	21:V:15:ARG:HH12	2.19	0.55
12:L:119:LYS:O	12:L:120:TYR:HB2	2.07	0.55
9:I:33:PHE:C	9:I:35:GLU:H	2.10	0.55
1:A:408:G:H2'	1:A:423:G:H21	1.71	0.55
1:A:701:G:C4'	11:K:117:ASN:ND2	2.68	0.55
1:A:1278:C:H1'	1:A:1279:C:H5	1.71	0.55
2:B:111:ARG:HB3	2:B:149:LEU:HD11	1.87	0.55
9:I:23:ASN:O	9:I:57:GLY:HA2	2.07	0.55
1:A:51:A:OP2	1:A:52:G:H8	1.90	0.55
10:J:8:LEU:CB	10:J:70:ARG:HB2	2.24	0.55
1:A:106:G:C1'	1:A:349:G:H5'	2.36	0.55
10:J:26:ALA:HB2	10:J:85:LEU:HD21	1.88	0.55
17:Q:100:LYS:HD2	17:Q:101:ARG:HE	1.71	0.55
1:A:1126:G:H3'	1:A:1126:G:H8	1.72	0.55
20:T:43:LEU:HD13	20:T:51:GLU:HG3	1.88	0.55
1:A:123:G:O2'	1:A:189:U:H5''	2.06	0.55
1:A:1209:C:OP1	13:M:115:LYS:HE3	2.06	0.55
14:N:9:LYS:HD3	14:N:9:LYS:C	2.26	0.55
1:A:1204:C:OP1	1:A:1205:G:H3'	2.06	0.55
2:B:114:ARG:NH1	2:B:118:LEU:HD11	2.20	0.55
5:E:101:ILE:HD12	5:E:119:LEU:HD23	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:127:LYS:HD2	9:I:127:LYS:N	2.22	0.55
9:I:11:LYS:O	9:I:12:GLU:HB3	2.06	0.55
1:A:1499:U:O2'	1:A:1500:G:H5'	2.06	0.55
1:A:1379:C:H4'	1:A:1380:A:OP2	2.05	0.55
1:A:952:A:C4'	1:A:953:G:H5''	2.36	0.55
14:N:3:ARG:NH1	14:N:6:LEU:HD11	2.21	0.55
10:J:46:ARG:HG2	10:J:46:ARG:NH1	2.19	0.55
1:A:1093:A:N6	3:C:177:THR:HG22	2.22	0.55
1:A:1202:G:O3'	19:S:77:THR:HG21	2.07	0.55
15:O:71:GLN:HB2	15:O:78:TYR:CD1	2.42	0.55
1:A:1294:U:H5	19:S:4:SER:HB2	1.70	0.55
3:C:188:LEU:O	3:C:189:ALA:HB2	2.07	0.55
1:A:603:C:C1'	4:D:135:LEU:HD13	2.37	0.55
1:A:353:U:H2'	1:A:354:U:H6	1.72	0.55
1:A:408:G:C2'	1:A:423:G:N2	2.67	0.55
1:A:1123:C:C2'	1:A:1124:G:H5'	2.37	0.55
1:A:542:A:O2'	1:A:543:U:OP2	2.19	0.55
1:A:1013:G:H2'	1:A:1014:G:C8	2.42	0.55
18:R:87:ARG:O	18:R:88:LYS:HB2	2.06	0.55
6:F:42:GLU:HG3	6:F:61:LEU:HD23	1.88	0.55
4:D:8:VAL:HG21	4:D:115:ARG:NH1	2.21	0.55
7:G:23:VAL:HG13	7:G:43:PHE:CE2	2.42	0.55
7:G:38:LEU:HD12	7:G:38:LEU:O	2.06	0.55
1:A:1259:U:C5'	1:A:1260:A:H5'	2.36	0.55
18:R:38:GLU:CD	18:R:38:GLU:H	2.10	0.55
2:B:118:LEU:CB	2:B:142:LEU:HD12	2.37	0.55
1:A:1113:G:C3'	1:A:1113:G:C8	2.89	0.55
1:A:930:G:C5'	1:A:942:A:H61	2.20	0.55
1:A:1119:C:H5'	1:A:1120:G:C6	2.42	0.55
13:M:81:LEU:O	13:M:86:CYS:HB3	2.07	0.55
3:C:134:ILE:HD11	3:C:153:VAL:CG2	2.36	0.55
2:B:189:ASP:HB3	2:B:203:GLY:O	2.07	0.55
1:A:49:U:HO2'	1:A:50:A:P	2.30	0.55
1:A:1267:A:H8	1:A:1268:A:H4'	1.71	0.55
2:B:17:PHE:CD1	2:B:18:GLY:N	2.75	0.55
1:A:275:C:H4'	1:A:276:G:OP2	2.05	0.55
1:A:1042:C:C6	3:C:2:GLY:HA2	2.41	0.55
9:I:118:LYS:O	9:I:119:ALA:HB3	2.07	0.55
7:G:13:GLN:NE2	7:G:14:PRO:HD2	2.21	0.55
1:A:1036:C:H2'	1:A:1037:A:H5''	1.89	0.54
5:E:64:ARG:HG2	5:E:64:ARG:NH1	2.17	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:984:C:N4	1:A:1002:G:H21	2.01	0.54
10:J:45:ARG:O	10:J:64:GLU:HA	2.07	0.54
1:A:776:U:H4'	1:A:777:A:OP2	2.07	0.54
12:L:111:LYS:HG2	12:L:112:ASP:N	2.21	0.54
6:F:69:GLU:HA	6:F:72:VAL:HG23	1.89	0.54
1:A:1296:U:OP2	19:S:6:LYS:NZ	2.39	0.54
1:A:48:C:HO2'	1:A:49:U:P	2.19	0.54
1:A:775:A:O2'	1:A:777:A:N7	2.39	0.54
1:A:500:G:O2'	1:A:501:C:OP2	2.19	0.54
4:D:199:ASN:ND2	4:D:201:GLN:H	2.05	0.54
1:A:1348:C:H2'	1:A:1349:C:H6	1.72	0.54
1:A:1121:G:N2	1:A:1126:G:H22	2.06	0.54
1:A:245:A:H4'	1:A:246:G:O5'	2.07	0.54
1:A:415:U:O2'	1:A:416:U:H5''	2.07	0.54
1:A:418:G:H2'	1:A:419:G:O4'	2.08	0.54
3:C:111:LEU:HD11	3:C:144:SER:O	2.07	0.54
5:E:35:GLY:HA2	5:E:40:ARG:O	2.07	0.54
1:A:1023:A:H2'	1:A:1024:G:C8	2.41	0.54
7:G:120:ILE:H	7:G:120:ILE:HD12	1.72	0.54
1:A:1261:A:O4'	10:J:41:PRO:HG3	2.08	0.54
13:M:115:LYS:O	13:M:117:VAL:HG23	2.07	0.54
1:A:611:G:H2'	1:A:612:G:C8	2.42	0.54
9:I:43:ALA:O	9:I:45:ALA:N	2.41	0.54
2:B:59:GLU:O	2:B:63:MET:HG2	2.07	0.54
1:A:475:G:O2'	1:A:476:G:H5'	2.08	0.54
10:J:17:ASP:C	10:J:19:SER:H	2.11	0.54
5:E:152:ARG:HA	8:H:64:LYS:HZ3	1.71	0.54
1:A:1046:G:O2'	1:A:1171:G:N2	2.39	0.54
18:R:25:THR:HG22	18:R:42:ARG:HH12	1.72	0.54
1:A:437:C:H2'	1:A:438:C:H6	1.73	0.54
1:A:56:U:H2'	1:A:57:G:C8	2.43	0.54
1:A:637:G:O6	1:A:638:A:C6	2.61	0.54
10:J:51:ARG:HG3	10:J:59:SER:OG	2.07	0.54
17:Q:45:HIS:NE2	17:Q:47:PRO:HG3	2.22	0.54
6:F:10:LEU:N	6:F:10:LEU:HD12	2.22	0.54
1:A:1036:C:N3	23:X:34:70U:H4'	2.22	0.54
1:A:1123:C:H2'	1:A:1124:G:C5'	2.37	0.54
7:G:16:LEU:HD22	7:G:16:LEU:N	2.23	0.54
1:A:1220:A:H4'	1:A:1221:U:O5'	2.08	0.54
2:B:178:ARG:HH21	2:B:196:LEU:C	2.12	0.54
1:A:1197:G:O2'	1:A:1198:C:H5'	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:7:LYS:CD	19:S:7:LYS:O	2.56	0.54
1:A:352:G:O2'	1:A:353:U:H5'	2.08	0.54
13:M:23:TYR:O	13:M:25:ILE:N	2.41	0.54
10:J:60:ARG:HH11	10:J:60:ARG:HG2	1.73	0.54
1:A:1304:G:H2'	1:A:1305:A:C8	2.43	0.54
6:F:98:LEU:HD22	6:F:101:ALA:HB3	1.90	0.54
2:B:17:PHE:HA	2:B:44:LEU:CD2	2.38	0.54
13:M:34:LEU:CD1	13:M:41:PRO:HA	2.37	0.54
1:A:316:A:H4'	1:A:1417:G:O2'	2.08	0.54
1:A:748:G:H1	1:A:795:C:HO2'	1.55	0.54
7:G:144:MET:O	7:G:147:ALA:HB3	2.08	0.54
1:A:500:G:H5'	1:A:502:C:C2	2.43	0.54
2:B:69:LEU:HD12	2:B:155:LEU:HD11	1.89	0.54
3:C:167:TRP:O	3:C:168:ALA:HB3	2.08	0.54
1:A:455:C:O2'	1:A:456:G:OP1	2.23	0.54
11:K:69:ALA:O	11:K:73:MET:HG2	2.08	0.54
1:A:670:A:N6	1:A:686:G:H1'	2.23	0.53
2:B:9:GLU:HG2	2:B:217:ARG:CZ	2.37	0.53
2:B:213:LEU:O	2:B:217:ARG:HG2	2.07	0.53
1:A:1281:G:O2'	1:A:1282:U:P	2.66	0.53
1:A:636:A:H5'	8:H:56:LYS:CE	2.33	0.53
1:A:1254:G:H2'	1:A:1255:G:O4'	2.08	0.53
15:O:78:TYR:CZ	15:O:82:ILE:HD11	2.42	0.53
1:A:1062:A:H5''	5:E:16:THR:HG21	1.89	0.53
1:A:1236:G:H1	1:A:1263:C:N4	2.05	0.53
5:E:148:VAL:O	5:E:152:ARG:HG3	2.08	0.53
20:T:57:ARG:NH2	20:T:102:GLY:HA2	2.23	0.53
1:A:396:C:H1'	1:A:605:A:H1'	1.90	0.53
4:D:182:LYS:HZ3	4:D:182:LYS:HB2	1.72	0.53
1:A:637:G:C4	1:A:638:A:C8	2.97	0.53
1:A:201:A:H4'	20:T:68:LYS:CE	2.36	0.53
4:D:162:LEU:HD22	4:D:181:MET:HE2	1.89	0.53
15:O:45:VAL:O	15:O:46:HIS:C	2.47	0.53
1:A:1236:G:H1	1:A:1263:C:H42	1.56	0.53
19:S:44:MET:O	19:S:62:ILE:HG21	2.07	0.53
1:A:1014:G:H2'	1:A:1015:G:H5'	1.90	0.53
2:B:84:GLU:HB3	2:B:219:VAL:HG21	1.90	0.53
17:Q:67:LYS:O	17:Q:69:LYS:N	2.39	0.53
5:E:101:ILE:O	5:E:120:THR:HB	2.08	0.53
4:D:199:ASN:HD21	4:D:201:GLN:HB3	1.72	0.53
7:G:120:ILE:HD12	7:G:120:ILE:N	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:12:ASP:O	10:J:15:THR:HG22	2.09	0.53
2:B:108:ILE:CG2	2:B:108:ILE:O	2.56	0.53
2:B:144:ARG:HA	2:B:147:LYS:CD	2.37	0.53
5:E:144:THR:O	5:E:148:VAL:HG23	2.08	0.53
12:L:33:ARG:HG2	12:L:60:LEU:HG	1.91	0.53
7:G:113:GLU:CG	7:G:119:ARG:HG2	2.38	0.53
6:F:30:LEU:HB3	6:F:35:ALA:HB3	1.91	0.53
5:E:99:GLY:O	5:E:117:ASP:HA	2.09	0.53
2:B:212:GLN:HE22	2:B:235:SER:CB	2.20	0.53
18:R:87:ARG:HD2	18:R:88:LYS:H	1.74	0.53
12:L:25:PRO:C	12:L:27:LEU:N	2.59	0.53
20:T:50:GLU:H	20:T:99:LEU:HD12	1.73	0.53
1:A:79:U:C6	1:A:79:U:C3'	2.91	0.53
7:G:146:GLU:HA	7:G:149:ARG:HG2	1.90	0.53
1:A:738:G:OP2	15:O:65:ARG:HG2	2.08	0.53
9:I:5:TYR:CG	9:I:6:GLY:N	2.77	0.53
5:E:87:SER:HB3	5:E:131:ILE:HD13	1.90	0.53
1:A:1063:G:H5'	5:E:18:ARG:HG3	1.90	0.53
1:A:484:C:H2'	1:A:485:G:H8	1.73	0.53
1:A:600:G:H5'	16:P:45:THR:HG22	1.89	0.53
15:O:60:VAL:O	15:O:64:ARG:HG2	2.08	0.53
10:J:47:PHE:HD2	14:N:34:TYR:CD2	2.26	0.53
1:A:648:A:N3	1:A:715:C:H2'	2.24	0.53
1:A:377:A:H2'	1:A:378:A:C8	2.43	0.53
2:B:28:PHE:HE2	2:B:42:ILE:HD12	1.72	0.53
1:A:1238:U:OP2	3:C:27:LYS:HE3	2.08	0.53
13:M:8:GLU:C	13:M:9:ILE:HD12	2.29	0.53
12:L:59:ARG:HH11	12:L:65:GLU:HG3	1.73	0.53
1:A:1004:G:H2'	1:A:1005:C:H5'	1.90	0.53
3:C:58:GLU:O	3:C:59:ARG:HG2	2.09	0.53
20:T:69:GLY:O	20:T:73:HIS:CD2	2.62	0.53
1:A:1288:U:H2'	1:A:1289:U:C6	2.44	0.53
4:D:31:CYS:O	4:D:33:MET:N	2.35	0.53
11:K:101:SER:O	11:K:103:LEU:N	2.42	0.53
4:D:64:LEU:HD22	4:D:75:PHE:HE1	1.73	0.53
20:T:86:ARG:HH11	20:T:86:ARG:HG2	1.72	0.53
1:A:811:A:H2'	1:A:812:G:O4'	2.08	0.53
8:H:9:MET:HG3	8:H:26:VAL:HG21	1.91	0.53
1:A:50:A:N6	1:A:356:G:C4'	2.67	0.53
3:C:99:VAL:O	3:C:99:VAL:HG23	2.09	0.53
9:I:10:ARG:HG2	9:I:75:ASP:HB2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:121:VAL:O	4:D:134:ASP:HA	2.09	0.53
1:A:17:U:H1'	1:A:1062:A:N3	2.24	0.53
15:O:87:ILE:HG22	15:O:88:ARG:N	2.24	0.53
12:L:42:THR:HG21	12:L:52:LEU:HB3	1.91	0.53
1:A:125:C:H2'	1:A:126:C:H6	1.73	0.53
20:T:67:ALA:O	20:T:73:HIS:ND1	2.42	0.53
4:D:199:ASN:HD21	4:D:201:GLN:CB	2.22	0.53
18:R:25:THR:CG2	18:R:42:ARG:HH12	2.23	0.53
1:A:1262:U:H5'	1:A:1263:C:C5	2.42	0.52
3:C:156:ARG:H	3:C:163:ALA:HA	1.73	0.52
1:A:1125:G:O5'	1:A:1125:G:H8	1.92	0.52
17:Q:96:GLN:HB2	17:Q:105:ALA:HB2	1.91	0.52
1:A:1170:C:OP1	10:J:51:ARG:NH2	2.42	0.52
1:A:925:C:OP1	13:M:109:THR:HG22	2.09	0.52
3:C:13:GLY:HA3	14:N:57:ARG:HH21	1.74	0.52
1:A:425:A:H2'	1:A:426:A:H5'	1.91	0.52
18:R:19:LYS:HE2	18:R:54:ARG:CZ	2.39	0.52
8:H:68:ARG:HH11	8:H:68:ARG:HG2	1.73	0.52
1:A:1286:G:H22	1:A:1312:G:H2'	1.74	0.52
4:D:70:ILE:HG22	4:D:71:SER:O	2.10	0.52
2:B:25:ASN:ND2	2:B:27:LYS:H	2.07	0.52
4:D:122:ARG:NH2	4:D:134:ASP:OD2	2.42	0.52
3:C:84:ILE:HG13	3:C:88:ARG:NH1	2.23	0.52
12:L:87:GLY:HA2	12:L:98:TYR:HA	1.90	0.52
1:A:353:U:H2'	1:A:354:U:C6	2.44	0.52
1:A:1084:A:H2'	1:A:1085:C:C6	2.45	0.52
2:B:84:GLU:OE1	2:B:216:SER:HA	2.09	0.52
6:F:91:VAL:CG1	6:F:92:LYS:N	2.72	0.52
2:B:92:TYR:HH	2:B:150:SER:HG	1.57	0.52
8:H:13:ILE:O	8:H:17:THR:HG23	2.08	0.52
1:A:472:C:H6	1:A:472:C:O5'	1.92	0.52
18:R:86:VAL:O	18:R:87:ARG:CB	2.57	0.52
2:B:71:VAL:CG2	2:B:164:VAL:HG22	2.39	0.52
1:A:1110:C:C5'	9:I:16:ARG:NH2	2.72	0.52
2:B:91:PRO:HG3	2:B:154:LEU:HB2	1.91	0.52
9:I:95:LYS:O	9:I:98:PRO:HD2	2.08	0.52
3:C:23:TYR:CD2	3:C:24:ALA:N	2.77	0.52
3:C:193:TYR:HE1	3:C:196:LEU:HD11	1.73	0.52
1:A:1311:U:OP1	13:M:23:TYR:O	2.26	0.52
5:E:52:PRO:O	5:E:56:GLN:HG3	2.09	0.52
16:P:51:VAL:O	16:P:52:ASP:CB	2.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:A:O2'	1:A:311:G:OP2	2.22	0.52
1:A:952:A:C5'	1:A:953:G:H5''	2.40	0.52
1:A:1014:G:C2'	1:A:1015:G:H5'	2.40	0.52
4:D:32:ALA:C	4:D:34:GLU:N	2.63	0.52
8:H:121:ASP:O	8:H:125:ARG:HB2	2.10	0.52
18:R:22:VAL:O	18:R:26:LEU:HD13	2.09	0.52
2:B:239:VAL:HG23	2:B:239:VAL:O	2.10	0.52
6:F:82:ARG:HB2	6:F:85:VAL:CG2	2.40	0.52
10:J:60:ARG:NH1	10:J:60:ARG:HG2	2.25	0.52
1:A:1112:A:P	1:A:1113:G:OP2	2.68	0.52
20:T:67:ALA:HB2	20:T:77:ALA:HB2	1.92	0.52
1:A:816:U:H2'	1:A:817:C:H6	1.75	0.52
1:A:926:A:N7	13:M:106:ASN:ND2	2.57	0.52
1:A:1035:G:OP1	1:A:1036:C:H5	1.93	0.52
13:M:117:VAL:HG12	13:M:118:ALA:N	2.18	0.52
20:T:54:LYS:HA	20:T:57:ARG:NH1	2.25	0.52
1:A:603:C:N1	4:D:135:LEU:HD13	2.24	0.52
16:P:74:LEU:O	16:P:79:VAL:HG23	2.09	0.52
12:L:55:VAL:HG12	12:L:56:ALA:N	2.25	0.51
2:B:78:GLN:NE2	2:B:96:ARG:NH1	2.56	0.51
1:A:1193:U:H6	1:A:1193:U:H3'	1.75	0.51
2:B:17:PHE:HD1	2:B:18:GLY:H	1.58	0.51
2:B:211:ILE:HG22	2:B:215:LEU:HD12	1.92	0.51
16:P:36:ILE:O	16:P:51:VAL:O	2.28	0.51
1:A:916:G:H2'	1:A:917:C:C6	2.45	0.51
12:L:109:GLY:HA3	12:L:121:GLY:O	2.10	0.51
1:A:392:A:N7	1:A:530:A:O2'	2.35	0.51
3:C:38:ARG:NH1	3:C:38:ARG:HG3	2.25	0.51
1:A:453:G:H3'	1:A:454:A:C5'	2.40	0.51
1:A:31:G:H4'	1:A:32:A:OP2	2.10	0.51
1:A:1236:G:H2'	1:A:1260:A:H62	1.76	0.51
10:J:16:LEU:HD23	10:J:94:VAL:HG22	1.93	0.51
10:J:96:ILE:N	10:J:96:ILE:HD12	2.25	0.51
3:C:70:VAL:HG21	3:C:76:VAL:CG2	2.34	0.51
1:A:1303:C:C4'	1:A:1304:G:OP1	2.56	0.51
1:A:167:U:H5''	1:A:203:A:O4'	2.10	0.51
2:B:118:LEU:HB3	2:B:142:LEU:HD12	1.92	0.51
10:J:80:LYS:HD3	10:J:83:GLU:OE1	2.10	0.51
1:A:1293:G:N7	19:S:3:ARG:O	2.43	0.51
16:P:45:THR:HB	16:P:46:PRO:HD2	1.91	0.51
1:A:798:A:H5''	1:A:800:C:N4	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:8:GLU:HA	5:E:33:VAL:O	2.10	0.51
1:A:108:G:H1'	1:A:109:A:N7	2.26	0.51
1:A:1027:C:H2'	1:A:1028:A:O5'	2.10	0.51
1:A:1130:U:H2'	1:A:1131:C:O4'	2.10	0.51
1:A:1015:G:H2'	1:A:1016:G:C8	2.45	0.51
1:A:988:G:N2	1:A:998:U:H1'	2.25	0.51
1:A:1469:A:H1'	22:W:2:A:O2'	2.10	0.51
13:M:49:THR:HG22	13:M:51:ALA:N	2.22	0.51
5:E:103:GLY:O	5:E:106:PRO:HD2	2.11	0.51
5:E:36:ASP:CG	5:E:40:ARG:HB2	2.31	0.51
1:A:1073:U:O2	1:A:1075:A:C8	2.63	0.51
1:A:66:G:C8	1:A:66:G:OP1	2.64	0.51
1:A:1348:C:H2'	1:A:1349:C:C6	2.45	0.51
2:B:222:ILE:O	2:B:226:ARG:HG3	2.11	0.51
1:A:982:A:H62	1:A:1019:C:H42	1.58	0.51
1:A:512:G:O6	12:L:49:ASN:HA	2.11	0.51
6:F:50:TYR:CE1	18:R:77:GLY:HA2	2.46	0.51
1:A:49:U:N3	1:A:359:A:N6	2.59	0.51
13:M:22:ILE:CD1	13:M:25:ILE:HD12	2.40	0.51
2:B:15:VAL:HG21	2:B:209:ARG:HB3	1.91	0.51
1:A:239:U:H4'	1:A:240:C:O5'	2.10	0.51
1:A:383:G:O2'	1:A:384:A:P	2.69	0.51
1:A:379:G:H2'	1:A:380:C:H6	1.75	0.51
6:F:100:ASN:OD1	18:R:23:LYS:O	2.28	0.51
1:A:1295:C:O2'	1:A:1296:U:H5'	2.11	0.51
1:A:1145:C:H2'	1:A:1146:G:H8	1.76	0.51
1:A:1164:A:O2'	1:A:1165:G:OP1	2.24	0.51
2:B:48:MET:O	2:B:52:GLU:HB2	2.11	0.51
1:A:961:C:H2'	1:A:962:C:H6	1.75	0.51
8:H:4:ASP:CG	8:H:85:ARG:HH11	2.14	0.51
7:G:15:ASP:HB3	7:G:19:GLY:H	1.75	0.51
2:B:97:TRP:CH2	2:B:176:GLU:OE2	2.64	0.51
1:A:1108:U:C2'	1:A:1109:G:H5'	2.40	0.51
7:G:75:VAL:HG21	7:G:144:MET:HE1	1.93	0.51
2:B:91:PRO:HG3	2:B:154:LEU:CB	2.40	0.51
1:A:1238:U:OP2	3:C:27:LYS:CE	2.58	0.51
2:B:98:LEU:O	2:B:101:MET:HG3	2.10	0.51
2:B:218:ALA:O	2:B:222:ILE:HG13	2.11	0.51
12:L:27:LEU:C	12:L:29:GLY:H	2.13	0.51
1:A:1206:A:N3	1:A:1206:A:H2'	2.26	0.51
1:A:385:C:H2'	1:A:386:G:C8	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:74:GLY:HA3	5:E:116:THR:HG22	1.91	0.51
5:E:47:LYS:HD3	5:E:47:LYS:N	2.25	0.51
1:A:705:A:H5''	1:A:706:U:OP1	2.10	0.51
1:A:701:G:H4'	11:K:117:ASN:ND2	2.25	0.51
4:D:194:LEU:HD22	4:D:194:LEU:N	2.25	0.51
7:G:69:VAL:HG12	7:G:69:VAL:O	2.11	0.51
1:A:1182:A:H4'	1:A:1183:G:O5'	2.11	0.51
1:A:190:G:H4'	1:A:191:G:OP2	2.11	0.51
1:A:49:U:N3	1:A:359:A:C6	2.78	0.51
12:L:57:LYS:HG2	12:L:67:THR:HG22	1.92	0.51
19:S:15:LEU:O	19:S:19:VAL:N	2.39	0.51
1:A:1126:G:H3'	1:A:1126:G:C8	2.46	0.51
2:B:223:ILE:HD12	2:B:230:VAL:H	1.75	0.51
1:A:984:C:C3'	1:A:984:C:C6	2.93	0.51
5:E:144:THR:H	5:E:147:ASP:HB2	1.76	0.51
20:T:50:GLU:HB2	20:T:99:LEU:HD12	1.92	0.51
18:R:53:ARG:NH1	18:R:59:SER:HA	2.26	0.51
5:E:50:GLU:HB2	5:E:53:LEU:HD12	1.93	0.51
4:D:175:SER:OG	4:D:184:LYS:HB3	2.09	0.51
19:S:55:LYS:O	19:S:56:GLN:HG3	2.11	0.51
1:A:980:G:H3'	1:A:980:G:C8	2.45	0.51
1:A:669:U:O4	1:A:686:G:O2'	2.29	0.50
3:C:157:ILE:HG21	3:C:164:ARG:NH2	2.26	0.50
1:A:123:G:C2	1:A:189:U:H5'	2.46	0.50
2:B:223:ILE:HG13	2:B:224:GLN:H	1.76	0.50
1:A:983:A:H5'	1:A:984:C:C2	2.45	0.50
3:C:179:ARG:O	3:C:179:ARG:CG	2.56	0.50
4:D:189:PRO:HB2	4:D:194:LEU:HD21	1.93	0.50
1:A:690:C:H2'	1:A:691:C:C6	2.46	0.50
1:A:858:G:P	12:L:12:ARG:HH22	2.33	0.50
1:A:1376:A:O5'	1:A:1376:A:H8	1.93	0.50
3:C:91:LEU:HB3	3:C:99:VAL:HG21	1.92	0.50
3:C:64:VAL:CG2	3:C:99:VAL:HG12	2.40	0.50
11:K:18:ARG:NH1	11:K:36:ASP:HA	2.26	0.50
1:A:1093:A:C6	3:C:177:THR:HG22	2.46	0.50
20:T:53:LEU:HB2	20:T:100:ILE:HG22	1.93	0.50
3:C:38:ARG:HH11	3:C:38:ARG:HG3	1.76	0.50
15:O:53:HIS:CE1	15:O:57:LEU:HD11	2.47	0.50
1:A:423:G:H4'	1:A:424:U:O5'	2.11	0.50
2:B:21:ARG:NE	2:B:23:ARG:HD2	2.26	0.50
12:L:33:ARG:CD	12:L:62:SER:HB3	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:78:ARG:HH11	7:G:154:TYR:HB3	1.76	0.50
1:A:961:C:H2'	1:A:962:C:C6	2.46	0.50
1:A:699:A:H2'	1:A:700:C:O4'	2.11	0.50
1:A:330:C:H2'	1:A:331:C:C6	2.46	0.50
10:J:95:GLU:C	10:J:96:ILE:HD12	2.31	0.50
3:C:46:GLU:HB3	3:C:83:ARG:HH21	1.77	0.50
1:A:635:U:O5'	1:A:635:U:H6	1.94	0.50
17:Q:92:ARG:HG3	17:Q:92:ARG:NH1	2.27	0.50
1:A:334:C:H2'	1:A:335:U:C6	2.47	0.50
1:A:1011:G:O2'	1:A:1012:A:H5'	2.12	0.50
1:A:685:A:HO2'	1:A:686:G:P	2.34	0.50
1:A:1286:G:N2	1:A:1312:G:H2'	2.27	0.50
1:A:1253:G:H2'	1:A:1254:G:C5'	2.41	0.50
1:A:1193:U:C6	1:A:1193:U:C3'	2.95	0.50
16:P:43:LYS:HA	16:P:48:TRP:HB3	1.94	0.50
1:A:895:A:H2'	1:A:896:A:C8	2.47	0.50
3:C:86:VAL:O	3:C:89:GLU:HB3	2.12	0.50
3:C:14:ILE:H	3:C:14:ILE:CD1	2.17	0.50
20:T:43:LEU:HD11	20:T:55:ILE:HD12	1.92	0.50
5:E:61:TYR:O	5:E:64:ARG:O	2.30	0.50
1:A:249:G:OP1	17:Q:67:LYS:O	2.29	0.50
13:M:81:LEU:HD11	13:M:88:ARG:NH2	2.26	0.50
1:A:994:A:H2'	1:A:995:G:O4'	2.12	0.50
21:V:3:LYS:HG2	21:V:14:TRP:CD1	2.47	0.50
1:A:52:G:C6	1:A:355:A:C4	3.00	0.50
1:A:514:U:H4'	1:A:515:A:OP1	2.11	0.50
13:M:6:GLY:O	13:M:7:VAL:C	2.49	0.50
1:A:637:G:C5	1:A:638:A:N7	2.80	0.50
1:A:8:A:C6	4:D:209:ARG:HA	2.47	0.50
4:D:64:LEU:HD22	4:D:75:PHE:CE1	2.46	0.50
1:A:1210:A:H2'	1:A:1211:C:C6	2.47	0.50
1:A:684:C:H5''	1:A:686:G:O4'	2.11	0.50
1:A:685:A:O2'	1:A:686:G:OP1	2.29	0.50
9:I:46:ALA:HB1	9:I:77:ILE:HG22	1.93	0.50
11:K:12:ARG:O	11:K:13:GLN:C	2.50	0.50
3:C:34:LEU:HD11	3:C:38:ARG:HD3	1.94	0.50
1:A:65:U:O2'	1:A:66:G:OP2	2.26	0.50
1:A:1328:G:O2'	1:A:1329:U:OP2	2.30	0.50
1:A:1403:G:H1	1:A:1456:C:H42	1.60	0.50
1:A:249:G:OP1	17:Q:68:ARG:HB2	2.12	0.50
18:R:53:ARG:HH11	18:R:59:SER:HA	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:11:LYS:C	11:K:12:ARG:HD2	2.32	0.50
1:A:1326:U:O2'	1:A:1327:A:OP2	2.24	0.50
1:A:1051:C:O2'	1:A:1173:C:H1'	2.12	0.50
1:A:842:A:H5'	1:A:1060:U:O4	2.12	0.50
1:A:5:U:H4'	1:A:6:G:O5'	2.11	0.50
1:A:100:G:H2'	1:A:101:G:H5'	1.94	0.50
1:A:123:G:O2'	1:A:189:U:H3'	2.12	0.49
1:A:227:G:H1'	1:A:257:A:N1	2.27	0.49
1:A:936:A:C3'	1:A:937:U:H5''	2.37	0.49
12:L:102:ARG:HG3	12:L:109:GLY:HA2	1.94	0.49
11:K:121:PRO:HG2	11:K:126:ARG:HG2	1.92	0.49
20:T:100:ILE:O	20:T:101:GLY:C	2.51	0.49
1:A:1334:G:H2'	1:A:1335:C:C6	2.46	0.49
9:I:49:PRO:O	9:I:52:ALA:HB3	2.12	0.49
1:A:1295:C:C6	19:S:6:LYS:HE2	2.47	0.49
4:D:152:SER:O	4:D:158:ILE:HD12	2.12	0.49
1:A:1461:C:H6	1:A:1461:C:O5'	1.95	0.49
1:A:1463:G:H2'	1:A:1464:G:O4'	2.12	0.49
17:Q:80:GLY:O	17:Q:81:ARG:HB3	2.12	0.49
14:N:23:ARG:HH11	14:N:23:ARG:HG2	1.76	0.49
16:P:18:ARG:O	16:P:20:VAL:HG13	2.13	0.49
1:A:816:U:H2'	1:A:817:C:C6	2.47	0.49
6:F:97:PHE:HE2	18:R:62:GLU:HG2	1.76	0.49
1:A:1475:U:H2'	1:A:1520:C:OP1	2.12	0.49
1:A:578:G:O2'	1:A:579:C:OP2	2.23	0.49
18:R:36:ASN:HD21	18:R:38:GLU:HG2	1.74	0.49
1:A:982:A:C5'	1:A:982:A:N3	2.75	0.49
3:C:132:ARG:HH11	3:C:132:ARG:HG2	1.77	0.49
1:A:959:U:O2'	1:A:960:A:OP2	2.28	0.49
2:B:52:GLU:O	2:B:56:ARG:HG3	2.12	0.49
1:A:1049:A:H4'	1:A:1050:G:O5'	2.12	0.49
17:Q:4:LYS:HD2	17:Q:6:LEU:HD21	1.94	0.49
18:R:47:THR:HG22	18:R:48:GLY:N	2.27	0.49
1:A:1297:G:N2	1:A:1299:A:H3'	2.27	0.49
5:E:143:ARG:HH12	8:H:77:GLU:CD	2.15	0.49
1:A:1282:U:O2'	1:A:1283:U:OP1	2.25	0.49
19:S:18:LYS:HA	19:S:21:GLU:OE2	2.12	0.49
2:B:21:ARG:HE	2:B:23:ARG:CD	2.24	0.49
2:B:55:PHE:CD1	2:B:221:LEU:HD22	2.48	0.49
8:H:4:ASP:OD1	8:H:85:ARG:NH1	2.46	0.49
1:A:697:G:N2	1:A:760:A:H1'	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:A:C2	1:A:378:A:C4	3.01	0.49
2:B:7:VAL:HG23	2:B:8:LYS:HG3	1.93	0.49
1:A:1383:G:C2	1:A:1384:C:H1'	2.48	0.49
1:A:1257:G:O5'	1:A:1257:G:H8	1.95	0.49
1:A:50:A:C6	1:A:356:G:C4'	2.94	0.49
1:A:49:U:O3'	1:A:50:A:O3'	2.30	0.49
5:E:82:VAL:HG11	5:E:137:GLU:HB3	1.94	0.49
5:E:76:ILE:HG13	5:E:142:LEU:CD1	2.43	0.49
1:A:704:G:H4'	1:A:705:A:O5'	2.11	0.49
1:A:942:A:H4'	1:A:943:G:O5'	2.13	0.49
14:N:11:LYS:HG2	14:N:11:LYS:O	2.11	0.49
1:A:1294:U:C5	19:S:4:SER:HB2	2.48	0.49
4:D:18:LYS:HG3	4:D:33:MET:HG3	1.93	0.49
1:A:570:G:N2	1:A:737:C:OP2	2.43	0.49
1:A:75:G:O2'	1:A:76:G:H5'	2.13	0.49
1:A:1434:G:O2'	1:A:1435:G:H5'	2.13	0.49
12:L:46:LYS:CD	12:L:47:LYS:HG3	2.41	0.49
2:B:101:MET:N	2:B:108:ILE:HD12	2.27	0.49
1:A:340:C:O2'	1:A:341:G:OP2	2.29	0.49
1:A:1407:U:H2'	1:A:1408:C:C6	2.48	0.49
1:A:1139:A:O2'	1:A:1140:C:OP2	2.24	0.49
1:A:413:C:H6	1:A:413:C:O5'	1.95	0.49
1:A:382:U:H5'	1:A:383:G:P	2.53	0.49
1:A:495:U:H1'	4:D:42:GLN:HE22	1.78	0.49
9:I:48:GLU:N	9:I:49:PRO:HD2	2.27	0.49
7:G:79:ARG:HH11	7:G:83:ALA:HA	1.77	0.49
1:A:1295:C:C5	19:S:6:LYS:HE2	2.47	0.49
3:C:20:SER:O	14:N:54:PRO:HB3	2.12	0.49
2:B:12:GLU:OE2	2:B:12:GLU:HA	2.11	0.49
3:C:130:VAL:HG12	3:C:134:ILE:HD12	1.93	0.49
1:A:1210:A:C2	1:A:1211:C:C4	3.01	0.49
1:A:465:G:C5'	1:A:466:A:OP1	2.61	0.49
1:A:669:U:H2'	1:A:670:A:O5'	2.13	0.49
19:S:33:THR:CG2	19:S:34:TRP:H	2.26	0.49
1:A:1121:G:C5'	1:A:1122:C:OP1	2.55	0.49
12:L:28:LYS:O	12:L:30:ALA:N	2.46	0.49
1:A:1207:C:H5''	13:M:103:THR:HG1	1.78	0.49
5:E:120:THR:CG2	5:E:121:LYS:N	2.73	0.49
1:A:1278:C:O2'	1:A:1279:C:OP2	2.25	0.49
1:A:264:C:H2'	1:A:265:A:H8	1.76	0.49
1:A:911:C:H4'	1:A:912:A:OP1	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:6:GLU:CD	15:O:6:GLU:H	2.15	0.49
1:A:670:A:O2'	1:A:671:G:OP2	2.29	0.49
23:X:32:C:H5''	23:X:32:C:H6	1.77	0.49
1:A:1085:C:H5''	2:B:98:LEU:HD22	1.95	0.49
1:A:521:G:OP2	12:L:115:LYS:HG3	2.13	0.49
12:L:24:VAL:O	12:L:26:ALA:N	2.38	0.49
16:P:10:GLY:HA3	16:P:14:ASN:O	2.13	0.49
4:D:153:ARG:HH12	4:D:180:GLY:HA2	1.78	0.49
4:D:199:ASN:C	4:D:199:ASN:HD22	2.16	0.49
1:A:41:G:H2'	1:A:42:G:C8	2.48	0.49
7:G:115:ARG:HB2	7:G:118:VAL:HG23	1.94	0.49
1:A:417:C:O2'	1:A:418:G:OP2	2.28	0.49
4:D:36:ARG:N	4:D:37:PRO:CD	2.75	0.49
1:A:795:C:O2'	1:A:796:U:OP2	2.30	0.49
1:A:1197:G:H5''	14:N:5:ALA:HB2	1.95	0.49
1:A:992:A:C2	1:A:1200:U:H1'	2.48	0.49
13:M:54:VAL:O	13:M:58:GLU:HG2	2.13	0.49
1:A:294:G:H2'	1:A:295:A:C8	2.48	0.49
19:S:63:THR:HG22	19:S:64:GLU:N	2.26	0.49
1:A:763:A:O2'	1:A:764:A:H5''	2.13	0.49
1:A:670:A:HO2'	1:A:671:G:P	2.35	0.49
22:W:3:G:H1	23:X:34:70U:HN3	1.58	0.49
1:A:1281:G:H1'	1:A:1282:U:H5	1.76	0.49
1:A:1479:A:N3	1:A:1479:A:H2'	2.27	0.49
11:K:48:ILE:CD1	11:K:64:ALA:HA	2.40	0.49
4:D:63:LYS:O	4:D:67:ILE:HG13	2.13	0.49
13:M:90:LEU:HD23	13:M:93:ARG:NH1	2.27	0.49
8:H:22:GLU:OE2	8:H:22:GLU:HA	2.12	0.49
1:A:30:U:O2'	1:A:31:G:OP1	2.24	0.48
12:L:46:LYS:HD2	12:L:47:LYS:HG3	1.94	0.48
1:A:1135:C:OP1	10:J:13:HIS:HE1	1.96	0.48
10:J:46:ARG:HH11	10:J:46:ARG:CG	2.21	0.48
1:A:1206:A:H4'	1:A:1207:C:OP2	2.12	0.48
4:D:58:LEU:O	4:D:58:LEU:HD22	2.13	0.48
1:A:385:C:O3'	16:P:28:ARG:NH2	2.46	0.48
7:G:88:PRO:HB3	7:G:145:ALA:HB1	1.95	0.48
4:D:29:PRO:O	4:D:30:LYS:HG3	2.13	0.48
17:Q:15:MET:HE1	17:Q:43:LEU:HD22	1.95	0.48
1:A:705:A:H3'	1:A:705:A:N3	2.28	0.48
17:Q:100:LYS:HD2	17:Q:101:ARG:NE	2.27	0.48
1:A:417:C:H4'	1:A:418:G:O5'	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:121:PRO:HG2	11:K:126:ARG:HG3	1.95	0.48
17:Q:89:LEU:O	17:Q:92:ARG:HB3	2.13	0.48
1:A:99:C:O2	1:A:374:C:H4'	2.13	0.48
1:A:516:A:O2'	1:A:518:A:OP2	2.31	0.48
1:A:262:C:H2'	1:A:263:C:C6	2.48	0.48
12:L:78:GLN:O	12:L:80:HIS:N	2.38	0.48
1:A:1106:G:O5'	10:J:35:SER:O	2.31	0.48
1:A:1349:C:C5'	10:J:60:ARG:NH1	2.72	0.48
1:A:636:A:N3	1:A:636:A:C2'	2.73	0.48
3:C:14:ILE:CD1	3:C:14:ILE:N	2.75	0.48
14:N:22:THR:O	14:N:23:ARG:HB2	2.12	0.48
1:A:637:G:N1	1:A:638:A:C4	2.81	0.48
2:B:47:THR:O	2:B:51:LEU:HB2	2.13	0.48
2:B:195:ASP:O	8:H:74:PRO:HG3	2.13	0.48
2:B:97:TRP:CZ3	2:B:176:GLU:OE2	2.66	0.48
10:J:32:ALA:HB1	10:J:75:ILE:O	2.14	0.48
4:D:17:VAL:HG11	4:D:197:PRO:HB2	1.96	0.48
4:D:126:ILE:HG22	4:D:127:THR:N	2.28	0.48
2:B:220:ASP:O	2:B:224:GLN:HG3	2.13	0.48
2:B:132:LYS:HD2	2:B:135:GLN:HB2	1.96	0.48
1:A:1139:A:H4'	1:A:1140:C:O5'	2.13	0.48
2:B:115:LEU:HD11	2:B:146:GLN:HG2	1.94	0.48
4:D:36:ARG:NH1	4:D:36:ARG:HG2	2.28	0.48
1:A:775:A:O2'	1:A:776:U:OP2	2.29	0.48
1:A:1293:G:O2'	1:A:1294:U:H5'	2.14	0.48
2:B:91:PRO:HG2	2:B:155:LEU:CD2	2.43	0.48
8:H:107:LEU:N	8:H:107:LEU:HD23	2.29	0.48
1:A:969:U:O2'	1:A:970:G:OP2	2.23	0.48
17:Q:27:PHE:HB2	17:Q:28:PRO:HD2	1.94	0.48
13:M:3:ARG:HD3	13:M:7:VAL:HA	1.95	0.48
1:A:953:G:O2'	1:A:954:A:P	2.71	0.48
7:G:50:ILE:HG22	7:G:54:THR:HG22	1.96	0.48
18:R:55:ARG:HH11	18:R:55:ARG:HA	1.78	0.48
12:L:53:ARG:CG	12:L:93:LEU:HD21	2.41	0.48
10:J:54:PHE:CD2	10:J:55:LYS:HG2	2.49	0.48
2:B:27:LYS:HD3	2:B:195:ASP:OD2	2.13	0.48
14:N:57:ARG:HG2	14:N:58:LYS:H	1.79	0.48
1:A:927:U:C5	13:M:102:ARG:NE	2.82	0.48
8:H:88:LYS:HB2	8:H:89:PRO:HD2	1.95	0.48
1:A:207:C:OP2	1:A:207:C:H6	1.96	0.48
1:A:1136:G:H2'	1:A:1137:G:H8	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:10:LEU:HD12	8:H:85:ARG:CG	2.43	0.48
1:A:323:C:O2'	1:A:324:A:OP2	2.29	0.48
1:A:1182:A:O2'	1:A:1183:G:OP2	2.27	0.48
18:R:44:LEU:HD22	18:R:48:GLY:O	2.14	0.48
19:S:19:VAL:HG13	19:S:20:LEU:N	2.28	0.48
11:K:54:ARG:NH1	11:K:54:ARG:HB3	2.22	0.48
1:A:1267:A:H2	21:V:18:TYR:OH	1.96	0.48
1:A:983:A:OP2	1:A:984:C:C5	2.67	0.48
2:B:142:LEU:C	2:B:142:LEU:HD23	2.33	0.48
9:I:125:TYR:CE1	9:I:128:ARG:HB3	2.47	0.48
10:J:82:ILE:O	10:J:86:MET:HB2	2.14	0.48
1:A:705:A:H4'	1:A:706:U:O5'	2.12	0.48
4:D:62:GLN:NE2	4:D:65:ARG:NH1	2.62	0.48
10:J:20:ALA:CB	10:J:37:PRO:HG3	2.44	0.48
4:D:52:SER:O	4:D:53:ASP:C	2.51	0.48
1:A:647:G:OP1	18:R:64:ARG:HD2	2.13	0.48
11:K:54:ARG:O	11:K:57:THR:CG2	2.55	0.48
20:T:10:LEU:O	20:T:13:LEU:HG	2.14	0.48
1:A:981:G:H2'	1:A:982:A:O5'	2.14	0.48
9:I:12:GLU:HG3	9:I:12:GLU:O	2.14	0.48
1:A:927:U:OP2	13:M:102:ARG:HG2	2.14	0.48
1:A:1328:G:HO2'	1:A:1355:G:H1	1.62	0.48
1:A:332:C:H2'	1:A:333:A:C8	2.49	0.48
3:C:147:LYS:NZ	3:C:206:GLU:HB2	2.29	0.48
1:A:44:G:OP2	16:P:12:LYS:HB2	2.14	0.48
3:C:162:GLN:OE1	3:C:163:ALA:O	2.32	0.48
23:X:34:70U:H2'	23:X:35:U:C6	2.48	0.48
3:C:44:GLU:HA	3:C:52:LEU:HD11	1.95	0.48
1:A:701:G:C5'	11:K:117:ASN:HD22	2.27	0.48
1:A:322:A:H4'	1:A:323:C:OP1	2.13	0.48
1:A:960:A:HO2'	1:A:1031:U:HO2'	1.58	0.48
1:A:525:G:H2'	1:A:526:C:H6	1.78	0.48
16:P:75:ARG:HH11	16:P:75:ARG:HG3	1.78	0.48
1:A:83:A:H2'	1:A:84:C:O4'	2.14	0.48
10:J:8:LEU:CD2	10:J:96:ILE:HG13	2.43	0.48
12:L:65:GLU:OE1	12:L:65:GLU:N	2.47	0.48
1:A:931:G:H2'	1:A:932:U:C6	2.49	0.48
1:A:1294:U:OP2	19:S:6:LYS:HA	2.14	0.48
9:I:97:LYS:HB3	9:I:98:PRO:HD3	1.95	0.48
1:A:66:G:OP1	1:A:66:G:H8	1.97	0.48
7:G:95:ARG:HG3	7:G:95:ARG:HH11	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:72:PRO:O	8:H:73:ASP:HB3	2.14	0.48
19:S:15:LEU:O	19:S:19:VAL:HG12	2.14	0.47
12:L:70:ILE:CD1	12:L:77:LEU:HD12	2.40	0.47
8:H:23:SER:HA	8:H:63:LEU:CD2	2.41	0.47
1:A:170:C:H2'	1:A:171:C:H6	1.79	0.47
3:C:5:ILE:HD13	3:C:10:PHE:HB2	1.96	0.47
1:A:330:C:H2'	1:A:331:C:H6	1.77	0.47
6:F:11:ASN:OD1	6:F:13:ASN:N	2.44	0.47
1:A:155:A:C2'	1:A:156:A:O5'	2.62	0.47
1:A:1259:U:H4'	1:A:1260:A:O4'	2.14	0.47
2:B:21:ARG:HE	2:B:23:ARG:HD2	1.79	0.47
14:N:23:ARG:NH1	14:N:30:ALA:HB2	2.30	0.47
1:A:1253:G:O2'	1:A:1254:G:H5'	2.14	0.47
3:C:58:GLU:HB2	3:C:65:ALA:HB2	1.96	0.47
11:K:34:ASP:OD1	11:K:38:ASN:HB2	2.14	0.47
2:B:17:PHE:HD1	2:B:18:GLY:N	2.11	0.47
12:L:50:SER:O	12:L:51:ALA:HB2	2.14	0.47
11:K:80:VAL:HG13	11:K:103:LEU:HD22	1.96	0.47
9:I:5:TYR:O	9:I:84:ALA:HA	2.13	0.47
1:A:1354:U:OP1	9:I:71:SER:HB3	2.13	0.47
15:O:4:THR:HB	15:O:6:GLU:OE2	2.14	0.47
19:S:19:VAL:HG23	19:S:47:HIS:CD2	2.49	0.47
1:A:1374:G:N2	1:A:1479:A:C8	2.80	0.47
9:I:69:GLY:O	9:I:73:GLN:HG3	2.14	0.47
2:B:230:VAL:CG1	2:B:231:GLU:H	2.20	0.47
1:A:1192:U:H4'	1:A:1193:U:H4'	1.97	0.47
1:A:942:A:C2	1:A:946:A:C2	3.02	0.47
1:A:760:A:H5''	1:A:760:A:C8	2.47	0.47
1:A:1509:U:O2	1:A:1510:C:H4'	2.14	0.47
9:I:100:GLY:O	9:I:102:LEU:N	2.47	0.47
1:A:1461:C:H2'	1:A:1462:U:O4'	2.14	0.47
5:E:143:ARG:NH1	8:H:77:GLU:OE2	2.47	0.47
3:C:193:TYR:CE1	3:C:196:LEU:HD11	2.49	0.47
1:A:1339:U:H2'	1:A:1340:C:O4'	2.15	0.47
1:A:446:A:O2'	1:A:447:A:P	2.71	0.47
3:C:12:LEU:HD11	14:N:51:GLY:HA3	1.96	0.47
17:Q:65:ILE:N	17:Q:65:ILE:HD12	2.29	0.47
2:B:62:ALA:O	2:B:64:ARG:N	2.38	0.47
10:J:42:THR:HB	10:J:67:THR:O	2.15	0.47
17:Q:51:TYR:C	17:Q:52:LYS:HD2	2.35	0.47
1:A:482:A:O2'	1:A:483:G:C8	2.68	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:42:THR:HG22	12:L:43:VAL:N	2.29	0.47
10:J:19:SER:O	10:J:23:ILE:HG13	2.14	0.47
9:I:40:LEU:C	9:I:42:ARG:H	2.17	0.47
1:A:1420:G:H2'	1:A:1421:C:C6	2.50	0.47
9:I:17:VAL:HG21	9:I:80:GLY:HA3	1.96	0.47
17:Q:12:SER:HB3	17:Q:20:THR:OG1	2.14	0.47
15:O:16:ALA:HB1	15:O:21:ASP:HB3	1.96	0.47
10:J:69:ASN:O	10:J:70:ARG:HD3	2.14	0.47
13:M:23:TYR:C	13:M:25:ILE:H	2.18	0.47
1:A:408:G:C2'	1:A:423:G:H22	2.27	0.47
1:A:1125:G:O5'	1:A:1125:G:C8	2.67	0.47
3:C:172:ARG:NH2	3:C:203:PHE:CZ	2.82	0.47
1:A:1170:C:C5'	1:A:1171:G:OP2	2.63	0.47
1:A:942:A:O2'	1:A:943:G:OP2	2.32	0.47
20:T:97:ALA:O	20:T:99:LEU:N	2.47	0.47
19:S:55:LYS:C	19:S:56:GLN:HG3	2.35	0.47
1:A:50:A:H5''	1:A:51:A:O3'	2.14	0.47
1:A:50:A:C6	1:A:356:G:H4'	2.47	0.47
19:S:33:THR:HG22	19:S:34:TRP:H	1.78	0.47
10:J:5:ARG:HA	10:J:73:ASP:OD1	2.14	0.47
1:A:1311:U:H2'	1:A:1312:G:H5'	1.96	0.47
2:B:15:VAL:CG2	2:B:209:ARG:HB3	2.44	0.47
1:A:545:C:O2'	12:L:15:ARG:CB	2.55	0.47
5:E:82:VAL:HG21	5:E:138:ALA:HA	1.95	0.47
2:B:71:VAL:HG21	2:B:164:VAL:HG22	1.96	0.47
13:M:37:THR:CG2	13:M:55:ARG:HB3	2.45	0.47
6:F:82:ARG:HB2	6:F:85:VAL:HG23	1.96	0.47
3:C:11:ARG:O	3:C:12:LEU:C	2.53	0.47
1:A:1068:U:H3	1:A:1081:G:N2	2.08	0.47
10:J:23:ILE:HA	10:J:85:LEU:HD22	1.96	0.47
13:M:15:VAL:CG2	13:M:48:LEU:HD21	2.43	0.47
17:Q:59:ILE:HD13	17:Q:73:VAL:HA	1.96	0.47
9:I:42:ARG:HH11	9:I:42:ARG:HG2	1.80	0.47
1:A:866:A:H4'	1:A:867:G:O5'	2.14	0.47
4:D:31:CYS:C	4:D:33:MET:N	2.67	0.47
1:A:1378:A:H4'	1:A:1379:C:H5''	1.97	0.47
3:C:110:ASN:C	3:C:111:LEU:HD12	2.35	0.47
18:R:45:SER:C	18:R:47:THR:N	2.68	0.47
2:B:74:LYS:HG2	2:B:76:GLN:H	1.80	0.47
12:L:18:VAL:HG12	12:L:19:ARG:N	2.30	0.47
1:A:141:G:O2'	1:A:142:G:H5'	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1100:C:H1'	1:A:1160:A:C4	2.49	0.47
7:G:37:ASN:OD1	9:I:41:VAL:HG22	2.15	0.47
1:A:1187:G:H1'	3:C:193:TYR:O	2.14	0.47
1:A:953:G:N7	1:A:1339:U:C2	2.83	0.47
1:A:544:U:O2'	1:A:545:C:P	2.72	0.47
15:O:26:GLU:HG3	15:O:81:LEU:HG	1.97	0.47
13:M:40:ASN:HD22	13:M:40:ASN:C	2.18	0.47
1:A:1328:G:N2	1:A:1355:G:H2'	2.30	0.47
1:A:518:A:H4'	1:A:519:C:OP1	2.12	0.47
12:L:59:ARG:HH12	12:L:65:GLU:HB3	1.78	0.47
17:Q:101:ARG:HE	17:Q:101:ARG:HA	1.79	0.47
14:N:8:GLU:OE1	14:N:8:GLU:C	2.54	0.47
10:J:32:ALA:CB	10:J:76:ASN:HB2	2.45	0.47
6:F:19:LEU:O	6:F:23:LYS:HG3	2.14	0.47
1:A:927:U:H5	13:M:102:ARG:NE	2.13	0.47
3:C:173:VAL:O	3:C:173:VAL:HG12	2.14	0.47
10:J:4:ILE:HA	10:J:100:THR:CB	2.45	0.47
1:A:1111:C:O2'	1:A:1112:A:P	2.73	0.47
1:A:1334:G:H2'	1:A:1335:C:H6	1.80	0.47
7:G:145:ALA:O	7:G:147:ALA:N	2.48	0.47
9:I:33:PHE:CE1	9:I:37:PHE:HD1	2.33	0.47
1:A:1024:G:H2'	1:A:1025:C:H5'	1.97	0.47
2:B:76:GLN:HG3	2:B:206:ASP:OD1	2.15	0.47
1:A:859:C:O2'	1:A:860:C:H5'	2.15	0.47
1:A:669:U:C2'	1:A:670:A:O5'	2.62	0.46
1:A:1125:G:N3	1:A:1126:G:N1	2.64	0.46
20:T:68:LYS:HA	20:T:68:LYS:HD2	1.77	0.46
9:I:32:ASP:OD2	9:I:33:PHE:N	2.49	0.46
17:Q:79:SER:O	17:Q:80:GLY:O	2.34	0.46
5:E:151:LEU:HD11	8:H:77:GLU:OE2	2.14	0.46
1:A:838:G:O2'	1:A:839:C:H5'	2.16	0.46
11:K:15:ALA:HA	11:K:76:GLY:O	2.15	0.46
1:A:1134:A:H2'	1:A:1135:C:O5'	2.15	0.46
10:J:39:PRO:O	10:J:40:LEU:HB2	2.14	0.46
23:X:32:C:C6	23:X:32:C:H5''	2.50	0.46
1:A:1006:C:C6	1:A:1006:C:H3'	2.51	0.46
2:B:103:THR:HA	2:B:180:LEU:HD11	1.97	0.46
13:M:88:ARG:HH11	19:S:3:ARG:HH21	1.63	0.46
4:D:148:VAL:CG1	4:D:158:ILE:HD13	2.46	0.46
1:A:1519:U:H6	1:A:1519:U:O5'	1.98	0.46
2:B:61:LEU:HD11	2:B:160:ASP:HB3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:V:21:TYR:O	21:V:22:ARG:HB2	2.13	0.46
1:A:49:U:C2	1:A:359:A:N6	2.84	0.46
10:J:12:ASP:HB3	10:J:15:THR:CG2	2.46	0.46
13:M:23:TYR:HB3	13:M:67:GLU:H	1.81	0.46
13:M:9:ILE:N	13:M:9:ILE:CD1	2.73	0.46
1:A:818:U:OP1	18:R:64:ARG:NH2	2.36	0.46
1:A:542:A:H4'	1:A:544:U:OP1	2.16	0.46
1:A:1222:G:H2'	1:A:1223:C:C6	2.50	0.46
12:L:71:PRO:O	12:L:102:ARG:NH1	2.48	0.46
8:H:65:TYR:HA	8:H:79:VAL:HG23	1.98	0.46
4:D:64:LEU:HD23	4:D:64:LEU:C	2.36	0.46
3:C:134:ILE:CG2	3:C:168:ALA:HB3	2.45	0.46
1:A:17:U:H2'	1:A:18:C:C6	2.50	0.46
17:Q:4:LYS:HD2	17:Q:6:LEU:CD2	2.46	0.46
1:A:794:C:H4'	1:A:877:A:N6	2.31	0.46
8:H:80:ILE:HG22	8:H:80:ILE:O	2.14	0.46
12:L:42:THR:CG2	12:L:52:LEU:HB3	2.45	0.46
1:A:208:U:H5''	1:A:209:U:OP2	2.14	0.46
3:C:186:PHE:CZ	3:C:188:LEU:HD23	2.50	0.46
19:S:7:LYS:HD2	19:S:7:LYS:O	2.15	0.46
1:A:577:G:C2'	1:A:578:G:H5'	2.45	0.46
10:J:34:VAL:HA	10:J:74:ILE:HG23	1.96	0.46
1:A:953:G:O2'	1:A:954:A:OP2	2.33	0.46
1:A:485:G:H2'	1:A:486:C:O4'	2.15	0.46
1:A:988:G:H2'	1:A:989:G:C8	2.51	0.46
7:G:15:ASP:O	7:G:19:GLY:HA2	2.14	0.46
1:A:613:G:H2'	1:A:614:G:H5'	1.98	0.46
1:A:795:C:H4'	1:A:796:U:O5'	2.14	0.46
20:T:54:LYS:HA	20:T:57:ARG:HH12	1.81	0.46
4:D:58:LEU:O	4:D:62:GLN:HG2	2.16	0.46
9:I:43:ALA:C	9:I:45:ALA:N	2.69	0.46
4:D:25:ARG:C	4:D:27:TYR:H	2.18	0.46
1:A:534:U:H2'	1:A:535:U:C6	2.50	0.46
13:M:23:TYR:HB2	13:M:67:GLU:CD	2.36	0.46
5:E:126:ARG:HG3	5:E:126:ARG:HH11	1.81	0.46
1:A:666:G:H21	11:K:38:ASN:ND2	2.07	0.46
2:B:178:ARG:HH22	8:H:68:ARG:NH2	2.13	0.46
2:B:178:ARG:O	8:H:71:GLY:HA2	2.14	0.46
20:T:45:GLN:HG2	20:T:91:LEU:CD2	2.41	0.46
7:G:78:ARG:NH1	7:G:154:TYR:HB3	2.31	0.46
11:K:51:LYS:O	11:K:55:LYS:HE2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:134:ILE:HG23	3:C:151:VAL:HB	1.98	0.46
2:B:92:TYR:OH	2:B:150:SER:OG	2.30	0.46
1:A:855:G:OP1	8:H:88:LYS:HG3	2.16	0.46
1:A:1413:C:H2'	1:A:1414:G:H5'	1.97	0.46
1:A:49:U:O2'	1:A:50:A:OP1	2.30	0.46
22:W:3:G:N2	23:X:34:70U:HN3	2.05	0.46
2:B:213:LEU:HD23	2:B:213:LEU:C	2.36	0.46
23:X:31:A:C2'	23:X:32:C:OP1	2.64	0.46
3:C:83:ARG:C	3:C:85:ARG:H	2.19	0.46
6:F:2:ARG:HH21	6:F:69:GLU:CG	2.28	0.46
8:H:10:LEU:CD1	8:H:85:ARG:HG2	2.45	0.46
1:A:241:A:C4'	1:A:242:G:OP1	2.62	0.46
8:H:24:THR:HG22	8:H:63:LEU:HD21	1.98	0.46
9:I:127:LYS:CD	9:I:127:LYS:H	2.28	0.46
20:T:57:ARG:CZ	20:T:102:GLY:HA2	2.46	0.46
3:C:139:GLN:HE21	3:C:139:GLN:HA	1.76	0.46
3:C:20:SER:HB3	3:C:40:ARG:HH22	1.80	0.46
1:A:100:G:C2'	1:A:101:G:H5'	2.46	0.46
10:J:48:THR:HG23	10:J:62:HIS:CD2	2.50	0.46
1:A:1302:C:H2'	1:A:1303:C:C5	2.51	0.46
1:A:1088:G:H5''	3:C:172:ARG:HG2	1.97	0.46
8:H:83:ILE:O	8:H:83:ILE:HG23	2.16	0.46
1:A:949:C:OP1	10:J:57:LYS:CD	2.61	0.46
1:A:416:U:HO2'	1:A:417:C:P	2.39	0.46
7:G:122:HIS:HD2	7:G:125:MET:CE	2.28	0.46
11:K:126:ARG:O	11:K:127:LYS:C	2.53	0.46
1:A:94:A:O2'	1:A:95:G:H5'	2.16	0.46
7:G:143:ARG:O	7:G:147:ALA:HB2	2.16	0.46
3:C:167:TRP:HB3	3:C:168:ALA:H	1.39	0.46
1:A:855:G:OP1	8:H:89:PRO:O	2.34	0.46
10:J:48:THR:OG1	10:J:62:HIS:CD2	2.68	0.46
10:J:6:ILE:HA	10:J:97:GLU:O	2.16	0.46
23:X:31:A:N3	23:X:31:A:H2'	2.31	0.46
14:N:45:ARG:HG3	14:N:45:ARG:HH11	1.81	0.46
1:A:424:U:H1'	1:A:425:A:H5''	1.97	0.46
2:B:231:GLU:HG3	2:B:232:PRO:HD2	1.98	0.46
1:A:705:A:HO2'	1:A:706:U:H3'	1.81	0.46
1:A:469:G:O2'	1:A:470:U:OP2	2.29	0.46
1:A:695:A:H2'	1:A:696:G:O4'	2.16	0.46
6:F:19:LEU:C	6:F:19:LEU:HD23	2.36	0.46
2:B:60:ASP:OD1	2:B:64:ARG:CZ	2.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:84:ILE:HG13	3:C:88:ARG:HH12	1.80	0.46
5:E:143:ARG:HA	5:E:143:ARG:HD3	1.58	0.46
1:A:627:G:O2'	1:A:628:C:H5'	2.16	0.46
1:A:949:C:P	10:J:57:LYS:HD3	2.56	0.46
1:A:697:G:H21	1:A:760:A:H1'	1.79	0.46
6:F:76:ALA:O	6:F:80:ARG:HG3	2.16	0.46
3:C:139:GLN:CA	3:C:139:GLN:NE2	2.73	0.46
19:S:28:LYS:HD3	19:S:29:ARG:H	1.80	0.46
12:L:111:LYS:HE3	12:L:112:ASP:OD1	2.15	0.46
5:E:116:THR:HG23	5:E:117:ASP:OD2	2.16	0.46
1:A:1355:G:H8	1:A:1355:G:O5'	1.98	0.46
1:A:1219:A:H5'	1:A:1317:C:N4	2.13	0.45
1:A:825:C:H2'	1:A:826:C:O5'	2.16	0.45
1:A:1481:G:OP2	1:A:1481:G:H3'	2.16	0.45
20:T:36:LEU:HD13	20:T:58:LYS:HG3	1.97	0.45
1:A:544:U:H4'	1:A:545:C:OP2	2.16	0.45
2:B:135:GLN:O	2:B:139:LYS:HB3	2.16	0.45
11:K:18:ARG:HH12	11:K:36:ASP:HA	1.81	0.45
3:C:29:TYR:CD2	3:C:29:TYR:C	2.89	0.45
1:A:929:U:O2'	1:A:930:G:H5'	2.16	0.45
1:A:1450:A:O2'	1:A:1451:G:H5'	2.16	0.45
16:P:26:ARG:HD2	16:P:31:LYS:O	2.16	0.45
1:A:1106:G:H5'	10:J:35:SER:OG	2.16	0.45
10:J:33:GLN:O	10:J:34:VAL:HB	2.17	0.45
3:C:107:GLN:O	3:C:108:ASN:CB	2.64	0.45
12:L:65:GLU:CD	12:L:65:GLU:N	2.69	0.45
4:D:151:LYS:N	4:D:151:LYS:CD	2.71	0.45
20:T:10:LEU:HD13	20:T:11:SER:N	2.30	0.45
7:G:115:ARG:HB2	7:G:118:VAL:CG2	2.46	0.45
19:S:69:HIS:HB3	19:S:74:PHE:HE1	1.81	0.45
15:O:34:LEU:O	15:O:34:LEU:HD23	2.16	0.45
12:L:56:ALA:O	12:L:67:THR:HA	2.16	0.45
1:A:1347:G:C6	1:A:1348:C:C4	3.05	0.45
3:C:68:VAL:HG12	3:C:70:VAL:HG13	1.98	0.45
1:A:1266:A:O2'	1:A:1267:A:OP2	2.32	0.45
1:A:1110:C:O2'	1:A:1112:A:N7	2.49	0.45
3:C:139:GLN:O	3:C:143:GLU:N	2.48	0.45
3:C:135:LYS:CE	5:E:50:GLU:HG2	2.47	0.45
16:P:81:ARG:HH11	16:P:83:GLU:CG	2.29	0.45
16:P:43:LYS:HA	16:P:48:TRP:CB	2.46	0.45
2:B:208:ILE:HG21	2:B:239:VAL:HB	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:50:ILE:HA	10:J:60:ARG:HD2	1.98	0.45
1:A:407:A:C2	4:D:35:ARG:HB3	2.52	0.45
1:A:613:G:C2'	1:A:614:G:H5'	2.46	0.45
1:A:726:U:H2'	1:A:727:C:H6	1.80	0.45
1:A:680:U:C2'	1:A:681:G:H5'	2.46	0.45
12:L:88:GLY:H	12:L:98:TYR:HA	1.81	0.45
1:A:332:C:H2'	1:A:333:A:H8	1.82	0.45
4:D:21:LEU:HD21	4:D:114:ARG:HB2	1.97	0.45
19:S:22:LEU:O	19:S:26:GLY:O	2.35	0.45
1:A:1286:G:O2'	1:A:1287:A:OP2	2.34	0.45
13:M:5:ALA:O	13:M:6:GLY:C	2.53	0.45
13:M:67:GLU:O	13:M:70:LEU:N	2.44	0.45
1:A:1345:A:O2'	1:A:1346:U:OP2	2.26	0.45
4:D:6:GLY:O	4:D:7:PRO:C	2.55	0.45
5:E:126:ARG:HG3	5:E:126:ARG:NH1	2.31	0.45
16:P:81:ARG:HH11	16:P:83:GLU:HG3	1.80	0.45
13:M:107:ALA:O	13:M:111:LYS:HG3	2.16	0.45
14:N:41:ARG:HG2	14:N:41:ARG:HH11	1.81	0.45
19:S:40:ILE:HB	19:S:67:VAL:O	2.16	0.45
1:A:1243:C:O5'	1:A:1243:C:H6	2.00	0.45
1:A:469:G:O2'	1:A:470:U:P	2.74	0.45
12:L:60:LEU:HD21	12:L:85:ILE:HD11	1.99	0.45
4:D:70:ILE:HD11	4:D:100:ARG:CD	2.46	0.45
15:O:11:VAL:HG21	15:O:34:LEU:HD12	1.99	0.45
10:J:12:ASP:HB3	10:J:15:THR:HG22	1.99	0.45
12:L:38:THR:HG21	12:L:59:ARG:HH21	1.81	0.45
1:A:849:A:C4'	1:A:850:A:OP1	2.58	0.45
1:A:915:A:C6	1:A:916:G:C5	3.05	0.45
10:J:46:ARG:NH1	10:J:46:ARG:CG	2.78	0.45
1:A:1170:C:H5'	1:A:1171:G:OP2	2.17	0.45
13:M:40:ASN:HB3	13:M:43:THR:HG23	1.99	0.45
1:A:433:G:C4'	1:A:434:A:OP1	2.62	0.45
7:G:145:ALA:C	7:G:147:ALA:N	2.68	0.45
1:A:1168:G:P	9:I:113:LYS:NZ	2.90	0.45
1:A:798:A:O2'	1:A:799:A:P	2.75	0.45
1:A:581:U:H4'	8:H:94:TYR:CD1	2.51	0.45
17:Q:3:LYS:HB3	17:Q:61:GLU:HB3	1.99	0.45
4:D:106:TYR:CE1	4:D:113:SER:HA	2.52	0.45
2:B:43:ASP:OD1	2:B:46:LYS:HG2	2.17	0.45
1:A:672:C:H2'	1:A:673:G:O4'	2.16	0.45
12:L:42:THR:CG2	12:L:43:VAL:N	2.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1126:G:C8	1:A:1126:G:C3'	3.00	0.45
9:I:3:GLN:HA	9:I:19:LEU:O	2.17	0.45
9:I:4:TYR:CE2	9:I:88:TYR:HA	2.52	0.45
4:D:148:VAL:HG11	4:D:158:ILE:HD13	1.98	0.45
1:A:465:G:H2'	1:A:467:C:H41	1.82	0.45
19:S:63:THR:HG21	19:S:65:ASN:HD21	1.81	0.45
1:A:627:G:C2'	1:A:628:C:H5'	2.47	0.45
3:C:159:GLY:HA2	3:C:193:TYR:CD2	2.52	0.45
17:Q:100:LYS:HD2	17:Q:100:LYS:C	2.37	0.45
13:M:125:ARG:HD2	13:M:125:ARG:O	2.16	0.45
1:A:926:A:H2'	1:A:927:U:O4'	2.17	0.45
1:A:629:U:H2'	1:A:630:C:C6	2.52	0.45
1:A:1458:U:H2'	1:A:1459:G:O5'	2.17	0.45
1:A:1400:A:H2'	1:A:1401:G:H5'	1.98	0.45
1:A:963:A:H2'	1:A:964:G:O4'	2.16	0.45
5:E:120:THR:HG23	5:E:121:LYS:N	2.32	0.45
7:G:146:GLU:HG2	7:G:149:ARG:HD3	1.99	0.45
11:K:12:ARG:O	11:K:13:GLN:O	2.35	0.45
1:A:465:G:H2'	1:A:467:C:N4	2.31	0.45
1:A:1458:U:H2'	1:A:1459:G:C5'	2.47	0.45
16:P:6:LEU:HD12	16:P:6:LEU:N	2.32	0.45
1:A:52:G:N7	1:A:355:A:C2	2.85	0.44
1:A:1134:A:OP2	10:J:68:HIS:CE1	2.70	0.44
1:A:562:G:H5'	1:A:711:A:C1'	2.36	0.44
2:B:82:ARG:HG2	2:B:82:ARG:HH11	1.82	0.44
2:B:39:ILE:HG22	2:B:40:HIS:H	1.82	0.44
20:T:57:ARG:NE	20:T:102:GLY:HA2	2.32	0.44
9:I:78:LYS:O	9:I:78:LYS:HD2	2.16	0.44
2:B:41:ILE:HD12	2:B:41:ILE:H	1.81	0.44
3:C:188:LEU:HB3	3:C:189:ALA:H	1.58	0.44
3:C:89:GLU:O	3:C:93:LYS:HG2	2.18	0.44
1:A:852:C:H1'	8:H:15:ASN:HD21	1.82	0.44
5:E:13:ILE:O	5:E:13:ILE:HG13	2.17	0.44
10:J:71:LEU:O	10:J:72:VAL:CB	2.65	0.44
1:A:983:A:H3'	1:A:983:A:C8	2.53	0.44
4:D:3:ARG:O	4:D:4:TYR:HB3	2.17	0.44
9:I:36:TYR:CD2	9:I:37:PHE:CE2	3.05	0.44
1:A:1151:A:H2'	1:A:1152:G:H5'	1.99	0.44
7:G:64:GLN:HG2	7:G:128:ALA:HB1	1.98	0.44
1:A:752:G:H4'	1:A:1490:A:H4'	1.99	0.44
1:A:634:C:C5'	1:A:635:U:OP2	2.59	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:27:LEU:O	12:L:28:LYS:C	2.55	0.44
3:C:26:LYS:CD	3:C:26:LYS:H	2.17	0.44
1:A:1206:A:H5'	1:A:1207:C:OP2	2.18	0.44
12:L:119:LYS:O	12:L:120:TYR:CB	2.66	0.44
1:A:899:G:C6	1:A:900:A:C6	3.05	0.44
1:A:67:C:O2'	1:A:165:A:H1'	2.17	0.44
1:A:1262:U:C4'	1:A:1263:C:OP2	2.64	0.44
19:S:11:VAL:HA	19:S:38:SER:HA	1.99	0.44
13:M:67:GLU:HB3	13:M:68:GLY:H	1.58	0.44
23:X:30:G:C4	23:X:31:A:N7	2.86	0.44
13:M:65:LYS:HE3	13:M:69:GLU:CG	2.37	0.44
1:A:1305:A:O4'	1:A:1343:C:H4'	2.18	0.44
8:H:68:ARG:NH1	8:H:68:ARG:HG2	2.32	0.44
10:J:26:ALA:CB	10:J:85:LEU:HD11	2.47	0.44
1:A:949:C:O2'	10:J:55:LYS:HA	2.17	0.44
13:M:40:ASN:HD22	13:M:41:PRO:CD	2.31	0.44
20:T:70:SER:HA	20:T:73:HIS:CD2	2.52	0.44
1:A:1417:G:H2'	1:A:1418:U:H6	1.80	0.44
1:A:7:G:O2'	1:A:8:A:OP1	2.32	0.44
1:A:98:G:H2'	1:A:99:C:C6	2.52	0.44
1:A:145:A:H2'	1:A:146:A:O4'	2.17	0.44
7:G:56:GLN:HB3	7:G:60:LYS:HD3	1.98	0.44
14:N:61:TRP:N	14:N:61:TRP:CE3	2.85	0.44
10:J:6:ILE:O	10:J:6:ILE:HG13	2.17	0.44
2:B:119:GLU:O	2:B:122:PHE:HB2	2.18	0.44
3:C:6:HIS:CD2	3:C:8:ILE:HB	2.52	0.44
15:O:71:GLN:HB2	15:O:78:TYR:CG	2.52	0.44
1:A:1327:A:HO2'	1:A:1328:G:P	2.41	0.44
1:A:577:G:H2'	1:A:578:G:H5'	2.00	0.44
12:L:78:GLN:C	12:L:80:HIS:H	2.17	0.44
6:F:40:VAL:HG22	6:F:41:GLU:N	2.32	0.44
1:A:50:A:H4'	1:A:51:A:OP2	2.16	0.44
10:J:72:VAL:O	10:J:73:ASP:O	2.36	0.44
1:A:1311:U:C2'	1:A:1312:G:H5'	2.48	0.44
2:B:14:GLY:N	2:B:16:HIS:HE1	2.15	0.44
2:B:44:LEU:O	2:B:47:THR:HB	2.18	0.44
1:A:1110:C:O2'	1:A:1111:C:OP1	2.34	0.44
1:A:1111:C:OP2	9:I:62:TYR:HE2	2.00	0.44
9:I:108:VAL:HG12	9:I:109:VAL:N	2.33	0.44
3:C:20:SER:HB2	3:C:22:TRP:HE1	1.83	0.44
11:K:40:ILE:HG22	11:K:41:THR:HG23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:740:U:H2'	1:A:741:G:O4'	2.17	0.44
9:I:18:PHE:O	9:I:61:ALA:HA	2.17	0.44
14:N:45:ARG:O	14:N:49:HIS:CD2	2.71	0.44
9:I:79:LEU:CD1	9:I:83:ARG:HD2	2.46	0.44
1:A:1110:C:OP1	9:I:66:ARG:NH2	2.51	0.44
2:B:25:ASN:HD22	2:B:26:PRO:CD	2.30	0.44
12:L:89:ARG:HA	12:L:97:ARG:HA	1.99	0.44
10:J:32:ALA:HB2	10:J:76:ASN:HB2	2.00	0.44
1:A:1297:G:O2'	14:N:18:VAL:HG11	2.17	0.44
1:A:41:G:H2'	1:A:42:G:H8	1.82	0.44
1:A:1363:U:H2'	1:A:1364:C:H6	1.82	0.44
1:A:649:G:H5'	1:A:709:C:H1'	2.00	0.44
1:A:1476:A:H1'	1:A:1497:G:H5'	1.99	0.44
1:A:513:G:O2'	1:A:514:U:P	2.76	0.44
12:L:55:VAL:CG1	12:L:56:ALA:N	2.81	0.44
3:C:45:LYS:HE2	3:C:45:LYS:HB3	1.74	0.44
6:F:25:ILE:CD1	6:F:82:ARG:HH11	2.31	0.44
3:C:11:ARG:NH1	3:C:177:THR:O	2.51	0.44
20:T:67:ALA:O	20:T:73:HIS:CE1	2.71	0.44
1:A:1206:A:H5'	13:M:103:THR:HG1	1.81	0.44
9:I:127:LYS:HG2	13:M:126:LYS:HZ1	1.82	0.44
13:M:125:ARG:HH12	13:M:126:LYS:HG3	1.83	0.44
1:A:982:A:N6	1:A:1019:C:N4	2.64	0.44
20:T:57:ARG:HH22	20:T:100:ILE:CG1	2.29	0.44
1:A:492:A:H5''	4:D:55:ALA:HB2	2.00	0.44
18:R:34:TYR:HB3	18:R:69:THR:HG23	2.00	0.44
1:A:919:G:H2'	1:A:920:U:H6	1.83	0.44
1:A:1394:C:H2'	1:A:1395:A:C8	2.53	0.44
17:Q:78:GLU:O	17:Q:78:GLU:HG3	2.16	0.44
1:A:49:U:O4	1:A:359:A:C4	2.71	0.44
1:A:1039:G:C4	1:A:1185:A:C2	3.06	0.44
1:A:1478:C:OP2	1:A:1481:G:H2'	2.17	0.44
1:A:988:G:O2'	1:A:989:G:H5'	2.18	0.44
3:C:177:THR:OG1	3:C:180:ALA:HB2	2.18	0.44
9:I:20:ARG:O	9:I:22:GLY:N	2.51	0.44
13:M:108:ARG:NE	13:M:108:ARG:HA	2.33	0.44
3:C:131:ARG:O	3:C:135:LYS:HG3	2.17	0.44
1:A:1043:G:C6	1:A:1044:U:N3	2.86	0.44
1:A:1327:A:O2'	1:A:1328:G:P	2.76	0.44
1:A:12:U:H4'	1:A:509:C:O2'	2.18	0.44
9:I:13:ALA:HA	9:I:67:GLY:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:750:A:H2'	1:A:751:A:C8	2.53	0.44
1:A:1258:C:O2'	1:A:1260:A:H8	2.00	0.43
12:L:41:ARG:CB	12:L:41:ARG:CZ	2.96	0.43
1:A:406:A:N7	1:A:408:G:N3	2.66	0.43
2:B:112:VAL:O	2:B:115:LEU:HB3	2.18	0.43
7:G:15:ASP:OD2	7:G:17:VAL:HB	2.18	0.43
2:B:32:ILE:HD13	2:B:40:HIS:CE1	2.53	0.43
6:F:10:LEU:HB3	6:F:84:ASN:O	2.18	0.43
9:I:33:PHE:C	9:I:35:GLU:N	2.70	0.43
3:C:138:VAL:HG22	3:C:151:VAL:HG23	2.00	0.43
20:T:82:SER:O	20:T:86:ARG:HG3	2.18	0.43
20:T:86:ARG:HG2	20:T:86:ARG:NH1	2.33	0.43
1:A:993:A:H2'	1:A:994:A:C8	2.53	0.43
1:A:1384:C:H2'	1:A:1385:C:O4'	2.17	0.43
1:A:854:C:O2'	1:A:855:G:H5'	2.18	0.43
11:K:33:THR:HG22	11:K:39:PRO:HA	1.99	0.43
1:A:160:G:O2'	1:A:161:G:H5'	2.18	0.43
1:A:200:C:H6	1:A:200:C:O5'	2.01	0.43
13:M:5:ALA:HB2	13:M:22:ILE:HD13	2.00	0.43
3:C:76:VAL:HG11	3:C:103:VAL:CG2	2.47	0.43
9:I:83:ARG:O	9:I:86:VAL:N	2.50	0.43
14:N:6:LEU:HB3	14:N:23:ARG:HH21	1.83	0.43
1:A:102:A:C4'	1:A:103:C:OP2	2.64	0.43
9:I:97:LYS:HB2	9:I:102:LEU:HD12	1.99	0.43
1:A:980:G:C3'	1:A:980:G:C8	3.01	0.43
1:A:919:G:H2'	1:A:920:U:C6	2.52	0.43
2:B:15:VAL:C	2:B:16:HIS:CG	2.91	0.43
1:A:1281:G:C2'	1:A:1282:U:OP2	2.66	0.43
1:A:366:G:O2'	1:A:367:C:H5'	2.18	0.43
18:R:87:ARG:HG2	18:R:87:ARG:HH11	1.84	0.43
5:E:31:LEU:HD22	5:E:43:LEU:CD2	2.48	0.43
1:A:1206:A:C4'	1:A:1207:C:OP2	2.66	0.43
9:I:3:GLN:HG3	9:I:20:ARG:CG	2.45	0.43
7:G:88:PRO:CB	7:G:145:ALA:HB1	2.48	0.43
1:A:645:G:O2'	1:A:819:G:C5'	2.66	0.43
1:A:437:C:H2'	1:A:438:C:C6	2.51	0.43
7:G:93:PRO:HA	7:G:96:GLN:HE21	1.83	0.43
1:A:586:U:H2'	1:A:587:G:H8	1.83	0.43
1:A:52:G:C6	1:A:355:A:N3	2.87	0.43
2:B:14:GLY:N	2:B:16:HIS:CE1	2.86	0.43
1:A:1124:G:H2'	1:A:1125:G:H5'	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:A:H5'	16:P:72:ARG:HH21	1.79	0.43
1:A:637:G:C5	1:A:638:A:C5	3.07	0.43
1:A:1207:C:N4	13:M:104:ARG:HG3	2.33	0.43
1:A:468:G:O2'	1:A:469:G:H5''	2.19	0.43
6:F:92:LYS:HE3	6:F:92:LYS:HB2	1.74	0.43
2:B:69:LEU:CD1	2:B:155:LEU:HD11	2.48	0.43
4:D:145:GLU:OE2	4:D:182:LYS:HD2	2.18	0.43
1:A:465:G:C4'	1:A:466:A:OP1	2.66	0.43
1:A:558:G:H4'	1:A:559:G:O5'	2.18	0.43
7:G:45:ASP:O	7:G:49:ILE:HG13	2.18	0.43
14:N:26:ARG:HE	14:N:47:LEU:HD21	1.84	0.43
8:H:1:MET:HG2	8:H:2:LEU:N	2.33	0.43
1:A:48:C:O2'	1:A:49:U:P	2.71	0.43
1:A:406:A:C5	1:A:408:G:N3	2.86	0.43
9:I:82:ALA:O	9:I:86:VAL:HG23	2.17	0.43
2:B:178:ARG:NH2	8:H:68:ARG:HH22	2.16	0.43
8:H:6:ILE:O	8:H:10:LEU:HG	2.18	0.43
3:C:26:LYS:HB3	10:J:45:ARG:HH21	1.83	0.43
1:A:530:A:O2'	1:A:531:G:P	2.77	0.43
2:B:20:GLU:HB2	2:B:190:THR:HB	2.00	0.43
10:J:28:ARG:HG3	10:J:29:ARG:HG2	1.99	0.43
1:A:546:A:HO2'	1:A:549:G:HO2'	1.66	0.43
8:H:35:ILE:O	8:H:39:LEU:HD13	2.19	0.43
8:H:119:LEU:HD13	8:H:124:ALA:HA	2.01	0.43
13:M:10:PRO:CB	13:M:18:ALA:HB1	2.40	0.43
1:A:361:C:H4'	1:A:362:U:OP1	2.18	0.43
6:F:75:LEU:O	6:F:79:LEU:HG	2.19	0.43
1:A:413:C:H1'	1:A:421:G:N2	2.33	0.43
4:D:31:CYS:SG	4:D:31:CYS:O	2.76	0.43
1:A:1291:G:N7	19:S:2:PRO:HD3	2.34	0.43
10:J:13:HIS:HB3	10:J:68:HIS:CE1	2.53	0.43
19:S:20:LEU:HA	19:S:23:ASN:HD22	1.83	0.43
2:B:87:ARG:HB2	2:B:219:VAL:HG11	2.00	0.43
8:H:111:ILE:HD12	8:H:135:CYS:SG	2.59	0.43
6:F:44:GLY:HA2	6:F:59:TYR:CD1	2.52	0.43
1:A:1250:A:C2	1:A:1294:U:O4'	2.72	0.43
3:C:77:ILE:HA	3:C:84:ILE:HB	2.01	0.43
1:A:911:C:H5'	1:A:912:A:OP1	2.19	0.43
13:M:107:ALA:HB3	13:M:111:LYS:HD2	2.01	0.43
1:A:890:A:H4'	1:A:891:A:O5'	2.18	0.43
13:M:80:ARG:O	13:M:84:ILE:HG12	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:83:ARG:O	3:C:85:ARG:N	2.52	0.43
2:B:134:GLU:C	2:B:136:VAL:H	2.22	0.43
10:J:84:GLN:C	10:J:86:MET:H	2.21	0.43
12:L:102:ARG:HD2	12:L:102:ARG:HA	1.86	0.43
8:H:10:LEU:CD2	8:H:83:ILE:HD11	2.49	0.43
5:E:76:ILE:HG13	5:E:142:LEU:HD13	2.00	0.43
21:V:6:ARG:HB3	21:V:15:ARG:NH1	2.33	0.43
1:A:7:G:H21	5:E:121:LYS:HG2	1.83	0.43
1:A:250:G:H1'	17:Q:16:GLN:NE2	2.34	0.43
1:A:250:G:O6	1:A:261:G:O6	2.37	0.43
17:Q:59:ILE:CG2	17:Q:71:PHE:HB3	2.48	0.43
1:A:814:U:H2'	1:A:815:C:C6	2.50	0.43
19:S:5:LEU:O	19:S:6:LYS:HB2	2.18	0.43
2:B:124:SER:C	2:B:126:GLU:H	2.22	0.43
16:P:42:ARG:C	16:P:43:LYS:HG3	2.38	0.43
14:N:26:ARG:NE	14:N:47:LEU:HD21	2.33	0.43
3:C:6:HIS:CD2	3:C:8:ILE:H	2.34	0.43
9:I:114:TYR:CE1	10:J:59:SER:O	2.71	0.43
1:A:470:U:O5'	1:A:470:U:H6	2.01	0.43
4:D:70:ILE:HG23	4:D:74:GLN:HB2	2.00	0.43
2:B:25:ASN:ND2	2:B:25:ASN:C	2.70	0.43
1:A:494:C:O2'	1:A:495:U:H6	2.02	0.43
1:A:208:U:H4'	1:A:209:U:OP1	2.19	0.43
2:B:92:TYR:CD2	2:B:151:GLY:HA3	2.54	0.43
9:I:95:LYS:O	9:I:99:LEU:HD23	2.19	0.43
1:A:798:A:H4'	1:A:799:A:OP2	2.19	0.43
1:A:1519:U:H2'	1:A:1520:C:O4'	2.19	0.43
1:A:399:U:H2'	1:A:400:U:C6	2.54	0.43
3:C:76:VAL:O	3:C:83:ARG:CG	2.66	0.43
3:C:83:ARG:C	3:C:85:ARG:N	2.71	0.43
4:D:8:VAL:HG21	4:D:115:ARG:HH11	1.84	0.43
4:D:24:GLU:C	4:D:26:CYS:H	2.18	0.43
16:P:18:ARG:CG	16:P:35:LYS:HE3	2.47	0.43
9:I:9:ARG:CG	9:I:14:VAL:HG22	2.48	0.43
1:A:1158:G:O5'	1:A:1158:G:H8	2.02	0.43
1:A:1168:G:P	9:I:113:LYS:HZ1	2.42	0.43
1:A:872:G:H2'	1:A:873:C:C6	2.54	0.43
6:F:45:LEU:H	6:F:45:LEU:HD12	1.83	0.43
1:A:53:A:N1	1:A:54:C:C2	2.87	0.43
1:A:953:G:OP1	14:N:31:ARG:O	2.37	0.42
1:A:1374:G:H21	1:A:1479:A:H8	1.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:725:G:O2'	1:A:726:U:H5'	2.19	0.42
4:D:182:LYS:HB2	4:D:182:LYS:NZ	2.34	0.42
1:A:927:U:H3'	13:M:102:ARG:HH21	1.84	0.42
17:Q:81:ARG:HE	17:Q:81:ARG:HB2	1.64	0.42
1:A:143:A:H2'	1:A:144:C:C6	2.54	0.42
1:A:1213:U:H5''	9:I:124:GLN:O	2.20	0.42
11:K:95:ILE:O	11:K:99:GLN:HG3	2.19	0.42
4:D:76:ARG:O	4:D:80:GLU:HG2	2.19	0.42
1:A:46:G:O2'	1:A:360:U:H1'	2.19	0.42
1:A:278:C:O2'	1:A:279:G:H5'	2.19	0.42
2:B:204:ASN:HD22	2:B:205:ASP:N	2.17	0.42
19:S:11:VAL:HG22	19:S:39:THR:O	2.19	0.42
1:A:1481:G:O2'	1:A:1482:G:OP2	2.30	0.42
1:A:545:C:H1'	12:L:15:ARG:HD2	2.01	0.42
14:N:33:VAL:HG23	14:N:33:VAL:O	2.18	0.42
2:B:78:GLN:HE22	2:B:96:ARG:NH1	2.10	0.42
2:B:142:LEU:HD23	2:B:142:LEU:O	2.20	0.42
1:A:8:A:N6	4:D:205:GLU:O	2.50	0.42
3:C:34:LEU:CD1	3:C:38:ARG:HD3	2.49	0.42
9:I:33:PHE:O	9:I:35:GLU:N	2.52	0.42
11:K:114:VAL:HA	11:K:115:PRO:HD3	1.86	0.42
10:J:94:VAL:HG12	10:J:95:GLU:N	2.35	0.42
10:J:12:ASP:OD2	10:J:13:HIS:N	2.53	0.42
13:M:68:GLY:HA2	13:M:71:ARG:HD2	2.01	0.42
1:A:1302:C:H2'	1:A:1303:C:H5	1.84	0.42
1:A:915:A:N6	1:A:916:G:C6	2.87	0.42
2:B:178:ARG:NH2	8:H:68:ARG:NH2	2.67	0.42
20:T:72:LEU:O	20:T:73:HIS:O	2.36	0.42
1:A:319:G:N2	1:A:322:A:C8	2.87	0.42
4:D:17:VAL:N	4:D:33:MET:HE1	2.35	0.42
11:K:101:SER:C	11:K:103:LEU:N	2.72	0.42
1:A:1168:G:OP1	9:I:113:LYS:NZ	2.52	0.42
1:A:1062:A:C5'	5:E:16:THR:HG21	2.49	0.42
1:A:798:A:HO2'	1:A:799:A:P	2.41	0.42
1:A:911:C:C4'	1:A:912:A:OP1	2.67	0.42
1:A:155:A:H2'	1:A:156:A:O5'	2.19	0.42
1:A:1039:G:H5''	3:C:154:SER:OG	2.20	0.42
1:A:513:G:O2'	23:X:35:U:H4'	2.19	0.42
2:B:209:ARG:HH22	2:B:236:TYR:HA	1.85	0.42
1:A:952:A:C8	1:A:952:A:H5'	2.50	0.42
3:C:174:PRO:HB2	3:C:177:THR:HG23	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:50:ALA:HB2	3:C:75:VAL:HG23	2.00	0.42
1:A:1027:C:C2'	1:A:1028:A:O5'	2.68	0.42
1:A:1074:A:C2	1:A:1164:A:C6	3.08	0.42
21:V:2:GLY:C	21:V:4:GLY:H	2.23	0.42
17:Q:95:TYR:HA	17:Q:98:LEU:HD11	2.01	0.42
1:A:412:C:O5'	1:A:412:C:H6	2.01	0.42
1:A:972:C:H6	1:A:972:C:O5'	2.01	0.42
1:A:1106:G:C4'	1:A:1107:U:OP1	2.55	0.42
13:M:10:PRO:O	13:M:45:VAL:HG11	2.18	0.42
2:B:64:ARG:HG2	2:B:64:ARG:O	2.20	0.42
9:I:5:TYR:CD1	9:I:6:GLY:N	2.87	0.42
1:A:453:G:C3'	1:A:454:A:H5''	2.49	0.42
1:A:1210:A:H2'	1:A:1211:C:H6	1.83	0.42
1:A:53:A:C2	1:A:54:C:H1'	2.55	0.42
12:L:83:VAL:CG2	12:L:100:ILE:HG23	2.50	0.42
13:M:23:TYR:HB3	13:M:67:GLU:HA	2.01	0.42
5:E:64:ARG:CG	5:E:64:ARG:NH1	2.75	0.42
1:A:612:G:O2'	1:A:613:G:H5'	2.20	0.42
1:A:198:U:O3'	20:T:57:ARG:HD3	2.19	0.42
4:D:62:GLN:HE22	4:D:65:ARG:HH12	1.67	0.42
1:A:602:U:N3	4:D:134:ASP:OD1	2.52	0.42
1:A:1324:G:H2'	1:A:1325:C:C6	2.53	0.42
1:A:1162:G:O2'	1:A:1163:G:O5'	2.37	0.42
7:G:36:LYS:O	7:G:39:ALA:HB3	2.20	0.42
1:A:956:C:H2'	1:A:957:C:H5'	2.01	0.42
1:A:714:G:H5'	1:A:749:A:H4'	2.02	0.42
2:B:29:ALA:C	2:B:31:TYR:H	2.22	0.42
16:P:22:THR:HA	16:P:33:ILE:HG13	2.01	0.42
2:B:226:ARG:NH1	2:B:226:ARG:HG2	2.31	0.42
11:K:126:ARG:O	11:K:129:SER:C	2.58	0.42
4:D:199:ASN:C	4:D:199:ASN:ND2	2.73	0.42
6:F:45:LEU:O	6:F:46:ARG:HG2	2.20	0.42
1:A:607:C:H2'	1:A:608:G:H8	1.85	0.42
1:A:523:G:H2'	1:A:524:G:O4'	2.19	0.42
1:A:675:U:H2'	1:A:677:A:OP2	2.20	0.42
1:A:1186:U:H2'	1:A:1187:G:C8	2.55	0.42
5:E:11:ILE:HD12	5:E:31:LEU:HD13	2.01	0.42
7:G:89:MET:HB3	7:G:155:ARG:HH12	1.84	0.42
1:A:1042:C:O2'	1:A:1043:G:H5'	2.19	0.42
14:N:48:ALA:HB2	14:N:53:LEU:HD12	2.01	0.42
1:A:310:A:O2'	1:A:311:G:P	2.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:28:PHE:O	5:E:47:LYS:HA	2.20	0.42
1:A:1384:C:O2	1:A:1477:A:N1	2.53	0.42
5:E:78:HIS:HD2	8:H:107:LEU:HD12	1.85	0.42
1:A:1160:A:H2'	1:A:1161:A:O4'	2.20	0.42
1:A:135:A:H1'	1:A:176:U:O2	2.19	0.42
1:A:162:G:O2'	1:A:163:C:H5'	2.20	0.42
4:D:61:LYS:HE2	4:D:206:PHE:CE2	2.55	0.42
1:A:1367:G:O2'	1:A:1368:G:H5'	2.20	0.42
1:A:286:C:O2'	1:A:287:G:H5'	2.20	0.42
2:B:181:PHE:HD2	8:H:70:GLN:HB3	1.85	0.42
7:G:101:LEU:O	7:G:105:VAL:HG23	2.18	0.42
2:B:50:GLU:HB3	2:B:200:ILE:O	2.20	0.42
19:S:20:LEU:HA	19:S:23:ASN:ND2	2.34	0.42
9:I:83:ARG:C	9:I:85:LEU:N	2.72	0.42
1:A:543:U:C4'	1:A:544:U:H5''	2.44	0.42
1:A:1516:C:H5	7:G:82:GLY:CA	2.22	0.42
3:C:32:LEU:HD12	3:C:59:ARG:NH1	2.34	0.42
2:B:130:ARG:O	2:B:131:PRO:C	2.57	0.42
11:K:48:ILE:HD11	11:K:64:ALA:CA	2.43	0.42
18:R:88:LYS:HZ3	18:R:88:LYS:HB3	1.82	0.42
1:A:984:C:C5	1:A:985:C:C5	3.07	0.42
7:G:15:ASP:HB3	7:G:19:GLY:CA	2.50	0.42
1:A:1094:C:O2	3:C:179:ARG:HB3	2.20	0.42
1:A:645:G:O2'	1:A:819:G:H5'	2.19	0.42
1:A:839:C:O2'	1:A:840:U:H5'	2.20	0.42
16:P:26:ARG:NH2	16:P:31:LYS:HE2	2.35	0.42
9:I:26:VAL:HG12	9:I:28:VAL:HG23	2.02	0.42
1:A:1362:U:O2'	1:A:1363:U:OP2	2.30	0.42
20:T:8:ARG:HB3	20:T:9:ASN:H	1.71	0.42
10:J:5:ARG:H	10:J:100:THR:HA	1.84	0.42
1:A:423:G:OP2	4:D:7:PRO:HG3	2.20	0.42
1:A:485:G:P	12:L:118:SER:HB3	2.59	0.42
1:A:1006:C:H2'	1:A:1007:C:C5'	2.48	0.42
1:A:637:G:C2	1:A:638:A:H1'	2.55	0.42
2:B:187:LEU:HD12	2:B:201:ILE:O	2.19	0.42
6:F:33:TYR:CD1	6:F:75:LEU:HD23	2.54	0.42
17:Q:21:VAL:HG21	17:Q:59:ILE:HD11	2.01	0.42
3:C:207:VAL:HG12	3:C:207:VAL:O	2.20	0.42
9:I:58:ARG:HG2	9:I:58:ARG:NH1	2.33	0.42
9:I:118:LYS:NZ	9:I:118:LYS:CB	2.83	0.42
2:B:42:ILE:HD11	2:B:190:THR:OG1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1183:G:C2	14:N:42:ILE:HG21	2.55	0.42
1:A:586:U:H2'	1:A:587:G:C8	2.55	0.42
8:H:20:TYR:CE2	8:H:75:ARG:HD2	2.55	0.42
1:A:49:U:C4'	1:A:50:A:OP2	2.60	0.41
1:A:1237:A:C1'	1:A:1239:G:O4'	2.66	0.41
3:C:154:SER:OG	3:C:196:LEU:HA	2.20	0.41
1:A:1281:G:O2'	1:A:1282:U:H6	2.02	0.41
1:A:1123:C:O2'	1:A:1124:G:H5'	2.19	0.41
1:A:1124:G:C2'	1:A:1125:G:H5'	2.49	0.41
3:C:64:VAL:HG21	3:C:99:VAL:HG12	2.02	0.41
22:W:2:A:H5'	22:W:2:A:C8	2.46	0.41
1:A:637:G:C2	1:A:638:A:C1'	3.03	0.41
20:T:41:VAL:O	20:T:45:GLN:HB2	2.20	0.41
4:D:8:VAL:CG2	4:D:115:ARG:HH11	2.32	0.41
3:C:136:GLN:O	3:C:139:GLN:HB2	2.19	0.41
1:A:453:G:H2'	1:A:454:A:H5''	2.01	0.41
1:A:577:G:O2'	1:A:578:G:H5'	2.20	0.41
18:R:45:SER:O	18:R:47:THR:O	2.38	0.41
1:A:157:C:H2'	1:A:158:U:H6	1.83	0.41
19:S:80:TYR:CZ	19:S:81:ARG:HD2	2.55	0.41
1:A:1218:C:C4'	1:A:1315:G:N2	2.83	0.41
23:X:31:A:C2	23:X:32:C:C6	3.08	0.41
3:C:76:VAL:HG11	3:C:103:VAL:HG22	2.02	0.41
1:A:16:A:N1	1:A:896:A:H2	2.17	0.41
18:R:34:TYR:HA	18:R:69:THR:CG2	2.50	0.41
8:H:75:ARG:HA	8:H:76:PRO:HD3	1.83	0.41
9:I:89:ASN:O	9:I:92:TYR:HB2	2.20	0.41
1:A:584:C:C2	1:A:621:G:N2	2.88	0.41
1:A:566:A:H2'	1:A:567:G:O4'	2.20	0.41
1:A:1290:G:C5	1:A:1310:A:C2	3.08	0.41
1:A:639:C:O2'	15:O:28:GLN:OE1	2.25	0.41
1:A:80:U:O5'	1:A:80:U:H6	2.03	0.41
1:A:1259:U:H4'	1:A:1260:A:O5'	2.20	0.41
3:C:46:GLU:C	3:C:48:TYR:H	2.23	0.41
9:I:79:LEU:HD13	9:I:79:LEU:O	2.20	0.41
13:M:40:ASN:HD22	13:M:41:PRO:HD2	1.85	0.41
19:S:27:GLU:HB3	19:S:28:LYS:H	1.70	0.41
5:E:40:ARG:NH1	5:E:68:GLU:OE1	2.43	0.41
15:O:53:HIS:O	15:O:57:LEU:HD13	2.20	0.41
1:A:895:A:H2'	1:A:896:A:O4'	2.19	0.41
11:K:99:GLN:HG2	11:K:105:VAL:HG21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:148:ASN:C	7:G:150:ALA:N	2.73	0.41
3:C:113:ALA:HB3	3:C:114:PRO:HD3	2.02	0.41
11:K:32:ILE:CG2	11:K:77:MET:HE2	2.50	0.41
2:B:15:VAL:HB	2:B:209:ARG:HB3	2.02	0.41
10:J:49:VAL:O	10:J:61:GLU:N	2.51	0.41
2:B:100:GLY:C	2:B:108:ILE:HD12	2.40	0.41
6:F:69:GLU:O	6:F:72:VAL:HG23	2.21	0.41
17:Q:45:HIS:CD2	17:Q:47:PRO:HG3	2.55	0.41
1:A:1109:G:O2'	1:A:1129:C:N3	2.47	0.41
17:Q:63:ARG:O	17:Q:65:ILE:CD1	2.68	0.41
1:A:725:G:C2'	1:A:726:U:H5'	2.50	0.41
1:A:1024:G:C2'	1:A:1025:C:H5'	2.50	0.41
1:A:465:G:HO2'	1:A:467:C:N4	2.17	0.41
1:A:525:G:H2'	1:A:526:C:C6	2.56	0.41
1:A:522:A:H2'	1:A:523:G:C8	2.55	0.41
1:A:176:U:H6	1:A:176:U:H5'	1.86	0.41
1:A:1034:U:H2'	1:A:1181:C:H41	1.85	0.41
1:A:1371:C:H2'	1:A:1372:U:O4'	2.20	0.41
6:F:67:MET:HB2	6:F:68:PRO:CD	2.50	0.41
1:A:1485:G:H2'	1:A:1486:C:O4'	2.20	0.41
1:A:114:C:H4'	1:A:115:G:OP1	2.20	0.41
1:A:497:C:H2'	1:A:498:G:C8	2.55	0.41
1:A:31:G:H1	1:A:48:C:H5''	1.85	0.41
1:A:405:G:O6	1:A:424:U:O2'	2.39	0.41
9:I:7:THR:HG22	9:I:8:GLY:N	2.36	0.41
1:A:988:G:H2'	1:A:989:G:H8	1.84	0.41
18:R:19:LYS:HD2	18:R:19:LYS:N	2.25	0.41
1:A:450:C:H2'	1:A:451:C:C6	2.51	0.41
8:H:20:TYR:HE2	8:H:75:ARG:HD2	1.85	0.41
3:C:185:GLY:O	3:C:200:ALA:N	2.49	0.41
6:F:6:VAL:HG13	6:F:90:VAL:HG22	2.01	0.41
1:A:729:A:O2'	1:A:730:C:H5'	2.21	0.41
2:B:73:THR:HG23	2:B:95:GLN:O	2.21	0.41
8:H:63:LEU:HD22	8:H:63:LEU:H	1.85	0.41
12:L:89:ARG:NH2	12:L:97:ARG:HH21	2.16	0.41
4:D:135:LEU:HB2	4:D:138:TYR:HB2	2.01	0.41
5:E:96:PRO:HA	5:E:117:ASP:OD2	2.20	0.41
3:C:23:TYR:CG	3:C:24:ALA:N	2.89	0.41
1:A:481:U:H2'	1:A:482:A:O5'	2.20	0.41
9:I:26:VAL:HA	9:I:61:ALA:O	2.21	0.41
1:A:45:U:H2'	1:A:46:G:C8	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:32:VAL:HG12	5:E:58:ALA:HB1	2.02	0.41
12:L:104:VAL:O	12:L:105:TYR:HB2	2.20	0.41
22:W:3:G:H22	23:X:34:70U:C2	2.32	0.41
26:A:1786:PAR:O52	26:A:1786:PAR:C11	2.49	0.41
19:S:15:LEU:CD2	19:S:15:LEU:N	2.82	0.41
1:A:246:G:C4'	1:A:247:U:O5'	2.54	0.41
17:Q:97:SER:CB	17:Q:105:ALA:HB3	2.38	0.41
17:Q:100:LYS:CD	17:Q:101:ARG:NE	2.84	0.41
2:B:169:LYS:C	2:B:169:LYS:HD3	2.41	0.41
9:I:11:LYS:CG	9:I:11:LYS:O	2.69	0.41
5:E:36:ASP:OD2	5:E:40:ARG:HB2	2.19	0.41
10:J:47:PHE:CZ	14:N:37:PHE:HE1	2.38	0.41
1:A:1354:U:H2'	1:A:1355:G:O4'	2.20	0.41
1:A:1433:G:H2'	1:A:1434:G:O4'	2.21	0.41
8:H:72:PRO:O	8:H:73:ASP:CB	2.69	0.41
4:D:157:LEU:HA	4:D:160:GLN:HE21	1.86	0.41
1:A:1006:C:C3'	1:A:1006:C:C6	3.04	0.41
3:C:91:LEU:HD12	3:C:101:LEU:HD12	2.03	0.41
17:Q:66:SER:OG	17:Q:69:LYS:HB2	2.21	0.41
1:A:611:G:H2'	1:A:612:G:H8	1.85	0.41
1:A:701:G:H5''	1:A:702:C:OP2	2.21	0.41
20:T:57:ARG:HH21	20:T:102:GLY:HA2	1.86	0.41
7:G:146:GLU:HA	7:G:149:ARG:CG	2.50	0.41
7:G:146:GLU:OE1	7:G:146:GLU:O	2.39	0.41
4:D:173:TRP:CD2	4:D:189:PRO:HB3	2.56	0.41
6:F:42:GLU:HG3	6:F:61:LEU:CD2	2.50	0.41
3:C:10:PHE:CE2	3:C:178:LEU:HD13	2.56	0.41
1:A:1043:G:O4'	10:J:56:HIS:CE1	2.73	0.41
3:C:134:ILE:HD11	3:C:153:VAL:HG23	2.01	0.41
11:K:82:VAL:C	11:K:83:ILE:HG13	2.41	0.41
1:A:565:U:C2	1:A:743:G:C6	3.08	0.41
1:A:50:A:C6	1:A:356:G:O4'	2.74	0.41
1:A:1219:A:C8	1:A:1284:C:H1'	2.55	0.41
1:A:422:U:C4	1:A:423:G:C6	3.08	0.41
1:A:542:A:H4'	1:A:543:U:H5'	2.03	0.41
1:A:123:G:O2'	1:A:124:A:OP2	2.37	0.41
15:O:17:ARG:NH1	15:O:17:ARG:CG	2.81	0.41
15:O:26:GLU:HA	15:O:81:LEU:HD11	2.02	0.41
2:B:131:PRO:HG2	2:B:134:GLU:HG3	2.02	0.41
1:A:61:G:H2'	1:A:62:U:O4'	2.21	0.41
1:A:1002:G:H8	1:A:1002:G:H3'	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:8:ILE:O	3:C:11:ARG:N	2.41	0.41
3:C:172:ARG:HB3	3:C:174:PRO:HD3	2.03	0.41
1:A:1067:U:O3'	1:A:1068:U:H6	2.04	0.41
4:D:3:ARG:O	4:D:5:ILE:N	2.44	0.41
1:A:315:C:H2'	1:A:316:A:O4'	2.21	0.41
1:A:930:G:H2'	1:A:931:G:O4'	2.21	0.41
3:C:60:ALA:HB3	3:C:63:ASN:HB2	2.03	0.41
3:C:188:LEU:HD22	3:C:195:VAL:CG1	2.51	0.41
18:R:25:THR:CG2	18:R:42:ARG:NH1	2.83	0.41
14:N:37:PHE:CE2	14:N:53:LEU:HD13	2.56	0.41
20:T:86:ARG:O	20:T:90:GLN:HG3	2.20	0.41
15:O:87:ILE:CG2	15:O:88:ARG:N	2.83	0.41
3:C:84:ILE:O	3:C:88:ARG:NH1	2.53	0.41
1:A:627:G:C5	1:A:628:C:C5	3.09	0.41
1:A:400:U:H5''	1:A:479:A:C2	2.55	0.41
1:A:835:G:O2'	1:A:836:A:H5'	2.21	0.41
1:A:938:U:C2'	1:A:939:C:H5'	2.51	0.41
1:A:1396:U:H2'	1:A:1397:G:H8	1.86	0.41
1:A:173:A:O2'	1:A:174:U:H5'	2.21	0.41
13:M:29:ARG:HB3	13:M:64:TRP:CH2	2.56	0.41
13:M:121:LYS:HB2	13:M:121:LYS:HE3	1.85	0.41
1:A:1134:A:O2'	1:A:1135:C:H5'	2.21	0.41
1:A:1349:C:H2'	1:A:1350:G:O4'	2.21	0.41
1:A:425:A:C2'	1:A:426:A:H5'	2.51	0.41
9:I:82:ALA:CA	9:I:96:LEU:HD21	2.52	0.41
20:T:36:LEU:HA	20:T:39:LYS:HB2	2.03	0.41
1:A:105:G:C2'	1:A:106:G:H5'	2.51	0.41
2:B:135:GLN:O	2:B:139:LYS:HD2	2.21	0.41
1:A:944:C:H6	1:A:944:C:O5'	2.03	0.41
1:A:1093:A:N1	3:C:177:THR:CG2	2.78	0.41
1:A:1067:U:O3'	1:A:1068:U:C6	2.74	0.41
13:M:40:ASN:HD22	13:M:41:PRO:N	2.19	0.41
20:T:56:MET:HE2	20:T:88:VAL:HB	2.02	0.41
1:A:819:G:C6	1:A:828:G:C6	3.09	0.41
9:I:113:LYS:H	9:I:119:ALA:HA	1.86	0.41
1:A:511:C:H41	12:L:49:ASN:ND2	2.19	0.41
1:A:295:A:H8	1:A:295:A:O5'	2.04	0.41
21:V:2:GLY:C	21:V:4:GLY:N	2.74	0.41
17:Q:95:TYR:HA	17:Q:98:LEU:CD1	2.51	0.41
4:D:61:LYS:NZ	4:D:72:GLU:OE2	2.54	0.41
1:A:1308:C:O2'	1:A:1309:C:H5'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:539:C:O2'	1:A:540:G:H5'	2.21	0.41
1:A:1021:C:H2'	1:A:1022:U:C6	2.56	0.41
8:H:104:ARG:NH2	8:H:138:TRP:CZ3	2.88	0.41
1:A:484:C:OP1	12:L:117:ARG:NH2	2.53	0.40
1:A:983:A:OP1	1:A:983:A:O3'	2.38	0.40
2:B:119:GLU:CG	2:B:142:LEU:HD11	2.51	0.40
10:J:26:ALA:HB2	10:J:85:LEU:HD11	2.02	0.40
10:J:64:GLU:HB3	14:N:59:ALA:HB2	2.03	0.40
15:O:39:LEU:O	15:O:43:LEU:HG	2.21	0.40
1:A:421:G:P	4:D:36:ARG:HH21	2.44	0.40
11:K:126:ARG:O	11:K:129:SER:N	2.54	0.40
20:T:57:ARG:HH22	20:T:100:ILE:CD1	2.33	0.40
7:G:154:TYR:O	7:G:155:ARG:C	2.59	0.40
9:I:33:PHE:CZ	9:I:43:ALA:HB1	2.56	0.40
1:A:1363:U:H2'	1:A:1364:C:C6	2.56	0.40
3:C:117:ALA:HB2	3:C:200:ALA:HB2	2.04	0.40
1:A:538:C:H2'	1:A:539:C:C6	2.55	0.40
13:M:79:LYS:HD3	13:M:83:ASP:OD2	2.21	0.40
9:I:8:GLY:CA	9:I:79:LEU:HD12	2.39	0.40
1:A:916:G:H5''	7:G:102:ARG:CZ	2.51	0.40
1:A:942:A:HO2'	1:A:943:G:P	2.45	0.40
1:A:350:C:C1'	1:A:383:G:HO2'	2.34	0.40
19:S:5:LEU:O	19:S:6:LYS:CB	2.70	0.40
1:A:1167:G:N2	1:A:1168:G:H1'	2.35	0.40
1:A:810:U:H5''	1:A:811:A:OP2	2.20	0.40
1:A:453:G:C3'	1:A:454:A:C5'	2.99	0.40
1:A:549:G:H4'	1:A:550:G:OP1	2.21	0.40
1:A:173:A:H2'	1:A:174:U:C6	2.56	0.40
1:A:1194:A:H4'	1:A:1195:C:OP1	2.21	0.40
7:G:84:ASN:O	7:G:85:TYR:CD2	2.74	0.40
7:G:10:ARG:HG3	7:G:10:ARG:O	2.21	0.40
1:A:257:A:C6	1:A:258:A:C6	3.09	0.40
1:A:105:G:O2'	1:A:106:G:H5'	2.21	0.40
5:E:76:ILE:O	5:E:93:PRO:HB3	2.22	0.40
10:J:27:ALA:HB1	10:J:30:SER:OG	2.22	0.40
3:C:129:ALA:HB3	3:C:132:ARG:NH2	2.36	0.40
1:A:1044:U:H2'	1:A:1045:C:C6	2.57	0.40
1:A:481:U:O2'	1:A:482:A:H5'	2.22	0.40
1:A:837:A:H2'	1:A:838:G:O4'	2.21	0.40
1:A:113:A:O2'	1:A:114:C:H5'	2.21	0.40
13:M:96:LEU:O	13:M:110:ARG:NH1	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1409:U:O2'	1:A:1410:A:H5'	2.21	0.40
1:A:31:G:C2	1:A:48:C:H5''	2.56	0.40
13:M:25:ILE:HD11	13:M:60:VAL:CG1	2.52	0.40
1:A:409:A:OP2	1:A:423:G:N2	2.51	0.40
3:C:106:VAL:O	3:C:108:ASN:N	2.54	0.40
14:N:33:VAL:HA	14:N:39:LEU:O	2.22	0.40
15:O:17:ARG:NH1	15:O:77:ARG:NH1	2.69	0.40
2:B:78:GLN:O	2:B:94:ASN:ND2	2.55	0.40
2:B:71:VAL:HG23	2:B:71:VAL:O	2.21	0.40
2:B:188:ALA:O	2:B:202:PRO:HA	2.22	0.40
9:I:125:TYR:CD2	9:I:125:TYR:N	2.88	0.40
3:C:179:ARG:HG3	3:C:207:VAL:HA	2.03	0.40
1:A:995:G:H2'	1:A:996:C:C6	2.56	0.40
1:A:400:U:H5''	1:A:479:A:H2	1.86	0.40
7:G:39:ALA:O	7:G:42:ILE:HB	2.20	0.40
1:A:1194:A:O2'	1:A:1195:C:P	2.80	0.40
1:A:975:G:O2'	1:A:976:C:H5'	2.21	0.40
1:A:1095:C:O5'	1:A:1095:C:H6	2.05	0.40
1:A:1219:A:N7	1:A:1284:C:H1'	2.36	0.40
1:A:1283:U:O2'	1:A:1284:C:OP1	2.34	0.40
1:A:1345:A:H4'	1:A:1346:U:O5'	2.21	0.40
1:A:238:A:H4'	1:A:239:U:O5'	2.21	0.40
19:S:40:ILE:HG21	19:S:62:ILE:CD1	2.52	0.40
3:C:58:GLU:C	3:C:59:ARG:HG2	2.41	0.40
1:A:1046:G:N2	1:A:1171:G:O2'	2.55	0.40
1:A:434:A:C4	1:A:480:A:C2	3.09	0.40
20:T:57:ARG:NH2	20:T:100:ILE:HG12	2.35	0.40
7:G:114:ARG:HG2	7:G:114:ARG:NH1	2.31	0.40
1:A:690:C:H2'	1:A:691:C:H6	1.85	0.40
16:P:6:LEU:CD1	16:P:6:LEU:N	2.85	0.40
3:C:117:ALA:HB2	3:C:200:ALA:CB	2.51	0.40
5:E:69:VAL:HA	5:E:70:PRO:HD3	1.67	0.40
13:M:87:TYR:C	13:M:89:GLY:N	2.73	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	232/256 (91%)	178 (77%)	40 (17%)	14 (6%)	2	5
3	C	204/239 (85%)	149 (73%)	36 (18%)	19 (9%)	1	1
4	D	206/209 (99%)	171 (83%)	27 (13%)	8 (4%)	4	12
5	E	148/162 (91%)	136 (92%)	11 (7%)	1 (1%)	26	62
6	F	99/101 (98%)	86 (87%)	12 (12%)	1 (1%)	19	52
7	G	153/156 (98%)	130 (85%)	18 (12%)	5 (3%)	5	16
8	H	136/138 (99%)	125 (92%)	10 (7%)	1 (1%)	26	62
9	I	125/128 (98%)	94 (75%)	23 (18%)	8 (6%)	2	4
10	J	96/105 (91%)	69 (72%)	20 (21%)	7 (7%)	1	3
11	K	117/129 (91%)	101 (86%)	10 (8%)	6 (5%)	2	8
12	L	122/132 (92%)	95 (78%)	16 (13%)	11 (9%)	1	2
13	M	123/126 (98%)	90 (73%)	25 (20%)	8 (6%)	1	4
14	N	58/61 (95%)	42 (72%)	13 (22%)	3 (5%)	2	7
15	O	86/89 (97%)	75 (87%)	9 (10%)	2 (2%)	8	26
16	P	81/88 (92%)	68 (84%)	13 (16%)	0	100	100
17	Q	102/105 (97%)	90 (88%)	7 (7%)	5 (5%)	3	8
18	R	71/88 (81%)	65 (92%)	5 (7%)	1 (1%)	14	42
19	S	78/93 (84%)	58 (74%)	13 (17%)	7 (9%)	1	2
20	T	97/106 (92%)	80 (82%)	8 (8%)	9 (9%)	1	1
21	V	22/27 (82%)	17 (77%)	3 (14%)	2 (9%)	1	2
All	All	2356/2538 (93%)	1919 (82%)	319 (14%)	118 (5%)	3	8

All (118) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	17	PHE

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Mol	Chain	Res	Type
2	B	95	GLN
2	B	190	THR
3	C	16	ARG
3	C	18	TRP
3	C	61	ALA
3	C	154	SER
3	C	189	ALA
4	D	20	TYR
7	G	155	ARG
9	I	41	VAL
10	J	55	LYS
10	J	73	ASP
10	J	90	LEU
12	L	27	LEU
12	L	47	LYS
12	L	115	LYS
12	L	116	SER
13	M	23	TYR
13	M	67	GLU
14	N	8	GLU
14	N	22	THR
17	Q	80	GLY
17	Q	81	ARG
18	R	87	ARG
19	S	30	LEU
20	T	73	HIS
2	B	11	LEU
3	C	65	ALA
3	C	167	TRP
3	C	188	LEU
3	C	205	GLY
4	D	22	LYS
6	F	100	ASN
7	G	17	VAL
8	H	83	ILE
9	I	44	VAL
9	I	101	PHE
10	J	54	PHE
10	J	60	ARG
10	J	72	VAL
11	K	13	GLN
11	K	35	PRO

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Mol	Chain	Res	Type
11	K	52	GLY
11	K	88	GLY
12	L	28	LYS
12	L	79	GLU
12	L	80	HIS
13	M	7	VAL
13	M	24	GLY
13	M	86	CYS
17	Q	14	LYS
19	S	6	LYS
19	S	8	GLY
19	S	67	VAL
20	T	9	ASN
20	T	94	ALA
20	T	96	GLY
2	B	14	GLY
2	B	16	HIS
2	B	20	GLU
2	B	64	ARG
2	B	115	LEU
3	C	47	LEU
3	C	146	ALA
7	G	7	ALA
9	I	7	THR
9	I	12	GLU
9	I	34	ASN
9	I	56	LEU
13	M	121	LYS
15	O	86	GLY
17	Q	104	LYS
19	S	28	LYS
20	T	99	LEU
2	B	207	ALA
3	C	3	ASN
3	C	108	ASN
3	C	168	ALA
4	D	5	ILE
4	D	24	GLU
4	D	36	ARG
4	D	175	SER
9	I	21	PRO
12	L	29	GLY

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Mol	Chain	Res	Type
14	N	32	SER
19	S	9	VAL
20	T	95	ALA
20	T	97	ALA
20	T	98	PRO
20	T	102	GLY
21	V	9	ARG
2	B	229	VAL
3	C	107	GLN
5	E	65	ASN
7	G	81	GLY
11	K	127	LYS
12	L	105	TYR
17	Q	68	ARG
19	S	68	GLY
2	B	63	MET
4	D	29	PRO
10	J	34	VAL
12	L	51	ALA
12	L	91	LYS
2	B	127	ILE
2	B	130	ARG
3	C	51	GLY
3	C	66	VAL
13	M	68	GLY
21	V	22	ARG
3	C	84	ILE
3	C	130	VAL
4	D	88	VAL
7	G	82	GLY
11	K	102	GLY
13	M	124	PRO
15	O	23	GLY

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%)	187 (93%)	15 (7%)	17	43
3	C	160/188 (85%)	148 (92%)	12 (8%)	17	43
4	D	180/181 (99%)	167 (93%)	13 (7%)	18	45
5	E	115/123 (94%)	100 (87%)	15 (13%)	5	15
6	F	90/90 (100%)	84 (93%)	6 (7%)	20	50
7	G	126/127 (99%)	117 (93%)	9 (7%)	18	46
8	H	119/119 (100%)	110 (92%)	9 (8%)	16	42
9	I	98/99 (99%)	91 (93%)	7 (7%)	18	46
10	J	87/92 (95%)	84 (97%)	3 (3%)	44	78
11	K	90/99 (91%)	86 (96%)	4 (4%)	35	69
12	L	104/109 (95%)	99 (95%)	5 (5%)	31	66
13	M	100/101 (99%)	91 (91%)	9 (9%)	12	34
14	N	49/50 (98%)	43 (88%)	6 (12%)	6	18
15	O	79/80 (99%)	70 (89%)	9 (11%)	7	21
16	P	72/74 (97%)	68 (94%)	4 (6%)	26	59
17	Q	96/97 (99%)	88 (92%)	8 (8%)	14	38
18	R	64/77 (83%)	59 (92%)	5 (8%)	16	41
19	S	71/80 (89%)	67 (94%)	4 (6%)	26	59
20	T	76/82 (93%)	73 (96%)	3 (4%)	39	74
21	V	19/22 (86%)	18 (95%)	1 (5%)	28	61
All	All	1997/2110 (95%)	1850 (93%)	147 (7%)	17	43

All (147) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	16	HIS
2	B	21	ARG
2	B	24	TRP
2	B	25	ASN
2	B	40	HIS
2	B	83	MET
2	B	114	ARG
2	B	117	GLU
2	B	122	PHE
2	B	144	ARG
2	B	170	GLU

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Mol	Chain	Res	Type
2	B	178	ARG
2	B	204	ASN
2	B	215	LEU
2	B	231	GLU
3	C	3	ASN
3	C	14	ILE
3	C	26	LYS
3	C	42	LEU
3	C	105	GLU
3	C	127	ARG
3	C	139	GLN
3	C	162	GLN
3	C	167	TRP
3	C	188	LEU
3	C	192	THR
3	C	204	LEU
4	D	3	ARG
4	D	10	ARG
4	D	21	LEU
4	D	36	ARG
4	D	49	ARG
4	D	53	ASP
4	D	58	LEU
4	D	61	LYS
4	D	100	ARG
4	D	118	ARG
4	D	122	ARG
4	D	192	GLU
4	D	199	ASN
5	E	12	LEU
5	E	14	ARG
5	E	24	ARG
5	E	31	LEU
5	E	33	VAL
5	E	41	VAL
5	E	43	LEU
5	E	47	LYS
5	E	50	GLU
5	E	64	ARG
5	E	76	ILE
5	E	80	ILE
5	E	89	ILE

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Mol	Chain	Res	Type
5	E	120	THR
5	E	137	GLU
6	F	1	MET
6	F	10	LEU
6	F	18	GLN
6	F	27	GLN
6	F	55	ASP
6	F	82	ARG
7	G	5	ARG
7	G	8	GLU
7	G	12	LEU
7	G	16	LEU
7	G	45	ASP
7	G	72	ARG
7	G	73	MET
7	G	149	ARG
7	G	155	ARG
8	H	18	ARG
8	H	29	SER
8	H	30	ARG
8	H	85	ARG
8	H	88	LYS
8	H	91	ARG
8	H	92	ARG
8	H	112	LEU
8	H	133	LEU
9	I	29	ASN
9	I	38	GLN
9	I	41	VAL
9	I	60	ASP
9	I	92	TYR
9	I	113	LYS
9	I	121	ARG
10	J	60	ARG
10	J	71	LEU
10	J	73	ASP
11	K	29	ILE
11	K	54	ARG
11	K	114	VAL
11	K	116	HIS
12	L	41	ARG
12	L	60	LEU

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Mol	Chain	Res	Type
12	L	81	SER
12	L	89	ARG
12	L	118	SER
13	M	9	ILE
13	M	32	GLU
13	M	40	ASN
13	M	56	LEU
13	M	70	LEU
13	M	102	ARG
13	M	110	ARG
13	M	115	LYS
13	M	125	ARG
14	N	8	GLU
14	N	9	LYS
14	N	12	ARG
14	N	22	THR
14	N	31	ARG
14	N	41	ARG
15	O	31	LEU
15	O	38	ARG
15	O	39	LEU
15	O	44	LYS
15	O	64	ARG
15	O	70	LEU
15	O	81	LEU
15	O	83	GLU
15	O	88	ARG
16	P	1	MET
16	P	2	VAL
16	P	8	ARG
16	P	28	ARG
17	Q	9	VAL
17	Q	14	LYS
17	Q	34	LYS
17	Q	38	ARG
17	Q	70	ARG
17	Q	74	LEU
17	Q	98	LEU
17	Q	101	ARG
18	R	19	LYS
18	R	36	ASN
18	R	39	VAL

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Mol	Chain	Res	Type
18	R	54	ARG
18	R	87	ARG
19	S	7	LYS
19	S	15	LEU
19	S	32	LYS
19	S	65	ASN
20	T	9	ASN
20	T	75	ASN
20	T	84	LEU
21	V	3	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	25	ASN
2	B	78	GLN
2	B	204	ASN
2	B	212	GLN
3	C	3	ASN
3	C	6	HIS
3	C	123	GLN
3	C	139	GLN
3	C	170	GLN
3	C	176	HIS
4	D	42	GLN
4	D	45	GLN
4	D	62	GLN
4	D	123	HIS
4	D	160	GLN
4	D	199	ASN
5	E	56	GLN
5	E	73	ASN
6	F	7	ASN
6	F	18	GLN
6	F	27	GLN
6	F	73	ASN
6	F	100	ASN
7	G	13	GLN
7	G	56	GLN
7	G	68	ASN
7	G	96	GLN
7	G	106	GLN

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Mol	Chain	Res	Type
7	G	122	HIS
8	H	15	ASN
9	I	23	ASN
9	I	73	GLN
10	J	13	HIS
10	J	56	HIS
10	J	62	HIS
10	J	78	ASN
10	J	84	GLN
11	K	38	ASN
11	K	62	GLN
11	K	93	GLN
11	K	117	ASN
12	L	49	ASN
13	M	40	ASN
13	M	62	ASN
15	O	13	GLN
15	O	37	ASN
16	P	16	HIS
16	P	76	GLN
17	Q	16	GLN
18	R	36	ASN
19	S	14	HIS
19	S	23	ASN
19	S	65	ASN
20	T	16	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1513/1513 (100%)	330 (21%)	188 (12%)
22	W	2/3 (66%)	1 (50%)	0
23	X	8/11 (72%)	4 (50%)	2 (25%)
All	All	1523/1527 (99%)	335 (21%)	190 (12%)

All (335) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	G
1	A	8	A
1	A	9	G

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Mol	Chain	Res	Type
1	A	13	U
1	A	14	U
1	A	31	G
1	A	32	A
1	A	39	G
1	A	47	C
1	A	48	C
1	A	49	U
1	A	50	A
1	A	51	A
1	A	52	G
1	A	61	G
1	A	65	U
1	A	66	G
1	A	94	A
1	A	102	A
1	A	103	C
1	A	108	G
1	A	109	A
1	A	113	A
1	A	114	C
1	A	115	G
1	A	124	A
1	A	125	C
1	A	138	G
1	A	156	A
1	A	157	C
1	A	167	U
1	A	168	C
1	A	176	U
1	A	189	U
1	A	190	G
1	A	191	G
1	A	201	A
1	A	203	A
1	A	204	G
1	A	207	C
1	A	208	U
1	A	209	U
1	A	210	U
1	A	211	G
1	A	212	C

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Mol	Chain	Res	Type
1	A	239	U
1	A	240	C
1	A	242	G
1	A	246	G
1	A	247	U
1	A	261	G
1	A	262	C
1	A	270	G
1	A	275	C
1	A	276	G
1	A	277	A
1	A	284	G
1	A	301	G
1	A	311	G
1	A	323	C
1	A	324	A
1	A	325	C
1	A	327	G
1	A	340	C
1	A	341	G
1	A	347	C
1	A	348	A
1	A	349	G
1	A	362	U
1	A	363	U
1	A	367	C
1	A	368	A
1	A	384	A
1	A	389	G
1	A	392	A
1	A	393	C
1	A	401	G
1	A	407	A
1	A	408	G
1	A	409	A
1	A	416	U
1	A	417	C
1	A	418	G
1	A	423	G
1	A	424	U
1	A	425	A
1	A	434	A

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Mol	Chain	Res	Type
1	A	442	A
1	A	446	A
1	A	447	A
1	A	454	A
1	A	455	C
1	A	456	G
1	A	465	G
1	A	466	A
1	A	468	G
1	A	469	G
1	A	470	U
1	A	479	A
1	A	480	A
1	A	481	U
1	A	483	G
1	A	492	A
1	A	494	C
1	A	495	U
1	A	501	C
1	A	502	C
1	A	505	C
1	A	507	G
1	A	510	G
1	A	513	G
1	A	514	U
1	A	515	A
1	A	516	A
1	A	517	U
1	A	519	C
1	A	531	G
1	A	542	A
1	A	543	U
1	A	544	U
1	A	545	C
1	A	546	A
1	A	549	G
1	A	550	G
1	A	555	A
1	A	556	A
1	A	558	G
1	A	559	G
1	A	560	G

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Mol	Chain	Res	Type
1	A	579	C
1	A	590	A
1	A	624	U
1	A	625	A
1	A	634	C
1	A	635	U
1	A	636	A
1	A	637	G
1	A	648	A
1	A	670	A
1	A	671	G
1	A	678	A
1	A	684	C
1	A	685	A
1	A	686	G
1	A	687	A
1	A	701	G
1	A	704	G
1	A	705	A
1	A	706	U
1	A	707	G
1	A	714	G
1	A	731	C
1	A	732	C
1	A	737	C
1	A	738	G
1	A	760	A
1	A	764	A
1	A	775	A
1	A	776	U
1	A	777	A
1	A	795	C
1	A	796	U
1	A	798	A
1	A	799	A
1	A	800	C
1	A	801	G
1	A	802	A
1	A	803	U
1	A	804	G
1	A	810	U
1	A	811	A

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Mol	Chain	Res	Type
1	A	822	U
1	A	823	C
1	A	824	U
1	A	825	C
1	A	826	C
1	A	835	G
1	A	848	U
1	A	849	A
1	A	850	A
1	A	851	G
1	A	862	G
1	A	866	A
1	A	867	G
1	A	868	U
1	A	891	A
1	A	903	G
1	A	904	G
1	A	911	C
1	A	912	A
1	A	919	G
1	A	922	G
1	A	937	U
1	A	938	U
1	A	943	G
1	A	945	A
1	A	946	A
1	A	948	G
1	A	949	C
1	A	951	A
1	A	952	A
1	A	953	G
1	A	954	A
1	A	959	U
1	A	960	A
1	A	968	U
1	A	970	G
1	A	971	A
1	A	982	A
1	A	983	A
1	A	984	C
1	A	1003	U
1	A	1004	G

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Mol	Chain	Res	Type
1	A	1005	C
1	A	1006	C
1	A	1018	G
1	A	1024	G
1	A	1032	G
1	A	1036	C
1	A	1046	G
1	A	1047	U
1	A	1048	C
1	A	1050	G
1	A	1067	U
1	A	1068	U
1	A	1076	G
1	A	1077	U
1	A	1083	A
1	A	1084	A
1	A	1090	G
1	A	1106	G
1	A	1107	U
1	A	1108	U
1	A	1109	G
1	A	1111	C
1	A	1112	A
1	A	1113	G
1	A	1119	C
1	A	1120	G
1	A	1121	G
1	A	1122	C
1	A	1128	A
1	A	1134	A
1	A	1139	A
1	A	1140	C
1	A	1141	U
1	A	1142	G
1	A	1163	G
1	A	1164	A
1	A	1165	G
1	A	1172	A
1	A	1177	U
1	A	1178	G
1	A	1181	C
1	A	1182	A

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Mol	Chain	Res	Type
1	A	1183	G
1	A	1185	A
1	A	1193	U
1	A	1194	A
1	A	1195	C
1	A	1196	G
1	A	1199	C
1	A	1206	A
1	A	1207	C
1	A	1208	A
1	A	1221	U
1	A	1222	G
1	A	1231	A
1	A	1235	C
1	A	1236	G
1	A	1237	A
1	A	1238	U
1	A	1239	G
1	A	1243	C
1	A	1260	A
1	A	1261	A
1	A	1262	U
1	A	1263	C
1	A	1266	A
1	A	1267	A
1	A	1268	A
1	A	1270	A
1	A	1279	C
1	A	1280	A
1	A	1281	G
1	A	1282	U
1	A	1283	U
1	A	1284	C
1	A	1287	A
1	A	1303	C
1	A	1304	G
1	A	1317	C
1	A	1318	G
1	A	1319	G
1	A	1327	A
1	A	1328	G
1	A	1329	U

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Mol	Chain	Res	Type
1	A	1345	A
1	A	1346	U
1	A	1347	G
1	A	1361	G
1	A	1363	U
1	A	1376	A
1	A	1377	C
1	A	1379	C
1	A	1380	A
1	A	1382	C
1	A	1383	G
1	A	1424	G
1	A	1426	A
1	A	1427	G
1	A	1432	C
1	A	1433	G
1	A	1461	C
1	A	1469	A
1	A	1471	G
1	A	1476	A
1	A	1479	A
1	A	1480	A
1	A	1481	G
1	A	1482	G
1	A	1483	U
1	A	1484	A
1	A	1494	G
1	A	1506	G
1	A	1507	G
1	A	1510	C
1	A	1511	A
1	A	1516	C
1	A	1519	U
22	W	2	A
23	X	31	A
23	X	32	C
23	X	39	PSU
23	X	40	C

All (190) RNA pucker outliers are listed below:

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Mol	Chain	Res	Type
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Mol	Chain	Res	Type
1	A	5	U
1	A	7	G
1	A	8	A
1	A	13	U
1	A	30	U
1	A	31	G
1	A	47	C
1	A	48	C
1	A	49	U
1	A	50	A
1	A	51	A
1	A	60	A
1	A	64	G
1	A	65	U
1	A	102	A
1	A	108	G
1	A	112	A
1	A	114	C
1	A	123	G
1	A	124	A
1	A	155	A
1	A	167	U
1	A	175	G
1	A	188	U
1	A	189	U
1	A	190	G
1	A	203	A
1	A	208	U
1	A	209	U
1	A	238	A
1	A	239	U
1	A	241	A
1	A	245	A
1	A	246	G
1	A	261	G
1	A	269	A
1	A	274	A
1	A	275	C
1	A	276	G
1	A	300	G
1	A	310	A

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Mol	Chain	Res	Type
1	A	322	A
1	A	323	C
1	A	324	A
1	A	339	A
1	A	340	C
1	A	346	G
1	A	348	A
1	A	361	C
1	A	362	U
1	A	367	C
1	A	383	G
1	A	407	A
1	A	408	G
1	A	416	U
1	A	417	C
1	A	423	G
1	A	424	U
1	A	433	G
1	A	445	A
1	A	446	A
1	A	454	A
1	A	455	C
1	A	465	G
1	A	468	G
1	A	469	G
1	A	479	A
1	A	480	A
1	A	482	A
1	A	491	C
1	A	494	C
1	A	500	G
1	A	501	C
1	A	513	G
1	A	514	U
1	A	516	A
1	A	518	A
1	A	530	A
1	A	542	A
1	A	544	U
1	A	545	C
1	A	549	G
1	A	558	G

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Mol	Chain	Res	Type
1	A	559	G
1	A	578	G
1	A	624	U
1	A	636	A
1	A	669	U
1	A	670	A
1	A	684	C
1	A	685	A
1	A	686	G
1	A	700	C
1	A	704	G
1	A	705	A
1	A	731	C
1	A	735	G
1	A	736	A
1	A	775	A
1	A	776	U
1	A	795	C
1	A	798	A
1	A	800	C
1	A	801	G
1	A	802	A
1	A	803	U
1	A	823	C
1	A	847	U
1	A	848	U
1	A	849	A
1	A	850	A
1	A	861	U
1	A	866	A
1	A	867	G
1	A	890	A
1	A	911	C
1	A	937	U
1	A	942	A
1	A	945	A
1	A	948	G
1	A	951	A
1	A	952	A
1	A	953	G
1	A	959	U
1	A	969	U

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Mol	Chain	Res	Type
1	A	970	G
1	A	1031	U
1	A	1035	G
1	A	1046	G
1	A	1047	U
1	A	1049	A
1	A	1067	U
1	A	1083	A
1	A	1106	G
1	A	1110	C
1	A	1111	C
1	A	1121	G
1	A	1127	C
1	A	1133	A
1	A	1139	A
1	A	1141	U
1	A	1162	G
1	A	1163	G
1	A	1164	A
1	A	1171	G
1	A	1177	U
1	A	1182	A
1	A	1194	A
1	A	1195	C
1	A	1205	G
1	A	1206	A
1	A	1207	C
1	A	1220	A
1	A	1221	U
1	A	1261	A
1	A	1262	U
1	A	1266	A
1	A	1278	C
1	A	1279	C
1	A	1281	G
1	A	1282	U
1	A	1283	U
1	A	1286	G
1	A	1303	C
1	A	1316	C
1	A	1317	C
1	A	1318	G

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Mol	Chain	Res	Type
1	A	1326	U
1	A	1327	A
1	A	1328	G
1	A	1345	A
1	A	1346	U
1	A	1362	U
1	A	1376	A
1	A	1378	A
1	A	1379	C
1	A	1381	C
1	A	1382	C
1	A	1426	A
1	A	1431	A
1	A	1432	C
1	A	1475	U
1	A	1479	A
1	A	1480	A
1	A	1481	G
1	A	1483	U
1	A	1505	U
1	A	1506	G
23	X	31	A
23	X	39	PSU

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
23	70U	X	34	22,23	17,26,27	1.07	2 (11%)	20,37,40	3.25	3 (15%)
23	12A	X	37	23	24,36,37	3.48	10 (41%)	28,52,55	2.62	6 (21%)
23	PSU	X	39	23	13,21,22	1.60	4 (30%)	18,30,33	4.00	8 (44%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	70U	X	34	22,23	-	0/9/31/32	0/2/2/2
23	12A	X	37	23	-	0/17/43/44	0/3/3/3
23	PSU	X	39	23	-	0/7/25/26	0/2/2/2

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	X	37	12A	C8-N7	-3.71	1.27	1.34
23	X	37	12A	C4-N3	-2.16	1.32	1.35
23	X	39	PSU	C6-N1	2.12	1.39	1.34
23	X	37	12A	CA-N	2.43	1.51	1.46
23	X	37	12A	CB-CA	2.44	1.61	1.53
23	X	39	PSU	C2'-C1'	2.45	1.56	1.53
23	X	37	12A	C5-C4	2.49	1.46	1.40
23	X	37	12A	C2-N1	2.64	1.38	1.34
23	X	34	70U	C4-N3	2.68	1.38	1.33
23	X	39	PSU	C4-N3	2.87	1.38	1.33
23	X	34	70U	C6-N1	2.99	1.39	1.35
23	X	37	12A	O4'-C1'	3.20	1.45	1.41
23	X	39	PSU	C5-C1'	3.29	1.55	1.52
23	X	37	12A	OG1-CB	4.66	1.53	1.43
23	X	37	12A	C6-N6	6.63	1.49	1.36
23	X	37	12A	C2-S2	12.72	1.86	1.75

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	X	39	PSU	N1-C2-N3	-12.78	120.18	128.33
23	X	34	70U	C5-C4-N3	-9.07	114.77	125.04
23	X	37	12A	OO-CC-N6	-7.22	112.62	123.58
23	X	37	12A	C2M-S2-C2	-6.07	98.36	102.26
23	X	39	PSU	C5-C1'-C2'	-4.80	106.99	115.52
23	X	34	70U	C5M-C5-C4	-2.60	116.72	120.93
23	X	37	12A	N3-C2-N1	-2.25	122.49	126.79
23	X	37	12A	C4-C5-N7	-2.24	107.42	109.48
23	X	39	PSU	C5-C6-N1	-2.19	121.30	124.39
23	X	39	PSU	O4'-C1'-C2'	2.02	106.79	104.73
23	X	37	12A	O4'-C1'-N9	2.28	112.88	108.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	X	39	PSU	O4'-C4'-C3'	2.74	110.66	105.15
23	X	39	PSU	C6-N1-C2	3.24	120.68	115.47
23	X	39	PSU	C3'-C2'-C1'	4.62	107.15	101.79
23	X	39	PSU	C4-N3-C2	6.83	121.15	115.25
23	X	37	12A	N6-CC-N	7.96	126.48	113.81
23	X	34	70U	C2-N3-C4	10.64	127.62	115.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	X	34	70U	8	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 189 ligands modelled in this entry, 188 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	PAR	A	1786	-	45,45,45	0.59	1 (2%)	59,67,67	1.23	7 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PAR	A	1786	-	-	0/18/94/94	0/4/4/4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	1786	PAR	O43-C13	2.25	1.45	1.41

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	1786	PAR	C11-O51-C51	-2.72	108.47	113.75
26	A	1786	PAR	C64-C54-C44	-2.65	108.16	113.17
26	A	1786	PAR	C11-O11-C42	-2.41	111.72	118.01
26	A	1786	PAR	C13-O52-C52	-2.26	112.10	118.01
26	A	1786	PAR	C14-O33-C33	-2.14	112.41	118.01
26	A	1786	PAR	O52-C52-C62	2.23	112.93	107.17
26	A	1786	PAR	O33-C14-C24	3.03	113.57	107.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	A	1786	PAR	4	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1512/1513 (99%)	1.30	133 (8%) 12 6	28, 54, 117, 169	0
2	B	234/256 (91%)	1.30	48 (20%) 1 1	53, 89, 136, 146	0
3	C	206/239 (86%)	1.20	28 (13%) 4 2	52, 79, 118, 123	0
4	D	208/209 (99%)	0.83	18 (8%) 13 6	46, 64, 86, 96	0
5	E	150/162 (92%)	0.63	2 (1%) 79 71	33, 48, 67, 80	0
6	F	101/101 (100%)	0.96	13 (12%) 5 2	64, 87, 97, 100	0
7	G	155/156 (99%)	0.99	18 (11%) 6 3	51, 76, 105, 118	0
8	H	138/138 (100%)	0.71	2 (1%) 78 69	32, 47, 61, 71	0
9	I	127/128 (99%)	1.26	21 (16%) 2 1	43, 87, 103, 108	0
10	J	98/105 (93%)	2.29	47 (47%) 0 0	52, 113, 141, 145	0
11	K	119/129 (92%)	1.05	11 (9%) 11 5	38, 59, 81, 99	0
12	L	124/132 (93%)	0.85	6 (4%) 34 23	26, 53, 69, 92	0
13	M	125/126 (99%)	1.47	27 (21%) 1 1	57, 73, 126, 145	0
14	N	60/61 (98%)	1.37	15 (25%) 1 0	55, 68, 102, 104	0
15	O	88/89 (98%)	0.75	5 (5%) 27 17	45, 64, 82, 100	0
16	P	83/88 (94%)	0.82	1 (1%) 81 73	39, 49, 60, 84	0
17	Q	104/105 (99%)	1.01	8 (7%) 16 8	35, 50, 100, 129	0
18	R	73/88 (82%)	0.91	4 (5%) 29 18	53, 70, 111, 125	0
19	S	80/93 (86%)	1.62	22 (27%) 1 0	66, 96, 118, 120	0
20	T	99/106 (93%)	0.69	4 (4%) 42 30	32, 52, 74, 79	0
21	V	24/27 (88%)	1.02	3 (12%) 5 2	52, 61, 77, 90	0
22	W	3/3 (100%)	1.03	0 100 100	52, 52, 53, 54	0
23	X	8/11 (72%)	1.28	2 (25%) 1 0	61, 88, 115, 125	0
All	All	3919/4065 (96%)	1.16	438 (11%) 7 3	26, 61, 117, 169	0

All (438) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
17	Q	105	ALA	12.5
2	B	238	LEU	11.9
10	J	30	SER	11.8
19	S	3	ARG	11.8
10	J	28	ARG	10.7
13	M	124	PRO	10.6
11	K	128	ALA	9.8
2	B	237	ALA	9.0
10	J	29	ARG	8.6
13	M	126	LYS	7.7
13	M	120	LYS	7.1
2	B	19	HIS	7.1
1	A	1111	C	7.0
13	M	125	ARG	6.9
4	D	35	ARG	6.7
1	A	1516	C	6.5
19	S	20	LEU	6.4
13	M	123	ALA	6.3
13	M	4	ILE	6.2
18	R	16	PRO	6.2
13	M	116	THR	6.1
13	M	118	ALA	5.8
10	J	27	ALA	5.8
9	I	27	THR	5.7
14	N	13	THR	5.6
7	G	156	TRP	5.6
1	A	1510	C	5.4
3	C	61	ALA	5.4
10	J	31	GLY	5.3
2	B	136	VAL	5.3
19	S	37	ARG	5.2
17	Q	98	LEU	5.1
10	J	80	LYS	5.1
1	A	983	A	5.0
10	J	33	GLN	4.9
1	A	982	A	4.9
2	B	10	LEU	4.9
10	J	34	VAL	4.9
3	C	32	LEU	4.9
13	M	8	GLU	4.8
9	I	128	ARG	4.7
17	Q	103	GLY	4.7

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Mol	Chain	Res	Type	RSRZ
2	B	131	PRO	4.6
2	B	207	ALA	4.6
1	A	984	C	4.6
19	S	26	GLY	4.6
1	A	1009	G	4.6
1	A	1109	G	4.6
14	N	6	LEU	4.4
2	B	7	VAL	4.4
17	Q	104	LYS	4.4
4	D	2	GLY	4.3
1	A	1517	U	4.3
2	B	130	ARG	4.3
10	J	36	GLY	4.3
2	B	229	VAL	4.3
1	A	981	G	4.2
4	D	21	LEU	4.2
10	J	24	VAL	4.2
1	A	1518	U	4.2
7	G	155	ARG	4.2
2	B	133	LYS	4.1
13	M	9	ILE	4.1
18	R	17	SER	4.1
7	G	55	GLY	4.1
10	J	35	SER	4.1
17	Q	102	GLY	4.0
10	J	83	GLU	4.0
3	C	92	ALA	4.0
9	I	7	THR	4.0
10	J	93	GLY	3.9
3	C	21	ARG	3.9
2	B	15	VAL	3.9
10	J	90	LEU	3.9
13	M	119	GLY	3.9
19	S	2	PRO	3.8
1	A	1116	G	3.8
19	S	53	ASN	3.7
10	J	22	LYS	3.7
10	J	21	GLN	3.7
1	A	1005	C	3.7
9	I	84	ALA	3.7
3	C	96	GLY	3.6
16	P	83	GLU	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	1125	G	3.6
14	N	61	TRP	3.6
2	B	11	LEU	3.6
10	J	86	MET	3.6
19	S	49	ILE	3.6
6	F	98	LEU	3.6
9	I	96	LEU	3.6
13	M	115	LYS	3.6
1	A	1019	C	3.6
1	A	153	G	3.5
1	A	513	G	3.5
2	B	125	PRO	3.5
11	K	129	SER	3.5
14	N	60	SER	3.5
3	C	155	GLY	3.5
15	O	22	THR	3.5
10	J	89	ASP	3.4
4	D	9	CYS	3.4
13	M	117	VAL	3.4
9	I	15	ALA	3.4
10	J	20	ALA	3.4
13	M	2	ALA	3.4
1	A	1151	A	3.3
19	S	23	ASN	3.3
1	A	1237	A	3.3
1	A	1001	G	3.3
4	D	32	ALA	3.3
1	A	1119	C	3.3
10	J	70	ARG	3.3
9	I	19	LEU	3.3
10	J	79	ARG	3.2
10	J	71	LEU	3.2
3	C	33	LEU	3.2
19	S	60	VAL	3.2
2	B	240	GLN	3.2
9	I	102	LEU	3.2
10	J	10	GLY	3.2
1	A	1004	G	3.2
10	J	15	THR	3.1
1	A	1403	G	3.1
3	C	98	ASN	3.1
3	C	67	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	1020	C	3.1
3	C	77	ILE	3.1
9	I	94	ALA	3.1
1	A	1122	C	3.1
13	M	106	ASN	3.1
1	A	1018	G	3.1
1	A	1121	G	3.1
2	B	16	HIS	3.1
10	J	32	ALA	3.1
1	A	1036	C	3.1
4	D	3	ARG	3.1
18	R	18	ARG	3.1
1	A	1236	G	3.1
1	A	1455	C	3.1
2	B	234	PRO	3.1
7	G	63	LYS	3.0
19	S	17	GLU	3.0
7	G	12	LEU	3.0
10	J	72	VAL	3.0
10	J	38	ILE	3.0
6	F	61	LEU	3.0
9	I	92	TYR	3.0
7	G	2	ALA	3.0
11	K	54	ARG	3.0
10	J	5	ARG	3.0
1	A	1112	A	3.0
3	C	43	LEU	3.0
19	S	39	THR	3.0
3	C	81	GLY	3.0
1	A	515	A	3.0
1	A	1010	C	3.0
2	B	32	ILE	3.0
2	B	42	ILE	3.0
13	M	114	ARG	2.9
9	I	85	LEU	2.9
1	A	1127	C	2.9
10	J	87	THR	2.9
2	B	44	LEU	2.9
1	A	1012	A	2.9
10	J	75	ILE	2.9
2	B	227	GLY	2.9
9	I	17	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
3	C	57	ILE	2.9
19	S	62	ILE	2.9
14	N	16	PHE	2.9
1	A	211	G	2.9
14	N	2	ALA	2.9
9	I	38	GLN	2.9
13	M	35	GLU	2.9
1	A	987	G	2.8
19	S	31	ILE	2.8
2	B	108	ILE	2.8
11	K	79	SER	2.8
10	J	7	LYS	2.8
2	B	203	GLY	2.8
1	A	1002	G	2.8
4	D	25	ARG	2.8
3	C	70	VAL	2.8
4	D	20	TYR	2.8
1	A	1106	G	2.8
3	C	97	LYS	2.8
4	D	209	ARG	2.8
7	G	48	LYS	2.8
12	L	115	LYS	2.8
9	I	14	VAL	2.8
13	M	7	VAL	2.8
10	J	78	ASN	2.8
13	M	64	TRP	2.8
19	S	67	VAL	2.8
1	A	405	G	2.8
4	D	22	LYS	2.8
7	G	82	GLY	2.8
21	V	2	GLY	2.8
1	A	1348	C	2.7
19	S	4	SER	2.7
2	B	208	ILE	2.7
2	B	123	ALA	2.7
3	C	89	GLU	2.7
19	S	27	GLU	2.7
1	A	1152	G	2.7
12	L	19	ARG	2.7
1	A	1113	G	2.7
3	C	76	VAL	2.7
2	B	137	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
13	M	13	LYS	2.6
6	F	79	LEU	2.6
2	B	127	ILE	2.6
19	S	51	VAL	2.6
21	V	6	ARG	2.6
7	G	85	TYR	2.6
7	G	152	ALA	2.6
14	N	10	ALA	2.6
10	J	99	LYS	2.6
11	K	40	ILE	2.6
6	F	65	VAL	2.6
1	A	970	G	2.6
1	A	1120	G	2.6
2	B	23	ARG	2.6
7	G	50	ILE	2.6
4	D	7	PRO	2.6
2	B	28	PHE	2.5
12	L	18	VAL	2.6
1	A	417	C	2.5
1	A	1241	C	2.5
1	A	706	U	2.5
1	A	637	G	2.5
1	A	1015	G	2.5
8	H	2	LEU	2.5
10	J	85	LEU	2.5
10	J	43	ARG	2.5
1	A	825	C	2.5
1	A	1007	C	2.5
1	A	1424	G	2.5
20	T	44	ALA	2.5
2	B	132	LYS	2.5
7	G	70	LYS	2.5
10	J	55	LYS	2.5
10	J	57	LYS	2.5
2	B	89	GLY	2.5
14	N	14	PRO	2.5
1	A	1258	C	2.5
2	B	122	PHE	2.5
11	K	90	GLY	2.5
19	S	35	SER	2.5
2	B	232	PRO	2.5
6	F	57	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	157	C	2.5
7	G	60	LYS	2.5
9	I	70	LYS	2.5
1	A	465	G	2.4
17	Q	96	GLN	2.4
15	O	34	LEU	2.4
10	J	74	ILE	2.4
1	A	1172	A	2.4
1	A	985	C	2.4
1	A	479	A	2.4
7	G	61	VAL	2.4
1	A	1071	G	2.4
1	A	1204	C	2.4
2	B	8	LYS	2.4
2	B	236	TYR	2.4
10	J	47	PHE	2.4
14	N	12	ARG	2.4
1	A	961	C	2.4
2	B	224	GLN	2.4
3	C	23	TYR	2.4
1	A	1250	A	2.4
1	A	1519	U	2.4
9	I	87	GLN	2.4
1	A	413	C	2.4
12	L	31	PRO	2.4
21	V	10	ARG	2.4
10	J	40	LEU	2.3
4	D	160	GLN	2.3
14	N	29	ARG	2.3
1	A	1240	C	2.3
3	C	154	SER	2.3
1	A	1459	G	2.3
19	S	16	LEU	2.3
17	Q	101	ARG	2.3
2	B	223	ILE	2.3
3	C	55	VAL	2.3
6	F	6	VAL	2.3
1	A	433	G	2.3
20	T	68	LYS	2.3
1	A	317	C	2.3
1	A	1114	C	2.3
1	A	1480	A	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	383	G	2.3
1	A	1163	G	2.3
4	D	26	CYS	2.3
1	A	163	C	2.3
4	D	105	VAL	2.3
2	B	95	GLN	2.3
3	C	65	ALA	2.3
5	E	154	GLY	2.3
1	A	1426	A	2.3
11	K	28	THR	2.3
1	A	1117	U	2.3
12	L	60	LEU	2.3
9	I	13	ALA	2.3
15	O	89	GLY	2.3
1	A	1330	A	2.3
13	M	81	LEU	2.3
1	A	1263	C	2.3
6	F	35	ALA	2.3
9	I	36	TYR	2.3
13	M	109	THR	2.3
1	A	423	G	2.3
1	A	1035	G	2.3
11	K	77	MET	2.3
6	F	91	VAL	2.3
7	G	69	VAL	2.3
2	B	118	LEU	2.3
1	A	152	G	2.2
1	A	271	G	2.2
1	A	1032	G	2.2
1	A	1286	G	2.2
3	C	69	HIS	2.2
4	D	146	ILE	2.2
9	I	18	PHE	2.2
1	A	679	A	2.2
1	A	539	C	2.2
6	F	26	ILE	2.2
1	A	1479	A	2.2
7	G	5	ARG	2.2
14	N	17	LYS	2.2
11	K	27	ASN	2.2
1	A	531	G	2.2
1	A	1352	G	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	239	VAL	2.2
14	N	18	VAL	2.2
2	B	128	GLU	2.2
1	A	374	C	2.2
1	A	1325	C	2.2
6	F	63	TYR	2.2
1	A	1063	G	2.2
4	D	31	CYS	2.2
2	B	76	GLN	2.2
3	C	163	ALA	2.2
15	O	87	ILE	2.2
13	M	95	GLY	2.2
3	C	47	LEU	2.2
1	A	156	A	2.2
1	A	1062	A	2.2
13	M	66	LEU	2.2
4	D	49	ARG	2.2
13	M	42	ALA	2.2
2	B	206	ASP	2.2
1	A	321	G	2.2
1	A	527	G	2.2
1	A	613	G	2.2
1	A	1336	G	2.2
3	C	167	TRP	2.2
6	F	4	TYR	2.2
17	Q	97	SER	2.1
6	F	60	PHE	2.1
11	K	57	THR	2.1
3	C	176	HIS	2.1
1	A	501	C	2.1
1	A	1089	C	2.1
1	A	322	A	2.1
1	A	1238	U	2.1
7	G	80	VAL	2.1
12	L	28	LYS	2.1
8	H	1	MET	2.1
1	A	731	C	2.1
1	A	980	G	2.1
1	A	1474	G	2.1
1	A	1500	G	2.1
10	J	59	SER	2.1
1	A	1229	A	2.1

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Mol	Chain	Res	Type	RSRZ
19	S	6	LYS	2.1
10	J	76	ASN	2.1
1	A	396	C	2.1
13	M	31	LYS	2.1
1	A	1064	G	2.1
10	J	16	LEU	2.1
18	R	31	LEU	2.1
20	T	91	LEU	2.1
10	J	25	GLU	2.1
1	A	1126	G	2.1
1	A	1249	A	2.1
1	A	1239	G	2.1
14	N	31	ARG	2.1
10	J	4	ILE	2.1
15	O	3	ILE	2.1
1	A	124	A	2.1
1	A	1508	A	2.1
19	S	19	VAL	2.1
23	X	40	C	2.1
1	A	421	G	2.1
1	A	1090	G	2.1
3	C	119	ARG	2.1
23	X	30	G	2.1
2	B	190	THR	2.1
1	A	1202	G	2.0
10	J	6	ILE	2.0
6	F	72	VAL	2.0
1	A	617	C	2.0
2	B	139	LYS	2.0
14	N	11	LYS	2.0
4	D	187	ARG	2.0
1	A	249	G	2.0
1	A	649	G	2.0
1	A	1281	G	2.0
11	K	38	ASN	2.0
3	C	87	LEU	2.0
19	S	41	VAL	2.0
9	I	43	ALA	2.0
1	A	763	A	2.0
1	A	1049	A	2.0
10	J	54	PHE	2.0
1	A	1207	C	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	209	ARG	2.0
5	E	20	GLN	2.0
2	B	215	LEU	2.0
13	M	105	THR	2.0
1	A	190	G	2.0
1	A	373	G	2.0
1	A	1046	G	2.0
1	A	1174	G	2.0
1	A	1205	G	2.0
1	A	1347	G	2.0
1	A	1397	G	2.0
1	A	48	C	2.0
1	A	1181	C	2.0
7	G	76	ARG	2.0
9	I	111	ARG	2.0
20	T	83	ARG	2.0
14	N	39	LEU	2.0
2	B	210	SER	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
23	70U	X	34	25/26	0.90	0.26	-	61,70,80,82	0
23	PSU	X	39	20/21	0.81	0.30	-	88,88,91,91	0
23	12A	X	37	34/35	0.87	0.30	-	69,72,72,72	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
24	MG	A	1758	1/1	0.03	1.15	51.88	40,40,40,40	1
24	MG	A	1667	1/1	0.53	0.59	33.45	14,14,14,14	1
24	MG	A	1650	1/1	0.93	0.45	21.37	26,26,26,26	1
24	MG	A	1670	1/1	0.98	0.52	16.84	13,13,13,13	1
24	MG	A	1764	1/1	0.97	0.40	16.83	29,29,29,29	1
24	MG	A	1760	1/1	0.23	0.70	15.63	6,6,6,6	1
24	MG	A	1680	1/1	0.73	0.52	14.03	45,45,45,45	1
24	MG	A	1784	1/1	0.72	0.45	12.06	19,19,19,19	1
24	MG	A	1637	1/1	0.53	0.37	7.97	24,24,24,24	1
24	MG	A	1654	1/1	0.88	0.36	6.81	45,45,45,45	1
24	MG	A	1648	1/1	0.98	0.36	6.72	37,37,37,37	0
24	MG	A	1756	1/1	0.84	0.35	6.58	16,16,16,16	1
24	MG	A	1683	1/1	0.38	0.44	6.36	26,26,26,26	1
24	MG	A	1679	1/1	0.87	0.36	5.31	28,28,28,28	1
24	MG	A	1738	1/1	0.78	0.33	4.51	19,19,19,19	1
24	MG	A	1692	1/1	0.97	0.46	4.29	31,31,31,31	1
24	MG	A	1728	1/1	0.98	0.38	3.68	5,5,5,5	1
24	MG	A	1658	1/1	0.76	0.32	3.46	43,43,43,43	1
24	MG	A	1725	1/1	-0.15	0.32	3.20	38,38,38,38	1
24	MG	A	1762	1/1	0.96	0.32	3.19	28,28,28,28	1
26	PAR	A	1786	42/42	0.95	0.29	2.88	34,40,52,55	0
24	MG	A	1759	1/1	0.69	0.28	2.82	15,15,15,15	1
24	MG	A	1663	1/1	0.89	0.31	2.71	47,47,47,47	1
24	MG	A	1752	1/1	0.43	0.33	2.65	27,27,27,27	1
24	MG	A	1605	1/1	0.39	0.27	2.13	33,33,33,33	1
24	MG	A	1739	1/1	0.57	0.84	1.99	33,33,33,33	1
24	MG	A	1602	1/1	0.41	0.34	1.67	86,86,86,86	0
24	MG	A	1726	1/1	0.94	0.33	1.51	19,19,19,19	1
24	MG	A	1660	1/1	0.90	0.28	1.29	34,34,34,34	1
24	MG	A	1781	1/1	0.93	0.33	0.97	24,24,24,24	1
24	MG	A	1749	1/1	0.30	0.28	0.90	34,34,34,34	1
24	MG	A	1621	1/1	0.49	0.24	0.70	18,18,18,18	1
24	MG	A	1741	1/1	0.80	0.34	0.44	33,33,33,33	1
24	MG	A	1773	1/1	0.87	0.27	0.34	35,35,35,35	1
24	MG	A	1778	1/1	0.96	0.27	0.22	7,7,7,7	1
25	ZN	N	101	1/1	0.98	0.25	-0.05	60,60,60,60	0
24	MG	A	1625	1/1	0.69	0.29	-0.06	0,0,0,0	1
24	MG	A	1603	1/1	0.80	0.23	-0.33	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
24	MG	A	1742	1/1	0.85	0.24	-0.35	2,2,2,2	1
24	MG	A	1623	1/1	0.54	0.29	-0.35	67,67,67,67	1
24	MG	A	1673	1/1	0.90	0.22	-1.16	0,0,0,0	1
24	MG	A	1765	1/1	0.91	0.23	-1.29	0,0,0,0	1
24	MG	B	301	1/1	0.72	0.14	-1.68	26,26,26,26	1
24	MG	A	1782	1/1	0.89	0.22	-2.43	13,13,13,13	1
24	MG	A	1729	1/1	0.74	0.18	-3.32	20,20,20,20	1
24	MG	A	1691	1/1	0.83	0.13	-5.55	14,14,14,14	1
24	MG	A	1665	1/1	0.80	0.12	-5.70	28,28,28,28	1
24	MG	A	1763	1/1	0.81	0.15	-6.64	0,0,0,0	1
24	MG	A	1709	1/1	0.85	0.17	-7.71	8,8,8,8	1
24	MG	A	1727	1/1	0.65	0.30	-	6,6,6,6	1
24	MG	A	1780	1/1	0.69	0.73	-	0,0,0,0	1
24	MG	A	1770	1/1	0.44	0.64	-	36,36,36,36	1
24	MG	A	1612	1/1	0.93	0.35	-	25,25,25,25	1
24	MG	A	1674	1/1	0.94	0.43	-	36,36,36,36	1
24	MG	A	1783	1/1	0.51	0.42	-	24,24,24,24	1
24	MG	A	1713	1/1	0.85	0.21	-	31,31,31,31	1
24	MG	A	1775	1/1	0.69	0.29	-	16,16,16,16	1
24	MG	A	1641	1/1	0.91	0.34	-	19,19,19,19	1
24	MG	A	1745	1/1	0.63	0.49	-	13,13,13,13	1
24	MG	A	1766	1/1	0.93	0.52	-	43,43,43,43	1
24	MG	A	1743	1/1	0.88	0.51	-	17,17,17,17	1
24	MG	A	1678	1/1	0.71	0.47	-	40,40,40,40	1
24	MG	A	1601	1/1	0.56	0.20	-	51,51,51,51	0
24	MG	A	1611	1/1	0.94	0.40	-	37,37,37,37	0
24	MG	A	1684	1/1	0.17	0.75	-	16,16,16,16	1
24	MG	A	1608	1/1	0.84	0.40	-	62,62,62,62	1
24	MG	A	1716	1/1	0.63	0.30	-	19,19,19,19	1
24	MG	A	1652	1/1	0.61	0.45	-	30,30,30,30	1
24	MG	A	1767	1/1	0.55	0.34	-	17,17,17,17	1
24	MG	A	1724	1/1	0.66	0.35	-	19,19,19,19	1
24	MG	A	1697	1/1	0.24	1.16	-	55,55,55,55	1
24	MG	A	1607	1/1	-0.01	0.46	-	107,107,107,107	1
24	MG	A	1754	1/1	0.65	0.23	-	31,31,31,31	1
24	MG	A	1777	1/1	-0.25	0.93	-	34,34,34,34	1
24	MG	A	1676	1/1	0.84	0.30	-	44,44,44,44	1
24	MG	A	1704	1/1	0.94	0.63	-	10,10,10,10	1
24	MG	A	1750	1/1	0.51	0.45	-	43,43,43,43	1
24	MG	A	1645	1/1	0.70	0.28	-	36,36,36,36	1
24	MG	A	1606	1/1	0.91	0.27	-	47,47,47,47	1
24	MG	A	1675	1/1	0.84	0.42	-	29,29,29,29	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
24	MG	A	1710	1/1	0.88	0.38	-	25,25,25,25	1
24	MG	A	1769	1/1	0.63	0.36	-	2,2,2,2	1
24	MG	A	1620	1/1	0.56	0.39	-	52,52,52,52	1
24	MG	A	1619	1/1	0.27	0.76	-	57,57,57,57	1
24	MG	A	1656	1/1	0.92	0.49	-	24,24,24,24	1
24	MG	A	1634	1/1	0.88	0.33	-	26,26,26,26	1
24	MG	A	1685	1/1	0.77	0.46	-	37,37,37,37	1
24	MG	A	1618	1/1	0.83	0.23	-	20,20,20,20	1
24	MG	A	1695	1/1	-0.28	0.42	-	33,33,33,33	1
24	MG	A	1686	1/1	0.90	0.28	-	23,23,23,23	1
24	MG	A	1712	1/1	0.64	0.29	-	21,21,21,21	1
24	MG	A	1705	1/1	0.57	0.82	-	39,39,39,39	1
24	MG	A	1669	1/1	0.57	0.45	-	34,34,34,34	1
24	MG	A	1785	1/1	0.64	0.26	-	17,17,17,17	1
24	MG	A	1776	1/1	0.34	0.97	-	64,64,64,64	1
24	MG	A	1719	1/1	0.74	0.50	-	35,35,35,35	1
24	MG	A	1610	1/1	0.35	0.27	-	66,66,66,66	0
24	MG	A	1664	1/1	0.77	0.22	-	14,14,14,14	1
24	MG	A	1768	1/1	0.81	0.50	-	34,34,34,34	1
24	MG	A	1746	1/1	0.91	0.58	-	20,20,20,20	1
24	MG	A	1779	1/1	0.61	0.45	-	15,15,15,15	1
24	MG	A	1630	1/1	0.51	0.38	-	59,59,59,59	1
24	MG	A	1627	1/1	0.82	0.23	-	6,6,6,6	1
24	MG	A	1688	1/1	0.91	0.38	-	22,22,22,22	1
24	MG	A	1703	1/1	0.95	0.37	-	40,40,40,40	1
24	MG	A	1707	1/1	0.54	0.47	-	33,33,33,33	1
24	MG	A	1624	1/1	0.12	2.29	-	82,82,82,82	1
24	MG	A	1740	1/1	0.78	0.51	-	29,29,29,29	1
24	MG	A	1706	1/1	0.26	1.40	-	6,6,6,6	1
24	MG	A	1708	1/1	0.34	0.81	-	51,51,51,51	1
24	MG	A	1699	1/1	0.64	0.38	-	34,34,34,34	1
24	MG	A	1701	1/1	0.01	1.41	-	27,27,27,27	1
24	MG	A	1748	1/1	0.82	0.45	-	39,39,39,39	1
24	MG	A	1635	1/1	0.46	0.47	-	18,18,18,18	1
24	MG	A	1662	1/1	0.94	0.45	-	32,32,32,32	1
24	MG	A	1629	1/1	0.80	0.43	-	39,39,39,39	1
24	MG	A	1677	1/1	0.86	0.55	-	36,36,36,36	1
24	MG	A	1711	1/1	0.64	0.24	-	62,62,62,62	1
24	MG	A	1639	1/1	0.50	0.60	-	64,64,64,64	1
24	MG	A	1649	1/1	0.82	0.37	-	21,21,21,21	1
24	MG	A	1636	1/1	0.78	0.30	-	42,42,42,42	1
24	MG	A	1609	1/1	0.81	0.36	-	39,39,39,39	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
24	MG	A	1696	1/1	0.50	0.36	-	23,23,23,23	1
24	MG	A	1771	1/1	0.52	0.35	-	46,46,46,46	1
24	MG	A	1653	1/1	0.92	0.30	-	21,21,21,21	1
24	MG	A	1633	1/1	0.83	0.32	-	57,57,57,57	1
24	MG	A	1772	1/1	0.79	0.44	-	32,32,32,32	1
24	MG	A	1655	1/1	0.94	0.47	-	26,26,26,26	1
24	MG	A	1731	1/1	0.70	0.38	-	18,18,18,18	1
24	MG	A	1774	1/1	0.89	0.40	-	21,21,21,21	1
24	MG	A	1638	1/1	0.73	0.40	-	50,50,50,50	1
24	MG	A	1734	1/1	0.50	0.29	-	36,36,36,36	1
24	MG	A	1668	1/1	0.97	0.27	-	20,20,20,20	1
24	MG	A	1631	1/1	0.69	0.32	-	54,54,54,54	1
24	MG	A	1718	1/1	0.85	0.52	-	31,31,31,31	1
24	MG	A	1640	1/1	0.98	0.52	-	101,101,101,101	1
24	MG	A	1615	1/1	0.73	0.19	-	39,39,39,39	0
24	MG	A	1671	1/1	0.77	0.43	-	41,41,41,41	1
24	MG	A	1733	1/1	0.89	0.42	-	35,35,35,35	1
24	MG	A	1693	1/1	0.96	0.09	-	20,20,20,20	1
24	MG	A	1702	1/1	-0.08	0.40	-	57,57,57,57	1
24	MG	A	1687	1/1	0.90	0.54	-	22,22,22,22	1
24	MG	A	1698	1/1	0.87	0.18	-	24,24,24,24	1
24	MG	A	1694	1/1	0.70	0.37	-	69,69,69,69	1
24	MG	A	1736	1/1	0.21	0.46	-	26,26,26,26	1
24	MG	A	1666	1/1	0.12	0.44	-	55,55,55,55	1
24	MG	A	1646	1/1	0.30	0.48	-	42,42,42,42	1
24	MG	A	1730	1/1	0.81	0.30	-	23,23,23,23	1
24	MG	A	1642	1/1	0.67	0.44	-	44,44,44,44	1
24	MG	A	1689	1/1	0.69	0.29	-	27,27,27,27	1
24	MG	A	1647	1/1	0.82	0.48	-	55,55,55,55	1
24	MG	A	1643	1/1	0.95	0.25	-	31,31,31,31	1
24	MG	A	1682	1/1	0.93	0.45	-	34,34,34,34	1
24	MG	A	1735	1/1	0.69	0.37	-	3,3,3,3	1
24	MG	A	1604	1/1	-0.33	0.86	-	111,111,111,111	0
24	MG	A	1737	1/1	0.85	0.43	-	0,0,0,0	1
24	MG	A	1644	1/1	0.18	0.42	-	60,60,60,60	1
24	MG	A	1628	1/1	0.81	0.24	-	47,47,47,47	1
24	MG	A	1690	1/1	0.84	0.25	-	26,26,26,26	1
24	MG	A	1757	1/1	0.62	0.25	-	0,0,0,0	1
24	MG	A	1761	1/1	0.94	0.38	-	26,26,26,26	1
24	MG	A	1720	1/1	0.75	0.51	-	13,13,13,13	1
24	MG	A	1651	1/1	0.87	0.42	-	29,29,29,29	1
24	MG	A	1622	1/1	0.47	0.34	-	54,54,54,54	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
24	MG	A	1632	1/1	0.36	0.52	-	31,31,31,31	1
24	MG	A	1722	1/1	0.86	0.55	-	22,22,22,22	1
24	MG	A	1617	1/1	0.88	0.36	-	50,50,50,50	1
24	MG	A	1751	1/1	0.63	0.44	-	29,29,29,29	1
24	MG	A	1755	1/1	0.92	0.37	-	44,44,44,44	1
24	MG	A	1661	1/1	0.94	0.48	-	28,28,28,28	1
24	MG	A	1700	1/1	0.30	0.43	-	32,32,32,32	1
24	MG	A	1721	1/1	0.53	0.44	-	21,21,21,21	1
24	MG	A	1717	1/1	0.94	0.43	-	20,20,20,20	1
24	MG	A	1714	1/1	0.95	0.32	-	13,13,13,13	1
24	MG	A	1753	1/1	0.47	0.51	-	31,31,31,31	1
24	MG	A	1681	1/1	0.97	0.42	-	41,41,41,41	1
24	MG	A	1715	1/1	0.56	0.35	-	44,44,44,44	1
24	MG	A	1659	1/1	0.90	0.36	-	26,26,26,26	1
24	MG	A	1616	1/1	0.45	0.53	-	74,74,74,74	1
24	MG	A	1613	1/1	0.51	0.30	-	25,25,25,25	1
24	MG	A	1732	1/1	0.98	0.54	-	13,13,13,13	1
24	MG	A	1626	1/1	0.68	0.24	-	15,15,15,15	1
24	MG	A	1723	1/1	0.96	0.42	-	19,19,19,19	1
25	ZN	D	301	1/1	0.88	0.54	-	100,100,100,100	0
24	MG	A	1744	1/1	0.90	0.39	-	33,33,33,33	1
24	MG	A	1657	1/1	0.85	0.58	-	23,23,23,23	1
24	MG	A	1614	1/1	0.42	0.92	-	49,49,49,49	1
24	MG	A	1672	1/1	0.55	0.38	-	20,20,20,20	1
24	MG	A	1747	1/1	0.97	0.26	-	19,19,19,19	1

6.5 Other polymers [i](#)

There are no such residues in this entry.