



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 03:44 PM UTC

PDB ID : 1XMQ / pdb_00001xmq
Title : Crystal Structure of t6A37-ASLLysUUU AAA-mRNA Bound to the Decoding Center
Authors : Murphy, F.V.; Ramakrishnan, V.; Malkiewicz, A.; Agris, P.F.
Deposited on : 2004-10-04
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

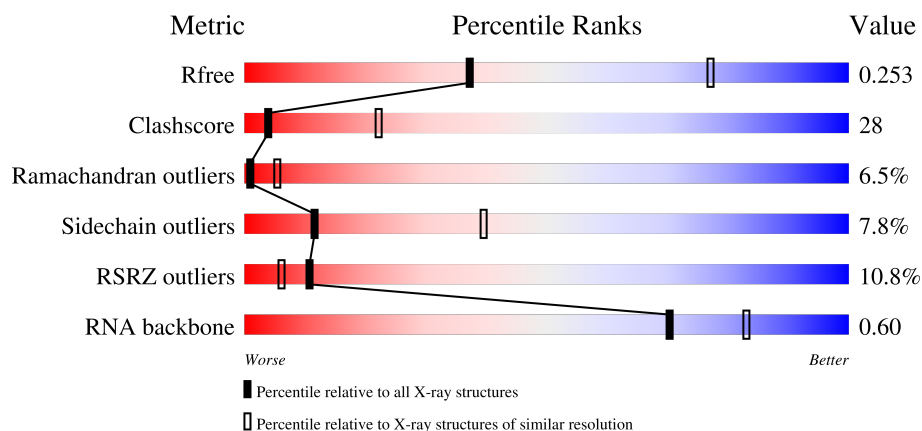
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

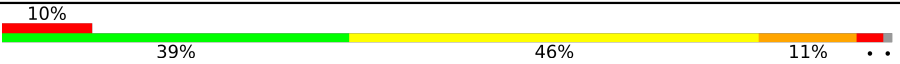
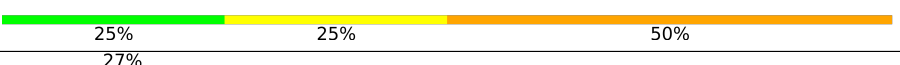
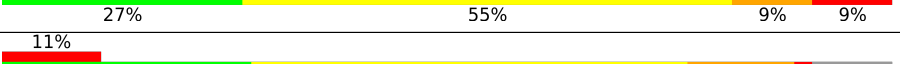
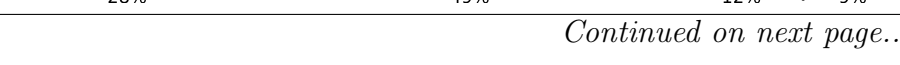
The reported resolution of this entry is 3.00 Å.

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



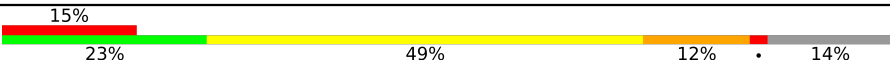
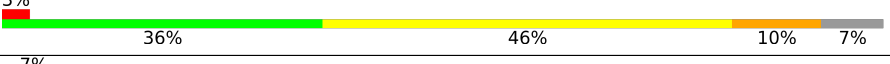
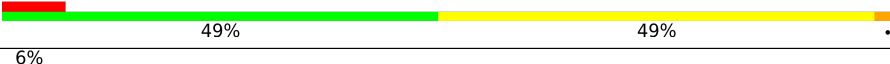
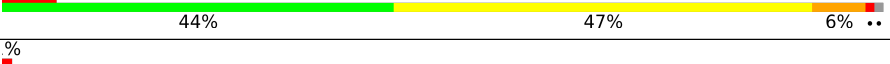
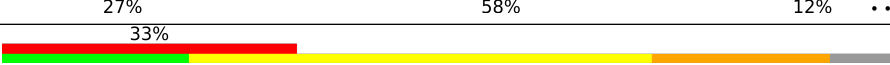
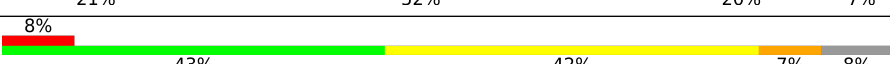
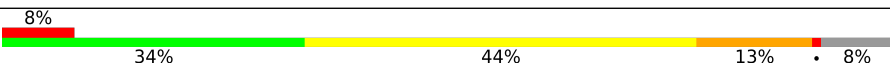
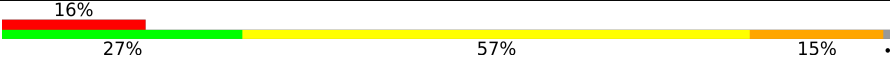
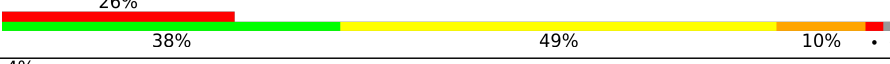
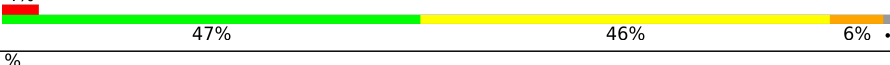
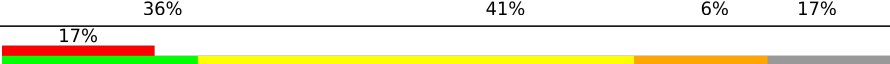
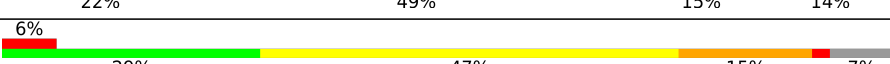
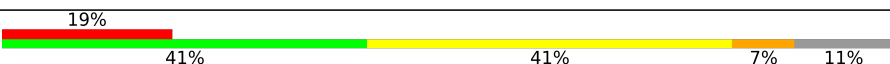
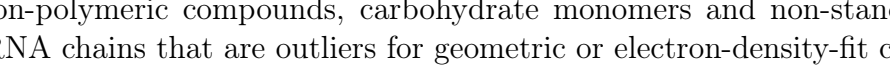
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)
RNA backbone	3983	1109 (3.20-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	1522	
2	W	4	
3	X	11	
4	B	256	

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Mol	Chain	Length	Quality of chain
5	C	239	
6	D	209	
7	E	162	
8	F	101	
9	G	156	
10	H	138	
11	I	128	
12	J	105	
13	K	129	
14	L	135	
15	M	126	
16	N	61	
17	O	89	
18	P	88	
19	Q	105	
20	R	88	
21	S	93	
22	T	106	
23	V	27	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	MG	A	1562	-	-	-	X
25	MG	A	1585	-	-	-	X
25	MG	A	1595	-	-	-	X
25	MG	A	1608	-	-	-	X
25	MG	A	1613	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	MG	A	1616	-	-	-	X
25	MG	A	214	-	-	-	X
25	MG	A	466	-	-	-	X
25	MG	A	493	-	-	-	X
25	MG	N	423	-	-	-	X
3	T6A	X	37	X	-	-	-

2 Entry composition

There are 26 unique types of molecules in this entry. The entry contains 52081 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1507	Total	C	N	O	P	22	0	0
			32380	14414	5990	10470	1506			

- Molecule 2 is a RNA chain called A-Site Messenger RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	W	4	Total	C	N	O	P	0	0	0
			85	40	20	22	3			

- Molecule 3 is a RNA chain called Anticodon RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	X	11	Total	C	N	O	P	0	0	0
			236	108	37	81	10			

- Molecule 4 is a protein called 30S Ribosomal Protein S2.

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

- Molecule 5 is a protein called 30S Ribosomal Protein S3.

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

- Molecule 6 is a protein called 30S Ribosomal Protein S4.

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

- Molecule 7 is a protein called 30S Ribosomal Protein S5.

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

- Molecule 8 is a protein called 30S Ribosomal Protein S6.

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

- Molecule 9 is a protein called 30S Ribosomal Protein S7.

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

- Molecule 10 is a protein called 30S Ribosomal Protein S8.

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

- Molecule 11 is a protein called 30S Ribosomal Protein S9.

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

- Molecule 12 is a protein called 30S Ribosomal Protein S10.

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

- Molecule 13 is a protein called 30S Ribosomal Protein S11.

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

- Molecule 14 is a protein called 30S Ribosomal Protein S12.

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

- Molecule 15 is a protein called 30S Ribosomal Protein S13.

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

- Molecule 16 is a protein called 30S Ribosomal Protein S14.

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

- Molecule 17 is a protein called 30S Ribosomal Protein S15.

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

- Molecule 18 is a protein called 30S Ribosomal Protein S16.

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

- Molecule 19 is a protein called 30S Ribosomal Protein S17.

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

- Molecule 20 is a protein called 30S Ribosomal Protein S18.

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

- Molecule 21 is a protein called 30S Ribosomal Protein S19.

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

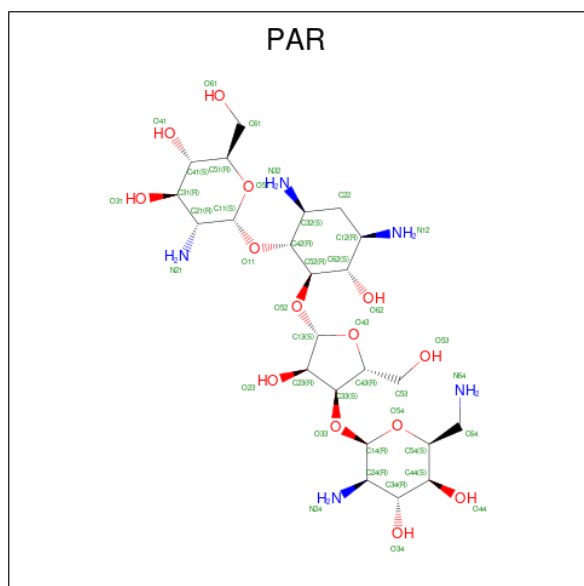
- Molecule 22 is a protein called 30S Ribosomal Protein S20.

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

- Molecule 23 is a protein called 30S Ribosomal Protein Thx.

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

- Molecule 24 is PAROMOMYCIN (CCD ID: PAR) (formula: $C_{23}H_{45}N_5O_{14}$).



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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	A	104	Total	Mg	0	0
			104	104		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	X	2	Total 2	Mg 2	0	0
25	N	1	Total 1	Mg 1	0	0

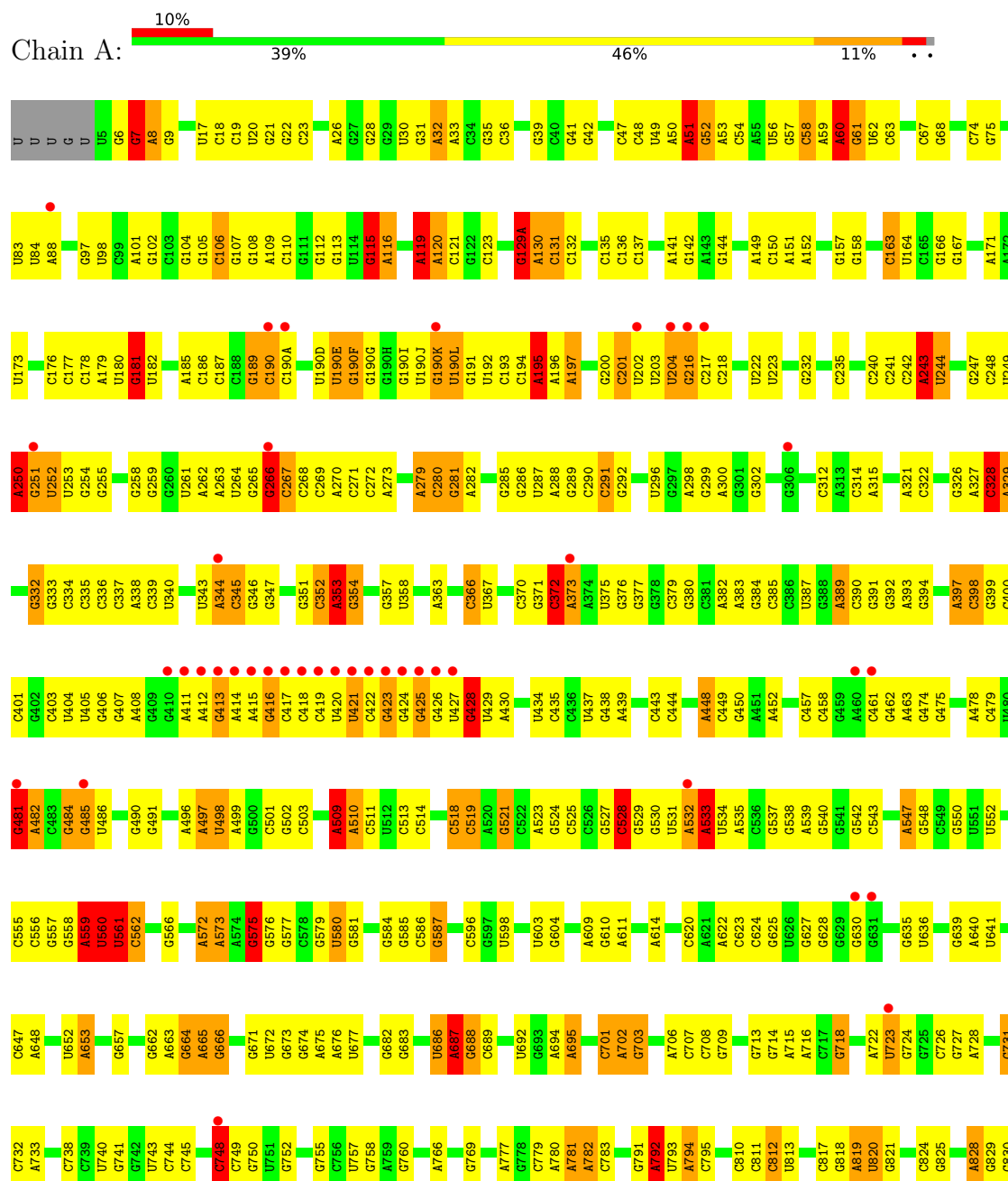
- Molecule 26 is ZINC ION (CCD ID: ZN) (formula: Zn).

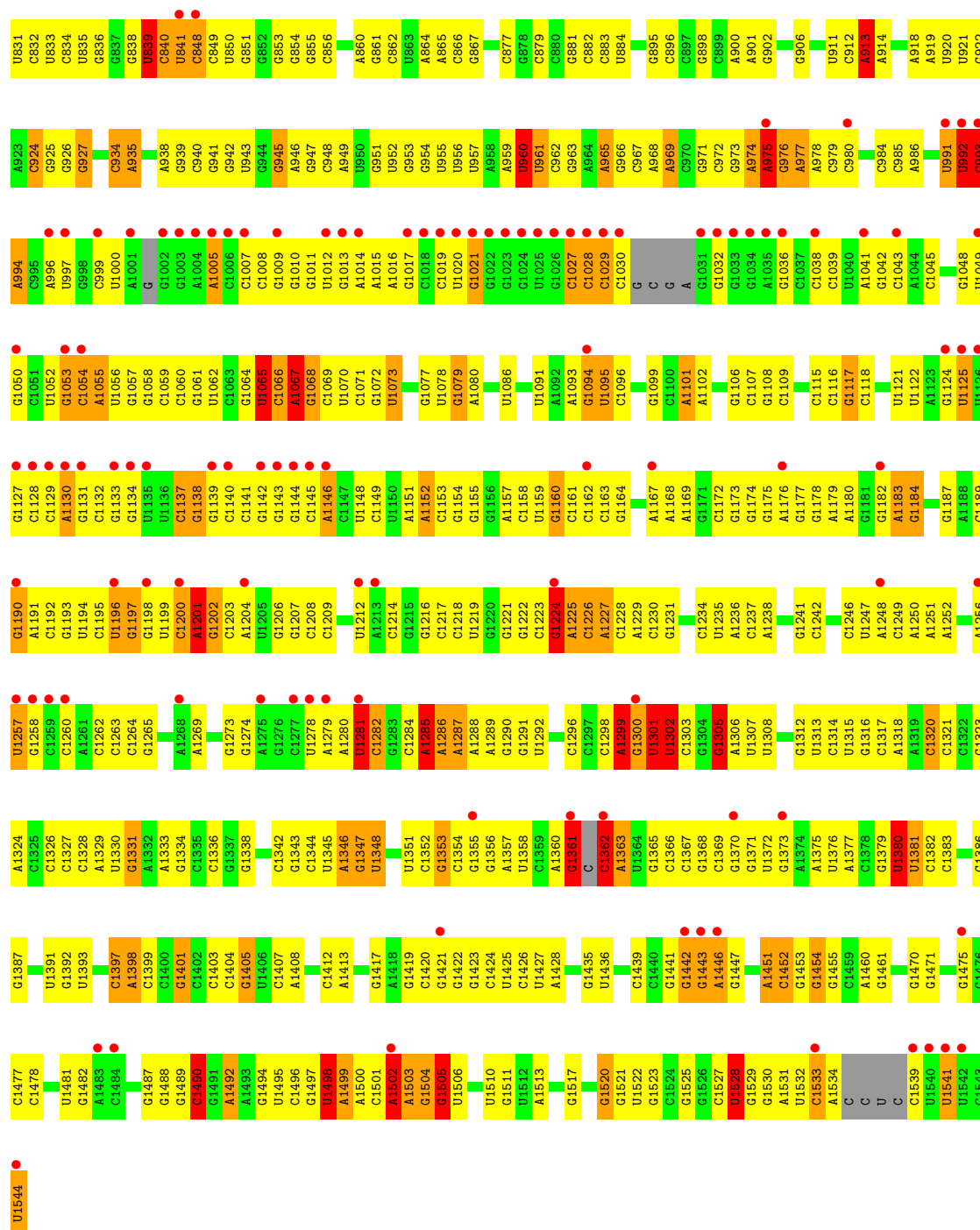
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
26	D	1	Total 1	Zn 1	0	0
26	N	1	Total 1	Zn 1	0	0

3 Residue-property plots

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

- Molecule 1: 16s ribosomal RNA





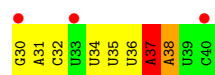
• Molecule 2: A-Site Messenger RNA

Chain W: 25% 25% 50%

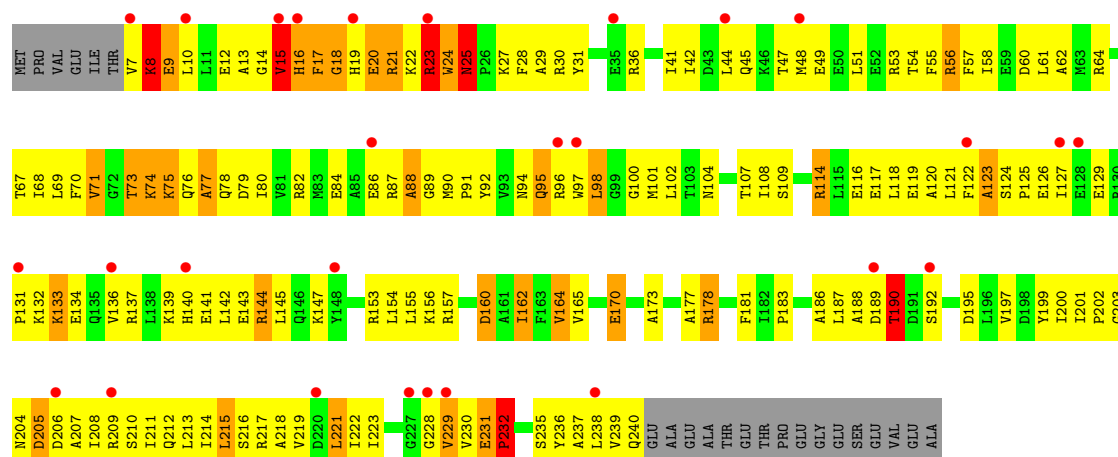


• Molecule 3: Anticodon RNA

Chain X: 27% 27% 55% 9% 9%

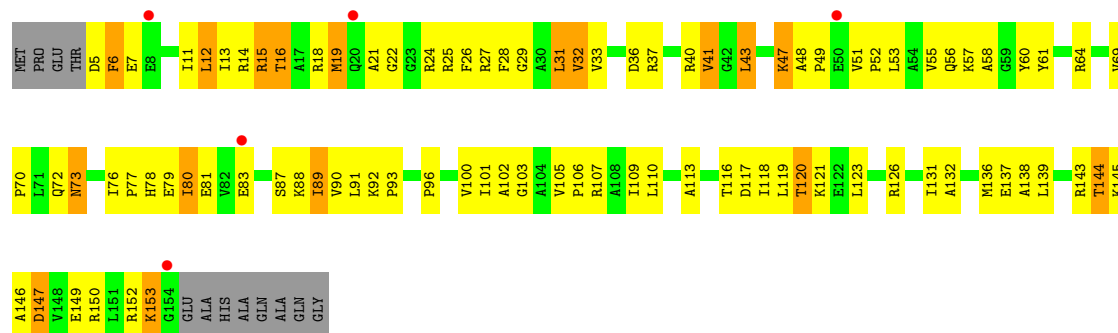


• Molecule 4: 30S Ribosomal Protein S2

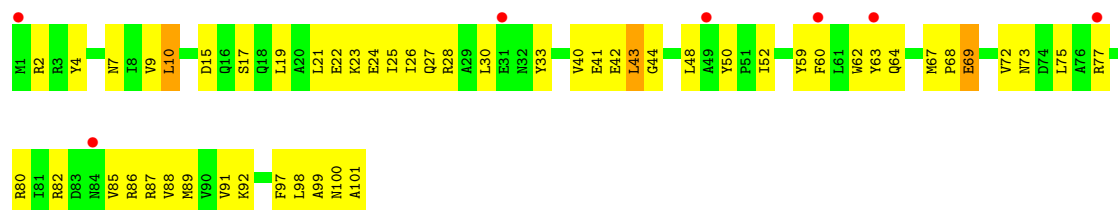




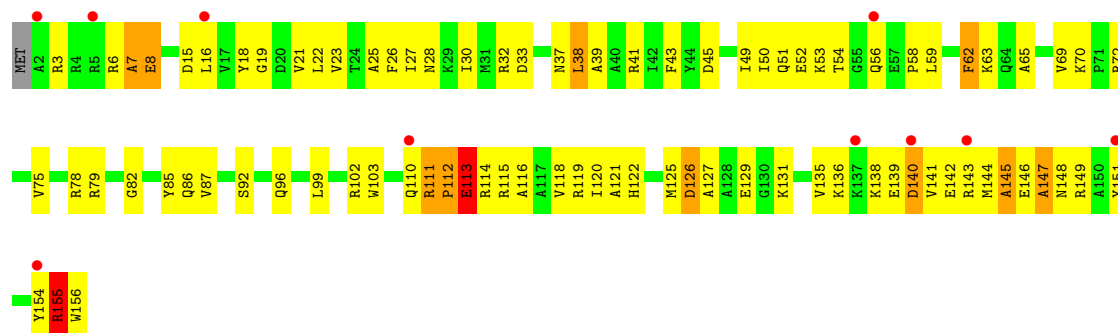
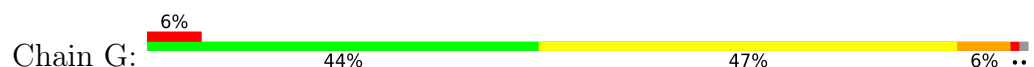
• Molecule 7: 30S Ribosomal Protein S5



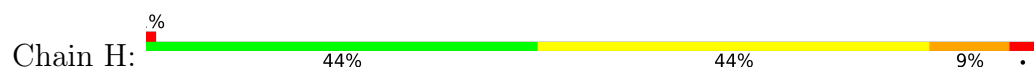
• Molecule 8: 30S Ribosomal Protein S6



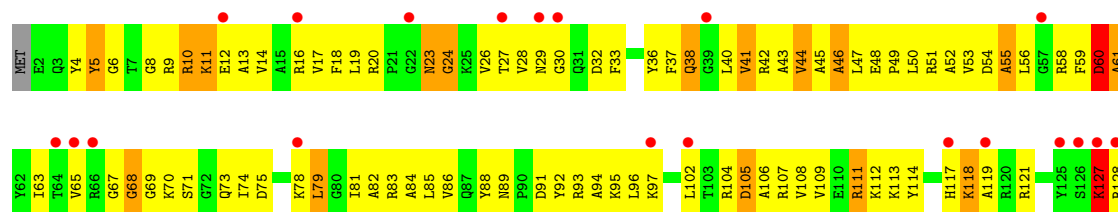
• Molecule 9: 30S Ribosomal Protein S7



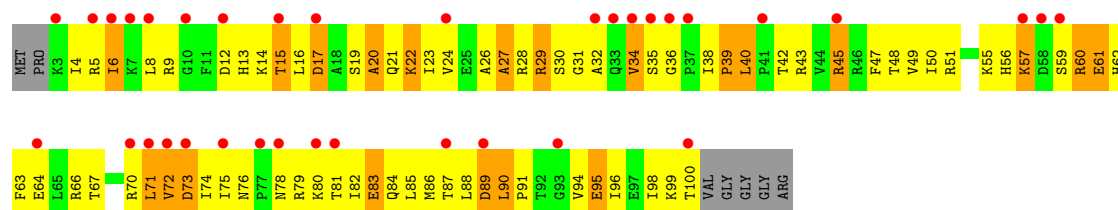
• Molecule 10: 30S Ribosomal Protein S8



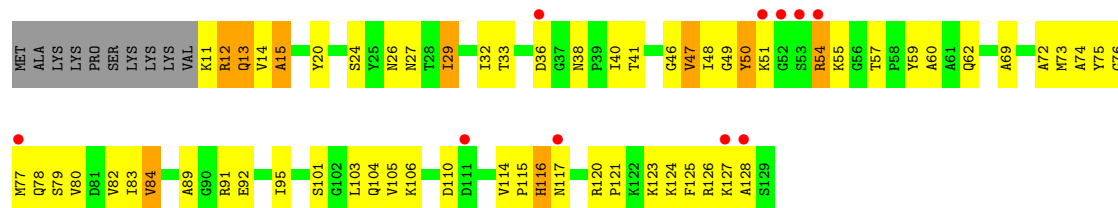
- Molecule 11: 30S Ribosomal Protein S9



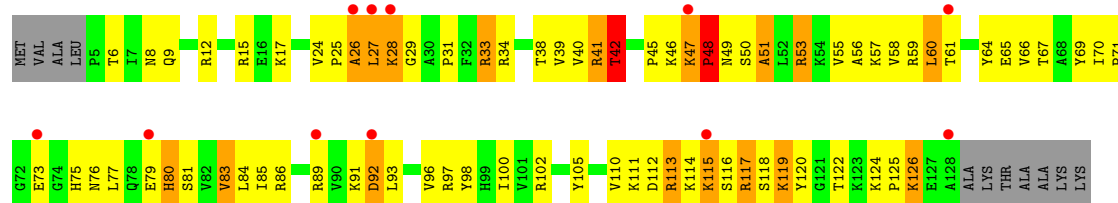
- Molecule 12: 30S Ribosomal Protein S10



- Molecule 13: 30S Ribosomal Protein S11

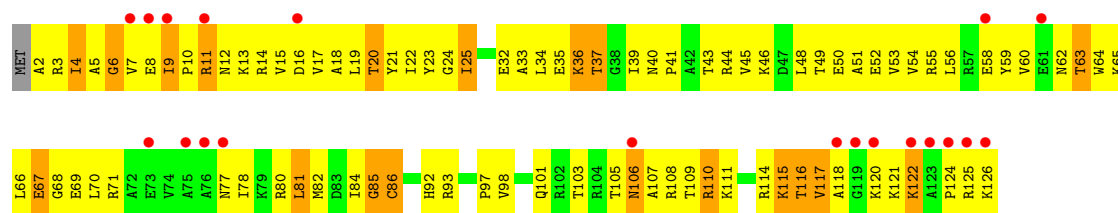


- Molecule 14: 30S Ribosomal Protein S12

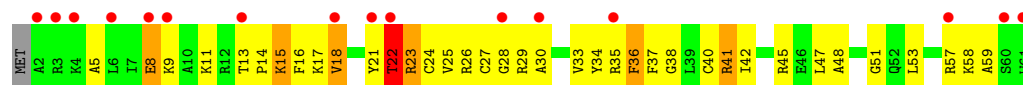


- Molecule 15: 30S Ribosomal Protein S13

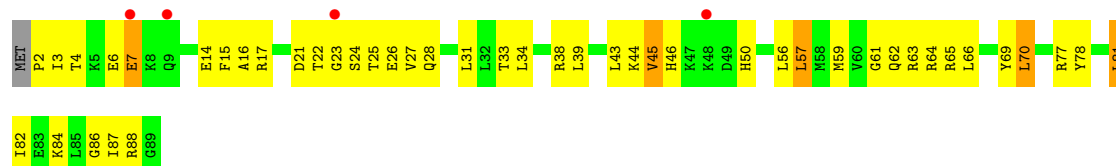




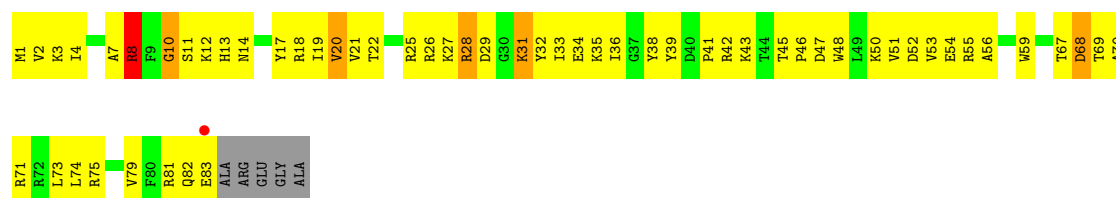
• Molecule 16: 30S Ribosomal Protein S14



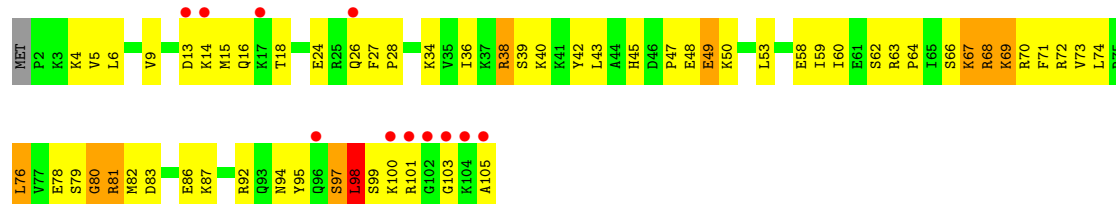
• Molecule 17: 30S Ribosomal Protein S15



• Molecule 18: 30S Ribosomal Protein S16

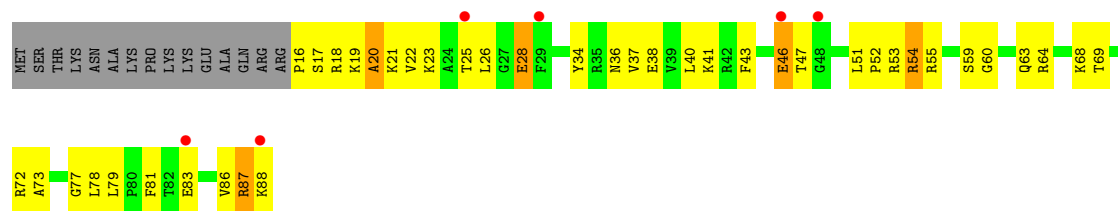


• Molecule 19: 30S Ribosomal Protein S17

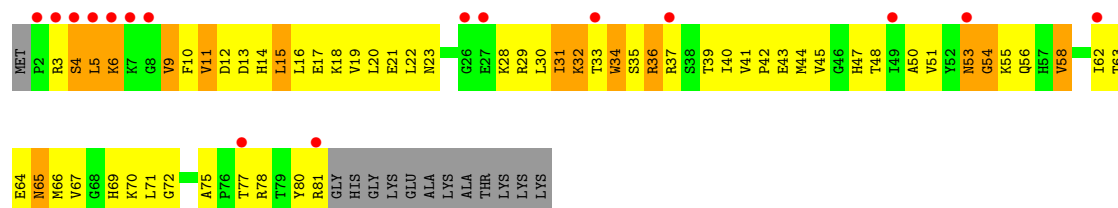


• Molecule 20: 30S Ribosomal Protein S18

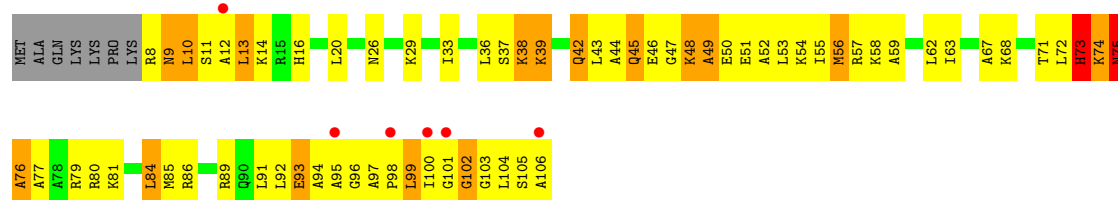




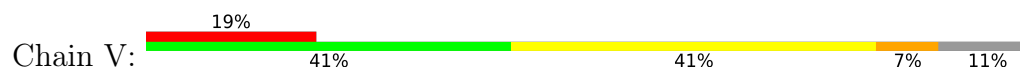
● Molecule 21: 30S Ribosomal Protein S19



● Molecule 22: 30S Ribosomal Protein S20



● Molecule 23: 30S Ribosomal Protein Thx



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	400.72Å 400.72Å 175.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	99.00 – 3.00 99.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (99.00-3.00) 93.6 (99.00-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.80 (at 3.01Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.222 , 0.236 0.216 , 0.253	Depositor DCC
R_{free} test set	13422 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	70.2	Xtriage
Anisotropy	0.240	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 78.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	52081	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.35% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, PAR, T6A, MG

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	0.43	3/36244 (0.0%)	0.72	76/56567 (0.1%)
2	W	0.43	0/96	0.94	2/148 (1.4%)
3	X	0.56	1/226 (0.4%)	0.73	0/349
4	B	0.36	0/1935	0.96	11/2609 (0.4%)
5	C	0.41	0/1636	0.94	4/2205 (0.2%)
6	D	0.42	0/1733	0.96	7/2318 (0.3%)
7	E	0.54	0/1162	1.03	5/1564 (0.3%)
8	F	0.36	0/856	0.91	1/1154 (0.1%)
9	G	0.40	0/1276	0.96	5/1709 (0.3%)
10	H	0.52	0/1136	1.14	10/1527 (0.7%)
11	I	0.39	0/1029	0.91	3/1378 (0.2%)
12	J	0.41	0/805	0.99	7/1082 (0.6%)
13	K	0.49	0/900	0.92	1/1213 (0.1%)
14	L	0.52	0/986	1.18	8/1320 (0.6%)
15	M	0.42	0/1008	0.97	3/1347 (0.2%)
16	N	0.42	0/501	1.02	3/664 (0.5%)
17	O	0.45	0/745	0.97	3/992 (0.3%)
18	P	0.54	0/716	1.03	5/963 (0.5%)
19	Q	0.51	0/870	1.05	3/1159 (0.3%)
20	R	0.38	0/603	0.92	2/799 (0.3%)
21	S	0.36	0/661	1.02	6/890 (0.7%)
22	T	0.52	0/764	1.18	7/1006 (0.7%)
23	V	0.47	0/212	0.89	0/277
All	All	0.43	4/56100 (0.0%)	0.82	172/83240 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	4	40
3	X	1	0
All	All	5	40

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1362	C	O5'-C5'	6.61	1.52	1.42
1	A	1361	G	O5'-C5'	5.88	1.51	1.42
3	X	37	T6A	O3'-P	5.41	1.61	1.56
1	A	1361	G	C3'-O3'	5.28	1.50	1.42

All (172) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	281	G	C2'-C3'-O3'	14.72	131.59	109.50
22	T	13	LEU	N-CA-C	-14.41	95.52	113.97
1	A	1498	U	C2'-C3'-O3'	14.36	131.04	109.50
1	A	243	A	C2'-C3'-O3'	13.90	130.35	109.50
1	A	1302	U	C2'-C3'-O3'	13.39	129.59	109.50
1	A	366	C	C2'-C3'-O3'	13.37	129.55	109.50
1	A	328	C	C2'-C3'-O3'	13.22	129.33	109.50
1	A	181	G	C2'-C3'-O3'	13.10	129.15	109.50
1	A	1528	U	C2'-C3'-O3'	12.55	128.33	109.50
1	A	965	A	C2'-C3'-O3'	12.19	127.78	109.50
1	A	792	A	C2'-C3'-O3'	12.15	127.72	109.50
1	A	484	G	C2'-C3'-O3'	12.08	127.63	109.50
1	A	559	A	C2'-C3'-O3'	12.05	127.58	109.50
1	A	812	C	C2'-C3'-O3'	11.98	127.47	109.50
1	A	575	G	C2'-C3'-O3'	11.42	126.63	109.50
1	A	913	A	C2'-C3'-O3'	10.83	125.75	109.50
14	L	26	ALA	N-CA-C	-10.55	101.07	113.21
1	A	60	A	C2'-C3'-O3'	10.47	125.21	109.50
1	A	1528	U	C4'-C3'-O3'	10.23	124.75	109.40
1	A	115	G	C2'-C3'-O3'	10.22	124.83	109.50
1	A	372	C	C2'-C3'-O3'	9.72	124.08	109.50
1	A	1346	A	C2'-C3'-O3'	9.56	123.84	109.50
1	A	497	A	C2'-C3'-O3'	9.30	123.44	109.50
1	A	366	C	C4'-C3'-O3'	9.11	123.06	109.40
17	O	44	LYS	N-CA-C	-9.08	101.29	111.82
1	A	533	A	C2'-C3'-O3'	8.97	122.96	109.50
1	A	1503	A	C2'-C3'-O3'	8.83	122.74	109.50
1	A	812	C	C4'-C3'-O3'	8.79	122.59	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	12	CYS	N-CA-C	-8.68	101.78	111.07
1	A	266	G	C2'-C3'-O3'	8.65	126.67	113.70
17	O	45	VAL	N-CA-C	-8.52	97.71	109.46
1	A	243	A	C4'-C3'-O3'	8.47	122.11	109.40
1	A	960	U	C2'-C3'-O3'	8.41	122.11	109.50
20	R	46	GLU	N-CA-C	-8.29	102.18	111.71
1	A	1380	U	C2'-C3'-O3'	8.22	121.83	109.50
1	A	1505	G	C2'-C3'-O3'	8.18	125.97	113.70
1	A	1301	U	C2'-C3'-O3'	8.05	121.58	109.50
1	A	1067	A	C2'-C3'-O3'	8.04	121.56	109.50
1	A	559	A	C4'-C3'-O3'	7.97	121.36	109.40
1	A	181	G	C4'-C3'-O3'	7.67	120.91	109.40
5	C	5	ILE	CB-CA-C	-7.65	103.18	111.59
12	J	20	ALA	N-CA-C	-7.59	105.19	114.75
18	P	20	VAL	N-CA-C	7.58	121.21	108.86
1	A	281	G	C4'-C3'-O3'	7.55	120.72	109.40
1	A	7	G	C2'-C3'-O3'	7.52	120.78	109.50
22	T	75	ASN	N-CA-C	-7.42	104.23	113.28
4	B	160	ASP	N-CA-C	-7.30	104.52	113.50
1	A	428	G	C2'-C3'-O3'	7.08	120.13	109.50
1	A	965	A	C4'-C3'-O3'	7.06	119.99	109.40
1	A	484	G	C4'-C3'-O3'	7.03	119.95	109.40
13	K	116	HIS	N-CA-C	-7.01	101.72	111.81
16	N	18	VAL	N-CA-C	6.99	117.13	110.42
2	W	1	A	O5'-C5'-C4'	6.88	121.81	111.50
1	A	1065	U	C2'-C3'-O3'	6.87	119.81	109.50
11	I	60	ASP	N-CA-C	-6.84	98.92	109.24
9	G	145	ALA	N-CA-C	-6.83	102.00	110.41
1	A	1544	U	C4'-C3'-O3'	6.81	119.62	109.40
14	L	119	LYS	N-CA-C	-6.79	100.43	110.48
1	A	1302	U	C4'-C3'-O3'	6.76	119.54	109.40
10	H	44	PHE	N-CA-C	-6.70	105.02	113.72
14	L	115	LYS	N-CA-C	6.69	119.52	108.48
1	A	509	A	C2'-C3'-O3'	6.69	123.74	113.70
5	C	19	GLU	N-CA-C	-6.68	105.45	112.93
2	W	4	A	C2'-C3'-O3'	-6.67	99.49	109.50
1	A	1281	U	C2'-C3'-O3'	6.65	119.48	109.50
20	R	81	PHE	N-CA-C	-6.63	105.32	113.41
6	D	28	SER	CA-C-N	6.54	128.01	119.84
6	D	28	SER	C-N-CA	6.54	128.01	119.84
10	H	89	PRO	N-CA-C	-6.53	100.95	111.14
21	S	58	VAL	N-CA-C	6.52	115.07	107.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1361	G	C4'-C3'-O3'	6.51	122.77	113.00
1	A	1299	A	N9-C1'-C2'	6.42	121.63	112.00
10	H	4	ASP	CA-C-N	6.38	125.61	118.97
10	H	4	ASP	C-N-CA	6.38	125.61	118.97
1	A	1224	G	C2'-C3'-O3'	6.38	119.07	109.50
22	T	93	GLU	N-CA-C	-6.34	100.12	109.62
19	Q	62	SER	N-CA-C	6.31	117.76	108.86
22	T	76	ALA	N-CA-C	-6.30	104.32	111.07
15	M	25	ILE	N-CA-C	6.26	117.49	108.48
8	F	60	PHE	N-CA-C	6.25	118.99	110.55
21	S	53	ASN	N-CA-C	-6.23	105.81	113.41
4	B	47	THR	N-CA-C	-6.22	104.42	111.07
1	A	250	A	C2'-C3'-O3'	6.20	118.80	109.50
21	S	36	ARG	N-CA-C	-6.20	105.47	113.16
9	G	148	ASN	N-CA-C	-6.17	103.23	112.54
1	A	975	A	C2'-C3'-O3'	6.09	118.63	109.50
15	M	11	ARG	N-CA-C	6.07	117.77	108.42
1	A	993	G	C2'-C3'-O3'	6.04	118.56	109.50
21	S	34	TRP	N-CA-C	-6.04	104.56	113.61
16	N	38	GLY	N-CA-C	-6.02	106.64	115.30
10	H	79	VAL	N-CA-C	-5.98	104.48	111.00
14	L	117	ARG	N-CA-C	5.97	118.56	111.33
5	C	4	LYS	N-CA-C	5.95	123.48	110.80
1	A	1490	C	C5'-C4'-O4'	-5.94	100.89	109.80
6	D	163	GLU	N-CA-C	-5.94	104.15	111.40
14	L	42	THR	N-CA-C	-5.93	100.03	109.23
7	E	26	PHE	N-CA-C	5.92	118.55	110.55
1	A	560	U	C2'-C3'-O3'	5.92	118.38	109.50
1	A	51	A	C2'-C3'-O3'	5.90	118.35	109.50
19	Q	58	GLU	N-CA-C	-5.90	100.94	110.32
12	J	62	HIS	N-CA-C	5.88	119.05	109.59
1	A	389	A	C2'-C3'-O3'	-5.86	104.91	113.70
12	J	60	ARG	N-CA-C	5.84	123.23	110.80
10	H	56	LYS	CA-C-N	5.81	127.10	119.84
10	H	56	LYS	C-N-CA	5.81	127.10	119.84
18	P	25	ARG	N-CA-C	5.81	120.36	113.16
1	A	1285	A	C2'-C3'-O3'	5.76	118.15	109.50
1	A	1201	A	C2'-C3'-O3'	5.73	118.10	109.50
16	N	8	GLU	N-CA-C	-5.73	105.60	112.59
1	A	389	A	C5'-C4'-C3'	5.67	124.51	116.00
10	H	80	ILE	CB-CA-C	-5.65	105.44	112.45
7	E	102	ALA	N-CA-C	5.64	116.84	108.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1331	G	N9-C1'-C2'	5.64	120.46	112.00
7	E	15	ARG	N-CA-C	5.64	119.33	112.23
4	B	73	THR	N-CA-C	-5.61	106.60	113.50
1	A	839	U	N1-C1'-C2'	5.60	120.41	112.00
12	J	15	THR	N-CA-C	-5.59	105.66	113.37
1	A	1331	G	C4'-C3'-O3'	-5.58	104.63	113.00
7	E	21	ALA	N-CA-C	-5.58	103.16	110.53
1	A	748	C	N1-C1'-C2'	5.57	120.36	112.00
1	A	353	A	C5'-C4'-O4'	-5.57	101.44	109.80
4	B	190	THR	N-CA-C	5.56	119.57	112.34
1	A	572	A	N9-C1'-C2'	5.55	120.32	112.00
9	G	87	VAL	N-CA-C	5.54	113.36	107.76
1	A	992	U	C2'-C3'-O3'	5.52	117.77	109.50
6	D	39	PRO	CA-C-N	5.49	125.69	120.31
6	D	39	PRO	C-N-CA	5.49	125.69	120.31
10	H	77	GLU	N-CA-C	-5.48	102.77	110.50
22	T	49	ALA	N-CA-C	5.48	117.68	111.11
1	A	1502	A	N9-C1'-C2'	5.45	122.17	114.00
11	I	61	ALA	N-CA-C	5.43	117.48	108.13
6	D	33	MET	N-CA-C	-5.43	106.73	113.19
14	L	92	ASP	N-CA-C	5.41	119.60	112.89
11	I	68	GLY	N-CA-C	5.40	119.29	111.24
22	T	92	LEU	N-CA-C	-5.39	106.74	113.15
1	A	119	A	C2'-C3'-O3'	5.38	117.57	109.50
1	A	129(A)	G	C2'-C3'-O3'	5.37	117.55	109.50
1	A	115	G	O4'-C1'-C2'	5.36	111.16	105.80
4	B	25	ASN	N-CA-C	-5.36	97.97	109.81
4	B	114	ARG	N-CA-C	-5.36	106.80	113.55
14	L	105	TYR	CB-CA-C	-5.33	110.44	116.63
1	A	63	C	C5'-C4'-C3'	-5.33	108.01	116.00
1	A	1498	U	C4'-C3'-O3'	5.32	117.38	109.40
1	A	687	A	C2'-C3'-O3'	5.30	117.45	109.50
14	L	118	SER	N-CA-C	-5.28	104.94	111.33
18	P	68	ASP	N-CA-C	-5.27	105.45	111.14
22	T	38	LYS	N-CA-C	-5.23	104.64	111.02
21	S	54	GLY	N-CA-C	-5.22	100.80	113.18
19	Q	67	LYS	N-CA-C	-5.22	102.33	110.10
12	J	22	LYS	N-CA-C	-5.21	105.20	112.45
1	A	533	A	C4'-C3'-O3'	5.21	117.22	109.40
7	E	19	MET	N-CA-C	5.19	117.43	109.07
12	J	66	ARG	N-CA-C	5.19	118.01	109.76
4	B	56	ARG	N-CA-C	-5.17	104.91	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	S	4	SER	N-CA-C	5.15	115.97	108.14
18	P	8	ARG	N-CA-C	5.15	116.65	108.67
12	J	95	GLU	N-CA-C	-5.14	101.48	109.24
15	M	60	VAL	N-CA-C	5.14	116.23	111.45
1	A	528	C	C5'-C4'-C3'	5.13	123.69	116.00
1	A	1305	G	C4'-C3'-O3'	-5.12	105.32	113.00
4	B	74	LYS	N-CA-C	-5.12	103.59	110.24
1	A	1190	G	C4'-C3'-O3'	-5.11	105.33	113.00
5	C	126	ARG	N-CA-C	-5.08	107.59	112.97
4	B	173	ALA	N-CA-C	-5.07	104.70	111.24
10	H	119	LEU	N-CA-C	5.07	116.76	108.76
9	G	111	ARG	CA-C-N	5.06	126.16	119.84
9	G	111	ARG	C-N-CA	5.06	126.16	119.84
17	O	50	HIS	N-CA-C	5.06	116.79	111.28
18	P	35	LYS	N-CA-C	-5.03	101.51	109.76
1	A	1200	C	N1-C1'-C2'	5.01	119.52	112.00
4	B	133	LYS	N-CA-C	-5.01	107.01	113.02
4	B	205	ASP	N-CA-C	-5.01	106.68	112.89

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	243	A	C3'
1	A	281	G	C3'
1	A	366	C	C3'
1	A	1528	U	C3'
3	X	37	T6A	C14

All (40) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1013	G	Sidechain
1	A	1048	G	Sidechain
1	A	106	C	Sidechain
1	A	1073	U	Sidechain
1	A	1077	G	Sidechain
1	A	1079	G	Sidechain
1	A	1281	U	Sidechain
1	A	1299	A	Sidechain
1	A	1301	U	Sidechain
1	A	1361	G	Sidechain
1	A	1405	G	Sidechain

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Mol	Chain	Res	Type	Group
1	A	1454	G	Sidechain
1	A	1490	C	Sidechain
1	A	1492	A	Sidechain
1	A	1498	U	Sidechain
1	A	190(K)	G	Sidechain
1	A	195	A	Sidechain
1	A	250	A	Sidechain
1	A	290	C	Sidechain
1	A	291	C	Sidechain
1	A	380	G	Sidechain
1	A	387	U	Sidechain
1	A	481	G	Sidechain
1	A	51	A	Sidechain
1	A	521	G	Sidechain
1	A	528	C	Sidechain
1	A	529	G	Sidechain
1	A	561	U	Sidechain
1	A	573	A	Sidechain
1	A	58	C	Sidechain
1	A	580	U	Sidechain
1	A	587	G	Sidechain
1	A	664	G	Sidechain
1	A	682	G	Sidechain
1	A	727	G	Sidechain
1	A	748	C	Sidechain
1	A	879	C	Sidechain
1	A	898	G	Sidechain
1	A	924	C	Sidechain
1	A	975	A	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32380	0	16346	885	0
2	W	85	0	46	4	0
3	X	236	0	122	13	0
4	B	1900	0	1951	195	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	1612	0	1677	209	0
6	D	1703	0	1764	118	0
7	E	1146	0	1207	105	0
8	F	843	0	857	60	0
9	G	1257	0	1296	93	0
10	H	1116	0	1177	89	0
11	I	1011	0	1043	119	0
12	J	792	0	835	122	0
13	K	885	0	904	73	0
14	L	970	0	1057	109	0
15	M	997	0	1072	103	0
16	N	492	0	529	46	0
17	O	734	0	771	39	0
18	P	700	0	720	58	0
19	Q	857	0	930	57	0
20	R	597	0	668	61	0
21	S	647	0	673	96	0
22	T	762	0	856	70	0
23	V	208	0	221	18	0
24	A	42	0	45	1	0
25	A	104	0	0	0	0
25	N	1	0	0	0	0
25	X	2	0	0	0	0
26	D	1	0	0	0	0
26	N	1	0	0	0	0
All	All	52081	0	36767	2505	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 28.

All (2505) 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:972:C:H4'	12:J:57:LYS:HG2	1.31	1.08
4:B:84:GLU:HB3	4:B:219:VAL:HG21	1.35	1.06
19:Q:98:LEU:H	19:Q:98:LEU:HD12	1.20	1.05
21:S:33:THR:HG22	21:S:35:SER:H	1.16	1.04
1:A:1490:C:H6	1:A:1490:C:H5'	1.18	1.04
21:S:55:LYS:HG2	21:S:56:GLN:HE21	1.19	1.03
5:C:3:ASN:HD22	5:C:3:ASN:N	1.56	1.01
1:A:243:A:H4'	1:A:244:U:H5'	1.43	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:G:O2'	1:A:190:C:H5''	1.60	1.00
21:S:28:LYS:HG2	21:S:29:ARG:H	1.25	0.99
5:C:26:LYS:H	5:C:26:LYS:HD3	1.27	0.99
1:A:1226:C:H4'	1:A:1227:A:OP1	1.62	0.98
18:P:28:ARG:HG2	18:P:28:ARG:HH11	1.30	0.96
12:J:32:ALA:HB2	12:J:76:ASN:HD22	1.29	0.96
4:B:18:GLY:HA2	4:B:41:ILE:HA	1.45	0.96
6:D:36:ARG:H	6:D:37:PRO:HD3	1.27	0.95
12:J:90:LEU:H	12:J:91:PRO:HD2	1.32	0.95
1:A:664:G:H22	1:A:741:G:H1	1.11	0.95
1:A:1190:G:OP1	5:C:4:LYS:HA	1.67	0.94
20:R:47:THR:HA	20:R:83:GLU:HB2	1.46	0.94
1:A:1502:A:H2	1:A:1505:G:H1	1.11	0.94
12:J:4:ILE:HD12	12:J:74:ILE:HB	1.50	0.94
14:L:41:ARG:HG2	14:L:42:THR:H	1.28	0.93
12:J:49:VAL:O	12:J:60:ARG:HA	1.68	0.93
14:L:47:LYS:HB3	14:L:48:PRO:CD	1.97	0.93
8:F:100:ASN:HD22	20:R:23:LYS:HG2	1.35	0.91
4:B:10:LEU:HD23	4:B:48:MET:HE2	1.52	0.91
14:L:75:HIS:HD2	14:L:77:LEU:H	1.18	0.91
1:A:1158:C:H5''	4:B:133:LYS:HE3	1.52	0.91
13:K:84:VAL:HG23	13:K:110:ASP:HA	1.50	0.91
12:J:45:ARG:HB3	12:J:45:ARG:HH11	1.35	0.90
6:D:162:LEU:HD12	6:D:181:MET:HE2	1.53	0.90
7:E:80:ILE:HD12	7:E:138:ALA:HB1	1.54	0.90
12:J:31:GLY:HA2	12:J:78:ASN:ND2	1.87	0.90
15:M:37:THR:HG23	15:M:55:ARG:HD2	1.53	0.90
15:M:17:VAL:O	15:M:20:THR:HB	1.72	0.89
12:J:5:ARG:H	12:J:100:THR:HA	1.36	0.89
5:C:188:LEU:HD13	5:C:189:ALA:H	1.38	0.88
12:J:6:ILE:HG23	12:J:98:ILE:HG12	1.56	0.88
22:T:39:LYS:HD2	22:T:55:ILE:HD13	1.54	0.87
6:D:98:GLU:HG2	6:D:189:PRO:HG3	1.57	0.87
3:X:37:T6A:H5'	3:X:37:T6A:H8	1.39	0.86
12:J:34:VAL:HG22	12:J:74:ILE:HG23	1.57	0.86
6:D:36:ARG:N	6:D:37:PRO:HD3	1.91	0.86
13:K:54:ARG:O	13:K:57:THR:HG22	1.76	0.85
1:A:1489:G:C2'	1:A:1490:C:H5''	2.06	0.85
4:B:77:ALA:HB2	4:B:211:ILE:HD13	1.58	0.85
1:A:1489:G:H2'	1:A:1490:C:H5''	1.58	0.85
14:L:53:ARG:HG2	14:L:93:LEU:HD11	1.59	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1305:G:O2'	1:A:1306:A:H8	1.59	0.84
5:C:191:THR:HG21	5:C:193:TYR:CZ	2.12	0.84
1:A:1490:C:H5'	1:A:1490:C:C6	2.10	0.84
5:C:34:LEU:HD12	16:N:25:VAL:HG21	1.57	0.84
1:A:939:G:H5''	9:G:102:ARG:NH2	1.93	0.84
22:T:50:GLU:HG2	22:T:54:LYS:HE3	1.60	0.83
9:G:155:ARG:CZ	9:G:155:ARG:HA	2.08	0.83
15:M:120:LYS:HE2	15:M:122:LYS:HB3	1.59	0.83
1:A:1223:C:P	21:S:78:ARG:HH12	2.01	0.82
5:C:3:ASN:N	5:C:3:ASN:ND2	2.24	0.82
8:F:7:ASN:HB2	8:F:89:MET:HB3	1.60	0.82
10:H:10:LEU:HD22	10:H:83:ILE:HD11	1.61	0.82
23:V:6:ARG:HG3	23:V:15:ARG:NH1	1.94	0.82
14:L:126:LYS:H	14:L:126:LYS:CD	1.90	0.82
13:K:54:ARG:HB3	13:K:54:ARG:NH1	1.94	0.82
5:C:119:ARG:HG2	5:C:140:ARG:HH12	1.44	0.82
15:M:65:LYS:HE3	15:M:69:GLU:HG2	1.62	0.82
1:A:1305:G:HO2'	1:A:1306:A:H8	0.87	0.82
9:G:54:THR:HG22	9:G:56:GLN:H	1.43	0.82
7:E:79:GLU:HG3	7:E:93:PRO:HD2	1.62	0.82
15:M:10:PRO:HB2	15:M:18:ALA:HB1	1.60	0.81
4:B:71:VAL:HG23	4:B:164:VAL:HA	1.59	0.81
3:X:37:T6A:H153	3:X:38:A:H2	1.46	0.81
16:N:57:ARG:HG2	16:N:58:LYS:H	1.43	0.81
1:A:371:G:O2'	1:A:372:C:H5'	1.80	0.81
1:A:877:C:O2	10:H:3:THR:HG21	1.80	0.81
7:E:51:VAL:HB	7:E:52:PRO:HD3	1.63	0.81
4:B:124:SER:HB2	4:B:125:PRO:HD2	1.63	0.80
12:J:90:LEU:H	12:J:91:PRO:CD	1.94	0.80
4:B:102:LEU:HD21	4:B:162:ILE:HD11	1.63	0.80
1:A:579:G:H5'	1:A:728:A:H1'	1.63	0.80
1:A:216:G:H2'	1:A:217:C:C6	2.17	0.80
11:I:46:ALA:HB2	11:I:74:ILE:HG23	1.62	0.80
14:L:47:LYS:HB3	14:L:48:PRO:HD3	1.60	0.80
1:A:1124:G:H3'	1:A:1145:C:N4	1.96	0.80
1:A:250:A:H4'	1:A:251:G:O5'	1.79	0.80
1:A:266:G:H5''	1:A:268:C:H41	1.46	0.79
5:C:14:ILE:HG22	5:C:15:THR:H	1.45	0.79
7:E:60:TYR:HE1	7:E:64:ARG:HH21	1.30	0.79
15:M:3:ARG:HG2	15:M:9:ILE:HG13	1.64	0.79
20:R:68:LYS:O	20:R:72:ARG:HG3	1.83	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:41:VAL:HG22	7:E:113:ALA:HA	1.64	0.79
4:B:12:GLU:OE2	4:B:213:LEU:HD11	1.82	0.79
5:C:64:VAL:HB	5:C:99:VAL:HG21	1.65	0.79
19:Q:101:ARG:HA	19:Q:101:ARG:HE	1.46	0.79
17:O:17:ARG:HG3	17:O:17:ARG:HH11	1.48	0.79
5:C:14:ILE:HG22	5:C:15:THR:N	1.98	0.78
20:R:55:ARG:NH1	20:R:55:ARG:HB3	1.98	0.78
5:C:77:ILE:HA	5:C:84:ILE:HB	1.65	0.78
21:S:30:LEU:HD23	21:S:31:ILE:N	1.98	0.78
1:A:1054:C:O2	1:A:1196:U:H2'	1.81	0.78
4:B:17:PHE:HB3	4:B:44:LEU:HD21	1.63	0.78
23:V:6:ARG:HG3	23:V:15:ARG:HH12	1.48	0.78
11:I:70:LYS:O	11:I:74:ILE:HG13	1.82	0.78
12:J:49:VAL:CG2	16:N:41:ARG:HB2	2.14	0.78
19:Q:59:ILE:HG22	19:Q:71:PHE:CD1	2.18	0.78
20:R:38:GLU:HA	20:R:41:LYS:HE2	1.63	0.78
1:A:946:A:H2'	1:A:947:G:C8	2.19	0.78
1:A:1148:U:H4'	11:I:14:VAL:HG11	1.64	0.78
18:P:28:ARG:HG2	18:P:29:ASP:OD2	1.84	0.78
1:A:975:A:H5'	1:A:975:A:H8	1.48	0.77
14:L:75:HIS:CD2	14:L:77:LEU:H	2.03	0.77
11:I:65:VAL:HG21	11:I:73:GLN:HB3	1.64	0.77
6:D:151:LYS:H	6:D:151:LYS:HD2	1.46	0.76
10:H:51:VAL:HG12	10:H:52:ASP:H	1.50	0.76
22:T:36:LEU:HD12	22:T:62:LEU:HD12	1.65	0.76
1:A:1367:C:H5'	12:J:60:ARG:NH1	2.01	0.76
1:A:1151:A:HO2'	1:A:1152:A:H8	1.32	0.76
14:L:57:LYS:HD3	14:L:67:THR:HG22	1.66	0.76
19:Q:27:PHE:HB2	19:Q:28:PRO:HD2	1.67	0.76
22:T:89:ARG:HG3	22:T:104:LEU:HD13	1.68	0.76
5:C:91:LEU:HD23	5:C:92:ALA:N	2.01	0.75
12:J:45:ARG:HB3	12:J:45:ARG:NH1	2.01	0.75
11:I:6:GLY:N	11:I:84:ALA:HB2	2.01	0.75
1:A:1016:A:H2'	1:A:1017:G:O4'	1.85	0.75
1:A:328:C:O2	1:A:328:C:H2'	1.85	0.75
7:E:105:VAL:HB	7:E:106:PRO:HD3	1.69	0.75
15:M:49:THR:HB	15:M:52:GLU:HG3	1.68	0.75
15:M:63:THR:HG23	15:M:64:TRP:N	2.01	0.75
20:R:54:ARG:HD3	20:R:55:ARG:HG2	1.67	0.75
1:A:1168:A:H2'	1:A:1169:A:C8	2.21	0.74
22:T:57:ARG:NH1	22:T:102:GLY:HA3	2.02	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1281:U:H5'	1:A:1282:C:H5	1.50	0.74
5:C:64:VAL:HG12	5:C:65:ALA:H	1.52	0.74
5:C:193:TYR:HE1	5:C:196:LEU:HD21	1.51	0.74
21:S:51:VAL:O	21:S:58:VAL:HG22	1.87	0.74
1:A:1250:A:H4'	11:I:68:GLY:H	1.49	0.74
8:F:10:LEU:HD12	8:F:59:TYR:HB3	1.69	0.74
7:E:144:THR:HB	7:E:147:ASP:OD1	1.88	0.74
10:H:9:MET:HG3	10:H:26:VAL:HG21	1.67	0.74
8:F:101:ALA:HB2	20:R:28:GLU:HG3	1.67	0.74
18:P:67:THR:HG22	18:P:68:ASP:N	2.00	0.74
12:J:38:ILE:HB	12:J:71:LEU:CB	2.17	0.74
1:A:1029:C:H2'	1:A:1030:C:O4'	1.87	0.74
4:B:178:ARG:HH11	4:B:178:ARG:HG3	1.51	0.74
18:P:20:VAL:HG11	18:P:32:TYR:CB	2.18	0.74
4:B:15:VAL:HG11	4:B:209:ARG:HG3	1.68	0.74
14:L:46:LYS:HD2	14:L:47:LYS:H	1.52	0.74
1:A:1132:C:H2'	1:A:1133:G:H8	1.51	0.73
5:C:64:VAL:HB	5:C:99:VAL:CG2	2.18	0.73
3:X:37:T6A:H153	3:X:38:A:C2	2.24	0.73
4:B:218:ALA:O	4:B:222:ILE:HG13	1.87	0.73
6:D:36:ARG:H	6:D:37:PRO:CD	2.01	0.73
7:E:11:ILE:HB	7:E:31:LEU:HB3	1.70	0.73
10:H:9:MET:SD	10:H:32:LYS:HG2	2.28	0.73
5:C:2:GLY:C	5:C:3:ASN:HD22	1.95	0.73
1:A:687:A:H4'	1:A:688:G:O5'	1.88	0.73
4:B:69:LEU:HD12	4:B:155:LEU:HD11	1.69	0.73
4:B:114:ARG:NH1	4:B:118:LEU:HD21	2.03	0.73
21:S:33:THR:HG22	21:S:35:SER:N	2.00	0.73
11:I:106:ALA:O	11:I:108:VAL:HG23	1.89	0.73
12:J:49:VAL:HG23	16:N:41:ARG:HB2	1.70	0.73
14:L:70:ILE:HD13	14:L:77:LEU:HD12	1.70	0.73
10:H:121:ASP:HB2	10:H:125:ARG:HH21	1.53	0.73
12:J:5:ARG:N	12:J:100:THR:HA	2.04	0.73
21:S:15:LEU:HA	21:S:18:LYS:HB3	1.71	0.73
1:A:969:A:H61	15:M:126:LYS:CB	2.01	0.72
7:E:11:ILE:HG22	7:E:12:LEU:HD12	1.70	0.72
4:B:143:GLU:O	4:B:147:LYS:HG3	1.88	0.72
1:A:1117:G:H4'	11:I:104:ARG:NH1	2.04	0.72
4:B:231:GLU:HB2	4:B:232:PRO:HD2	1.71	0.72
1:A:1152:A:H5''	12:J:13:HIS:CD2	2.24	0.72
1:A:1305:G:N2	1:A:1331:G:O2'	2.21	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:I:97:LYS:HG2	11:I:102:LEU:HD12	1.70	0.72
1:A:686:U:HO2'	1:A:687:A:H8	1.38	0.72
1:A:1238:A:H5'	1:A:1336:C:H41	1.53	0.72
8:F:86:ARG:O	8:F:87:ARG:HG2	1.89	0.72
18:P:38:TYR:CE2	18:P:50:LYS:HD3	2.24	0.72
1:A:344:A:H4'	1:A:345:C:OP2	1.89	0.72
1:A:840:C:H5''	1:A:841:U:OP1	1.89	0.72
11:I:118:LYS:O	11:I:119:ALA:HB3	1.89	0.72
12:J:38:ILE:HB	12:J:71:LEU:HB2	1.71	0.72
1:A:1106:G:H5''	5:C:172:ARG:HG2	1.71	0.71
4:B:8:LYS:CD	4:B:9:GLU:H	2.02	0.71
13:K:54:ARG:HB3	13:K:54:ARG:HH11	1.52	0.71
1:A:1417:G:H2'	1:A:1482:G:H22	1.55	0.71
15:M:15:VAL:HG23	15:M:43:THR:O	1.90	0.71
5:C:8:ILE:HG23	5:C:16:ARG:HG2	1.71	0.71
6:D:119:GLN:HG2	6:D:123:HIS:CD2	2.25	0.71
1:A:112:G:H4'	1:A:389:A:H5''	1.72	0.71
15:M:49:THR:HG22	15:M:51:ALA:N	2.06	0.71
1:A:1130:A:OP2	1:A:1131:G:H5''	1.91	0.71
1:A:518:C:HO2'	14:L:50:SER:HB3	1.56	0.70
1:A:677:U:H3	1:A:713:G:H22	1.39	0.70
1:A:1241:G:H2'	1:A:1242:C:C6	2.26	0.70
1:A:1497:G:O2'	1:A:1498:U:H5'	1.91	0.70
5:C:123:GLN:NE2	5:C:140:ARG:HH22	1.89	0.70
6:D:199:ASN:HD21	6:D:201:GLN:HB2	1.54	0.70
11:I:47:LEU:C	11:I:49:PRO:HD2	2.15	0.70
15:M:54:VAL:O	15:M:58:GLU:HG2	1.90	0.70
5:C:52:LEU:HD23	5:C:52:LEU:H	1.57	0.70
6:D:110:PHE:HD1	6:D:162:LEU:HD21	1.56	0.70
7:E:120:THR:HG23	7:E:121:LYS:N	2.05	0.70
1:A:1489:G:H2'	1:A:1490:C:C5'	2.21	0.70
14:L:89:ARG:NH2	14:L:97:ARG:HH11	1.89	0.70
4:B:51:LEU:HD22	4:B:55:PHE:HE1	1.56	0.70
14:L:25:PRO:C	14:L:27:LEU:H	1.99	0.70
4:B:18:GLY:H	4:B:41:ILE:HG23	1.56	0.70
4:B:68:ILE:HB	4:B:90:MET:HE3	1.73	0.70
7:E:76:ILE:HG23	7:E:77:PRO:HD2	1.72	0.70
1:A:180:U:H2'	1:A:181:G:H5'	1.74	0.70
1:A:1145:C:H5'	1:A:1146:A:OP1	1.91	0.70
20:R:17:SER:HB2	20:R:54:ARG:NH2	2.07	0.70
1:A:818:G:O2'	1:A:819:A:H5''	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:975:A:H5'	1:A:975:A:C8	2.25	0.70
5:C:36:ASP:HB3	5:C:40:ARG:HH12	1.56	0.70
6:D:25:ARG:C	6:D:27:TYR:H	2.00	0.70
7:E:57:LYS:HG2	7:E:61:TYR:CE2	2.26	0.70
8:F:2:ARG:CZ	8:F:69:GLU:HG2	2.21	0.70
21:S:17:GLU:HA	21:S:20:LEU:HG	1.74	0.70
1:A:1250:A:H4'	11:I:68:GLY:N	2.06	0.70
4:B:8:LYS:HD3	4:B:9:GLU:H	1.56	0.70
7:E:76:ILE:HG22	7:E:78:HIS:H	1.55	0.70
1:A:1064:G:H4'	1:A:1065:U:H5''	1.72	0.70
4:B:71:VAL:CG2	4:B:164:VAL:HG23	2.21	0.70
7:E:92:LYS:HB3	7:E:119:LEU:HB2	1.73	0.70
12:J:5:ARG:HA	12:J:73:ASP:OD1	1.91	0.70
15:M:49:THR:HG22	15:M:51:ALA:H	1.57	0.70
11:I:8:GLY:HA2	11:I:79:LEU:HD13	1.73	0.69
21:S:17:GLU:O	21:S:21:GLU:HG3	1.92	0.69
1:A:243:A:C4'	1:A:244:U:H5'	2.20	0.69
1:A:1356:G:H2'	1:A:1357:A:C8	2.27	0.69
4:B:97:TRP:HZ2	4:B:102:LEU:HD13	1.57	0.69
1:A:524:G:H2'	1:A:525:C:C6	2.28	0.69
4:B:98:LEU:O	4:B:101:MET:HG3	1.92	0.69
5:C:70:VAL:HG12	5:C:71:ALA:N	2.07	0.69
14:L:60:LEU:HD11	14:L:85:ILE:HD12	1.74	0.69
1:A:1256:A:H5'	1:A:1258:G:H1'	1.74	0.69
5:C:190:ARG:HG2	5:C:190:ARG:HH11	1.57	0.69
1:A:518:C:O2'	14:L:50:SER:HB3	1.93	0.69
6:D:146:ILE:N	6:D:146:ILE:HD12	2.06	0.69
16:N:9:LYS:HD3	16:N:9:LYS:C	2.17	0.69
1:A:243:A:H4'	1:A:244:U:C5'	2.21	0.69
5:C:15:THR:O	5:C:16:ARG:HB2	1.91	0.69
11:I:111:ARG:HD3	11:I:112:LYS:N	2.07	0.69
12:J:94:VAL:HG12	12:J:95:GLU:N	2.07	0.69
4:B:231:GLU:HB2	4:B:232:PRO:CD	2.22	0.69
5:C:178:LEU:O	5:C:179:ARG:HB3	1.93	0.69
1:A:235:C:H5'	19:Q:70:ARG:HG2	1.73	0.69
1:A:1435:G:H2'	1:A:1436:U:C6	2.27	0.69
6:D:78:LEU:HD22	6:D:96:LEU:HB3	1.73	0.69
14:L:41:ARG:HG2	14:L:42:THR:N	2.06	0.69
14:L:59:ARG:HD3	14:L:65:GLU:HG3	1.72	0.69
8:F:4:TYR:CE2	8:F:72:VAL:HG21	2.28	0.69
18:P:26:ARG:HD3	18:P:31:LYS:H	1.58	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:865:A:H5'	1:A:1078:U:O4	1.93	0.69
18:P:74:LEU:O	18:P:79:VAL:HG23	1.93	0.69
15:M:9:ILE:HD12	15:M:9:ILE:N	2.07	0.68
1:A:673:G:H2'	1:A:674:G:C8	2.28	0.68
1:A:1072:G:H2'	1:A:1073:U:C6	2.28	0.68
15:M:22:ILE:HD12	15:M:25:ILE:HD12	1.73	0.68
1:A:972:C:H4'	12:J:57:LYS:CG	2.18	0.68
1:A:1281:U:H5'	1:A:1282:C:C5	2.28	0.68
13:K:126:ARG:O	13:K:127:LYS:HB2	1.94	0.68
12:J:90:LEU:N	12:J:91:PRO:HD2	2.08	0.68
1:A:382:A:H2'	1:A:383:A:C8	2.29	0.68
1:A:113:G:H1'	1:A:354:G:H5'	1.76	0.68
1:A:1116:C:H2'	1:A:1117:G:H5''	1.74	0.68
5:C:23:TYR:CD2	5:C:24:ALA:N	2.61	0.68
5:C:26:LYS:H	5:C:26:LYS:CD	2.05	0.68
1:A:1195:C:H3'	1:A:1196:U:C5'	2.22	0.68
6:D:30:LYS:C	6:D:32:ALA:H	2.00	0.68
14:L:47:LYS:CB	14:L:48:PRO:HD3	2.22	0.68
1:A:1366:C:H2'	1:A:1367:C:H6	1.57	0.68
4:B:12:GLU:C	4:B:14:GLY:H	1.98	0.68
17:O:24:SER:OG	17:O:27:VAL:HG23	1.93	0.68
21:S:62:ILE:HD12	21:S:66:MET:HG3	1.76	0.68
5:C:91:LEU:HD11	5:C:99:VAL:HG13	1.75	0.68
5:C:112:SER:HB3	5:C:115:LEU:HD12	1.76	0.68
1:A:1137:C:H4'	1:A:1138:G:C2	2.28	0.68
1:A:1510:U:H2'	1:A:1511:G:C8	2.29	0.68
4:B:142:LEU:O	4:B:142:LEU:HD23	1.94	0.68
12:J:34:VAL:HG12	12:J:36:GLY:H	1.58	0.68
5:C:110:ASN:ND2	5:C:140:ARG:HB3	2.08	0.67
1:A:1121:U:H2'	1:A:1122:U:H6	1.59	0.67
19:Q:67:LYS:HA	19:Q:70:ARG:HH12	1.58	0.67
1:A:1182:G:O2'	1:A:1183:A:H5''	1.95	0.67
1:A:1391:U:H2'	1:A:1392:G:C8	2.29	0.67
6:D:199:ASN:HD22	6:D:199:ASN:C	2.02	0.67
11:I:8:GLY:HA3	11:I:79:LEU:HB3	1.75	0.67
12:J:35:SER:HB2	12:J:72:VAL:O	1.94	0.67
23:V:24:ARG:N	23:V:24:ARG:HD3	2.09	0.67
1:A:353:A:H5'	1:A:353:A:C8	2.30	0.67
18:P:28:ARG:HG2	18:P:28:ARG:NH1	2.04	0.67
9:G:15:ASP:HB3	9:G:19:GLY:N	2.08	0.67
1:A:853:G:O2'	1:A:854:G:H5'	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1224:G:H1	1:A:1362:C:H42	1.42	0.67
4:B:116:GLU:HG2	4:B:153:ARG:NH2	2.09	0.67
21:S:33:THR:HG22	21:S:34:TRP:H	1.58	0.67
9:G:50:ILE:O	9:G:54:THR:HB	1.95	0.67
11:I:48:GLU:N	11:I:49:PRO:HD2	2.10	0.67
12:J:32:ALA:HB2	12:J:76:ASN:ND2	2.06	0.67
13:K:47:VAL:O	13:K:47:VAL:HG12	1.94	0.67
1:A:254:G:OP1	19:Q:67:LYS:O	2.11	0.67
1:A:1132:C:H2'	1:A:1133:G:C8	2.29	0.67
7:E:80:ILE:HD11	7:E:91:LEU:HD12	1.77	0.67
9:G:146:GLU:HG2	9:G:149:ARG:HH21	1.60	0.67
14:L:27:LEU:O	14:L:29:GLY:N	2.28	0.67
1:A:1427:U:H2'	1:A:1428:A:H8	1.58	0.66
3:X:37:T6A:H5'	3:X:37:T6A:C8	2.28	0.66
16:N:29:ARG:HG2	16:N:29:ARG:HH11	1.60	0.66
1:A:992:U:H4'	1:A:993:G:O5'	1.94	0.66
7:E:43:LEU:HB2	7:E:136:MET:HE2	1.76	0.66
12:J:4:ILE:O	12:J:73:ASP:HA	1.96	0.66
21:S:50:ALA:HA	21:S:58:VAL:O	1.95	0.66
1:A:538:G:H5''	14:L:114:LYS:HG3	1.76	0.66
1:A:1305:G:H5'	23:V:4:GLY:HA3	1.75	0.66
1:A:1417:G:H2'	1:A:1482:G:N2	2.10	0.66
5:C:64:VAL:HB	5:C:99:VAL:CB	2.26	0.66
4:B:118:LEU:HB3	4:B:142:LEU:HD12	1.77	0.66
21:S:43:GLU:H	21:S:43:GLU:CD	2.04	0.66
1:A:190(L):U:O2'	1:A:191:G:H5'	1.95	0.66
1:A:1196:U:H5''	1:A:1197:G:H5'	1.77	0.66
1:A:1208:C:H2'	1:A:1209:C:H6	1.61	0.66
1:A:1320:C:O2	21:S:72:GLY:HA3	1.96	0.66
13:K:91:ARG:HH11	20:R:88:LYS:HZ3	1.44	0.66
1:A:1502:A:H2	1:A:1505:G:N1	1.88	0.66
1:A:969:A:H61	15:M:126:LYS:HB2	1.60	0.66
6:D:110:PHE:CD1	6:D:162:LEU:HD21	2.31	0.66
6:D:151:LYS:HD2	6:D:151:LYS:N	2.11	0.66
7:E:5:ASP:CG	7:E:6:PHE:H	2.04	0.66
19:Q:101:ARG:HA	19:Q:101:ARG:NE	2.11	0.66
1:A:216:G:H2'	1:A:217:C:H6	1.60	0.65
1:A:835:U:OP1	20:R:64:ARG:NH2	2.27	0.65
1:A:954:G:H2'	1:A:955:U:C6	2.31	0.65
4:B:101:MET:HA	4:B:108:ILE:HD12	1.78	0.65
5:C:191:THR:HB	5:C:194:GLY:O	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:8:VAL:HG13	6:D:21:LEU:HD13	1.78	0.65
6:D:131:ARG:H	6:D:131:ARG:HD2	1.61	0.65
1:A:19:C:H2'	1:A:20:U:H6	1.61	0.65
1:A:112:G:H21	1:A:354:G:H5'	1.61	0.65
1:A:1038:C:H2'	1:A:1039:C:C6	2.32	0.65
13:K:80:VAL:HG13	13:K:103:LEU:HD21	1.77	0.65
1:A:314:C:O2'	1:A:315:A:H5'	1.96	0.65
5:C:77:ILE:HD13	5:C:84:ILE:HD12	1.79	0.65
13:K:101:SER:C	13:K:103:LEU:H	2.04	0.65
1:A:1343:G:H2'	1:A:1344:C:C6	2.32	0.65
15:M:82:MET:HE2	15:M:93:ARG:HG3	1.78	0.65
20:R:86:VAL:O	20:R:87:ARG:HB2	1.96	0.65
1:A:738:C:P	8:F:92:LYS:HE3	2.36	0.65
5:C:10:PHE:CE2	5:C:178:LEU:HD13	2.32	0.65
14:L:27:LEU:C	14:L:29:GLY:H	2.02	0.65
21:S:33:THR:HG22	21:S:34:TRP:N	2.11	0.65
1:A:1251:A:H2'	1:A:1252:A:C8	2.31	0.65
1:A:1320:C:N3	21:S:36:ARG:HG3	2.12	0.65
5:C:35:GLU:CD	5:C:59:ARG:HH22	2.05	0.65
11:I:44:VAL:HG12	11:I:51:ARG:HH12	1.60	0.65
15:M:50:GLU:O	15:M:54:VAL:HG23	1.96	0.65
21:S:28:LYS:HG2	21:S:29:ARG:N	2.04	0.65
1:A:115:G:H1'	1:A:116:A:N7	2.11	0.65
1:A:1086:U:H3	1:A:1099:G:H22	1.44	0.65
1:A:1201:A:H4'	1:A:1202:G:O5'	1.97	0.65
4:B:197:VAL:HB	4:B:200:ILE:HG12	1.77	0.65
9:G:38:LEU:HA	9:G:41:ARG:HG3	1.78	0.65
1:A:1223:C:P	21:S:78:ARG:NH1	2.69	0.65
1:A:1392:G:H21	1:A:1502:A:H8	1.45	0.65
1:A:1368:G:O2'	1:A:1369:C:H5'	1.97	0.64
8:F:21:LEU:O	8:F:24:GLU:HB3	1.97	0.64
15:M:65:LYS:CE	15:M:69:GLU:HG2	2.26	0.64
17:O:70:LEU:HD12	17:O:78:TYR:HB2	1.78	0.64
1:A:1053:G:C4'	1:A:1054:C:H5'	2.27	0.64
1:A:1427:U:H2'	1:A:1428:A:C8	2.32	0.64
6:D:8:VAL:HG21	6:D:115:ARG:CZ	2.27	0.64
9:G:70:LYS:HB3	9:G:96:GLN:HG2	1.78	0.64
1:A:518:C:H5''	1:A:519:C:C6	2.32	0.64
1:A:714:G:H2'	1:A:715:A:C8	2.32	0.64
1:A:1116:C:C2'	1:A:1117:G:H5''	2.26	0.64
1:A:1355:G:H2'	1:A:1356:G:C8	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:J:14:LYS:C	12:J:16:LEU:H	2.06	0.64
1:A:686:U:O2'	1:A:687:A:H8	1.78	0.64
1:A:1367:C:H5'	12:J:60:ARG:HH12	1.63	0.64
4:B:28:PHE:CD2	4:B:190:THR:HA	2.33	0.64
1:A:1366:C:H2'	1:A:1367:C:C6	2.32	0.64
14:L:89:ARG:HG2	14:L:97:ARG:HA	1.80	0.64
20:R:36:ASN:HD21	20:R:38:GLU:HG2	1.62	0.64
1:A:1117:G:H5'	1:A:1117:G:H8	1.63	0.64
1:A:1286:A:H2'	1:A:1287:A:H4'	1.79	0.64
14:L:126:LYS:H	14:L:126:LYS:HD2	1.62	0.64
17:O:16:ALA:HB1	17:O:21:ASP:HB3	1.80	0.64
1:A:939:G:H2'	1:A:940:C:C6	2.33	0.64
4:B:71:VAL:O	4:B:165:VAL:HG23	1.98	0.64
4:B:91:PRO:HG3	4:B:154:LEU:HB2	1.79	0.64
5:C:154:SER:OG	5:C:155:GLY:N	2.28	0.64
1:A:166:G:O2'	1:A:167:G:H5'	1.97	0.64
1:A:1228:C:H4'	15:M:116:THR:HA	1.79	0.64
1:A:1305:G:C5'	23:V:4:GLY:HA3	2.27	0.64
4:B:98:LEU:HD23	4:B:98:LEU:N	2.13	0.64
5:C:188:LEU:CD1	5:C:189:ALA:H	2.10	0.64
1:A:912:C:O2'	1:A:913:A:H5'	1.98	0.63
1:A:1117:G:H4'	11:I:104:ARG:HH11	1.62	0.63
5:C:34:LEU:HD23	5:C:34:LEU:C	2.24	0.63
12:J:4:ILE:HA	12:J:100:THR:HA	1.78	0.63
14:L:47:LYS:CB	14:L:48:PRO:CD	2.73	0.63
6:D:76:ARG:HG2	6:D:76:ARG:HH11	1.64	0.63
21:S:5:LEU:O	21:S:6:LYS:HB2	1.98	0.63
1:A:35:G:H2'	1:A:36:C:C6	2.33	0.63
1:A:382:A:H2'	1:A:383:A:H8	1.64	0.63
1:A:975:A:O5'	1:A:976:G:H5'	1.98	0.63
1:A:1187:G:OP1	11:I:113:LYS:HE2	1.98	0.63
5:C:108:ASN:HD22	5:C:111:LEU:HG	1.64	0.63
22:T:51:GLU:HA	22:T:54:LYS:HD2	1.81	0.63
1:A:1285:A:H4'	1:A:1286:A:O5'	1.98	0.63
1:A:1347:G:N2	1:A:1373:G:H2'	2.14	0.63
1:A:1355:G:H2'	1:A:1356:G:H8	1.63	0.63
8:F:80:ARG:NH1	8:F:88:VAL:HB	2.13	0.63
14:L:27:LEU:C	14:L:29:GLY:N	2.53	0.63
7:E:78:HIS:HD2	10:H:107:LEU:HD12	1.61	0.63
7:E:144:THR:HG22	7:E:146:ALA:H	1.63	0.63
10:H:29:SER:OG	10:H:32:LYS:HB2	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:949:A:H62	15:M:106:ASN:HD21	1.47	0.63
1:A:1490:C:H6	1:A:1490:C:C5'	2.03	0.63
9:G:99:LEU:HD22	9:G:103:TRP:CZ2	2.34	0.63
1:A:838:G:H2'	1:A:839:U:H5''	1.81	0.63
1:A:1189:C:P	12:J:51:ARG:HH22	2.21	0.63
1:A:266:G:H5'	1:A:266:G:C8	2.34	0.63
1:A:662:G:H2'	1:A:663:A:C8	2.33	0.63
1:A:1053:G:C3'	1:A:1054:C:H5'	2.28	0.63
12:J:84:GLN:O	12:J:88:LEU:HD12	1.98	0.63
14:L:24:VAL:HG13	14:L:98:TYR:HE2	1.62	0.63
5:C:155:GLY:CA	5:C:164:ARG:H	2.12	0.62
9:G:38:LEU:C	9:G:38:LEU:HD12	2.24	0.62
15:M:62:ASN:O	15:M:63:THR:HB	1.98	0.62
17:O:56:LEU:HA	17:O:59:MET:HE2	1.81	0.62
20:R:36:ASN:ND2	20:R:38:GLU:HG2	2.14	0.62
20:R:46:GLU:H	20:R:46:GLU:CD	2.07	0.62
6:D:28:SER:O	6:D:30:LYS:N	2.32	0.62
7:E:88:LYS:HZ3	7:E:123:LEU:HD12	1.64	0.62
11:I:44:VAL:HG12	11:I:51:ARG:NH1	2.14	0.62
11:I:92:TYR:O	11:I:96:LEU:HD13	1.99	0.62
19:Q:48:GLU:O	19:Q:49:GLU:C	2.41	0.62
1:A:1015:A:H2'	1:A:1016:A:C8	2.34	0.62
3:X:36:U:H2'	3:X:37:T6A:H5''	1.81	0.62
5:C:191:THR:HG21	5:C:193:TYR:CE1	2.33	0.62
7:E:110:LEU:HD13	7:E:118:ILE:HD13	1.81	0.62
12:J:5:ARG:HD2	12:J:99:LYS:HB2	1.80	0.62
18:P:11:SER:OG	18:P:14:ASN:HB3	1.99	0.62
19:Q:68:ARG:N	19:Q:70:ARG:NH1	2.48	0.62
5:C:191:THR:HG22	5:C:192:THR:N	2.14	0.62
7:E:15:ARG:O	7:E:16:THR:O	2.18	0.62
17:O:25:THR:HG21	17:O:70:LEU:HD23	1.81	0.62
1:A:781:A:H2'	1:A:782:A:H5'	1.82	0.62
1:A:1351:U:O2'	1:A:1352:C:H5'	2.00	0.62
22:T:45:GLN:O	22:T:45:GLN:HG2	1.99	0.62
1:A:1291:G:H4'	11:I:38:GLN:O	2.00	0.62
4:B:95:GLN:O	4:B:96:ARG:HD2	1.99	0.62
5:C:119:ARG:CG	5:C:140:ARG:HH12	2.13	0.62
5:C:148:GLY:HA3	5:C:172:ARG:O	1.99	0.62
7:E:96:PRO:HA	7:E:117:ASP:OD2	1.99	0.62
21:S:55:LYS:HG2	21:S:56:GLN:NE2	2.04	0.62
1:A:419:C:C6	1:A:425:G:N2	2.68	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:36:U:C2'	3:X:37:T6A:H5''	2.29	0.62
7:E:36:ASP:OD2	7:E:40:ARG:HB2	2.00	0.62
13:K:14:VAL:HG21	13:K:40:ILE:HD11	1.81	0.62
13:K:57:THR:HG23	13:K:60:ALA:H	1.65	0.62
14:L:55:VAL:HG12	14:L:56:ALA:N	2.14	0.62
22:T:10:LEU:O	22:T:13:LEU:HD12	2.00	0.62
1:A:109:A:H2'	1:A:326:G:N2	2.15	0.61
1:A:1057:G:O2'	1:A:1058:G:H5'	1.99	0.61
5:C:118:GLN:O	5:C:122:GLU:HG3	2.00	0.61
1:A:1195:C:H3'	1:A:1196:U:H5'	1.80	0.61
13:K:54:ARG:HH11	13:K:54:ARG:CB	2.12	0.61
19:Q:68:ARG:H	19:Q:70:ARG:NH1	1.98	0.61
1:A:474:G:H5''	18:P:81:ARG:NH1	2.15	0.61
20:R:53:ARG:HH11	20:R:59:SER:HA	1.64	0.61
4:B:178:ARG:HG3	4:B:178:ARG:NH1	2.10	0.61
5:C:60:ALA:O	5:C:61:ALA:HB2	2.00	0.61
5:C:70:VAL:HG12	5:C:71:ALA:H	1.63	0.61
7:E:80:ILE:HG13	7:E:91:LEU:HB2	1.82	0.61
1:A:1161:C:H2'	1:A:1162:C:H6	1.64	0.61
6:D:35:ARG:O	6:D:36:ARG:HB2	1.99	0.61
6:D:127:THR:CG2	6:D:147:ALA:HB3	2.29	0.61
22:T:89:ARG:HH22	22:T:106:ALA:HA	1.66	0.61
1:A:918:A:H2'	1:A:919:A:C8	2.35	0.61
6:D:151:LYS:H	6:D:151:LYS:CD	2.13	0.61
7:E:41:VAL:HG21	7:E:113:ALA:HB2	1.81	0.61
12:J:12:ASP:HB3	12:J:15:THR:HG22	1.81	0.61
1:A:376:G:OP2	18:P:67:THR:HG21	2.00	0.61
8:F:100:ASN:HA	20:R:23:LYS:HE2	1.82	0.61
15:M:63:THR:HG23	15:M:64:TRP:H	1.65	0.61
1:A:299:G:H2'	1:A:300:A:C8	2.35	0.61
4:B:16:HIS:HE2	4:B:214:ILE:CG1	2.13	0.61
7:E:18:ARG:HH21	7:E:25:ARG:HB3	1.64	0.61
4:B:139:LYS:O	4:B:143:GLU:HG2	2.00	0.61
5:C:190:ARG:HG2	5:C:190:ARG:NH1	2.15	0.61
4:B:69:LEU:HD23	4:B:70:PHE:N	2.16	0.61
5:C:91:LEU:HD21	5:C:99:VAL:CG1	2.31	0.61
18:P:34:GLU:OE2	18:P:55:ARG:HD3	2.01	0.61
1:A:666:G:H5'	1:A:726:C:H1'	1.83	0.60
1:A:1061:G:O2'	1:A:1062:U:H5'	2.00	0.60
3:X:36:U:H2'	3:X:37:T6A:C5'	2.31	0.60
4:B:79:ASP:HB3	4:B:238:LEU:HD13	1.81	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:P:67:THR:CG2	18:P:68:ASP:N	2.63	0.60
1:A:371:G:C2'	1:A:372:C:H5'	2.31	0.60
1:A:1443:G:H5''	1:A:1446:A:H5'	1.82	0.60
4:B:51:LEU:HD22	4:B:55:PHE:CE1	2.35	0.60
1:A:1005:A:H5'	1:A:1038:C:H1'	1.83	0.60
6:D:8:VAL:HG21	6:D:115:ARG:NH1	2.17	0.60
14:L:110:VAL:H	14:L:122:THR:CG2	2.13	0.60
15:M:5:ALA:HB3	15:M:8:GLU:HG3	1.83	0.60
22:T:39:LYS:HD2	22:T:55:ILE:CD1	2.28	0.60
4:B:23:ARG:HH11	4:B:24:TRP:HA	1.66	0.60
11:I:36:TYR:HD2	11:I:37:PHE:CE2	2.20	0.60
14:L:89:ARG:CZ	14:L:97:ARG:HD2	2.32	0.60
22:T:56:MET:HE1	22:T:104:LEU:HG	1.84	0.60
1:A:1068:G:OP2	1:A:1068:G:H8	1.83	0.60
4:B:144:ARG:HA	4:B:147:LYS:HD2	1.84	0.60
4:B:164:VAL:HG12	4:B:186:ALA:HB2	1.84	0.60
5:C:10:PHE:CZ	5:C:178:LEU:HD13	2.37	0.60
5:C:26:LYS:HD3	5:C:26:LYS:N	2.08	0.60
6:D:7:PRO:HB2	6:D:10:ARG:HD2	1.83	0.60
9:G:155:ARG:O	9:G:156:TRP:HB3	2.02	0.60
10:H:6:ILE:O	10:H:10:LEU:HG	2.01	0.60
22:T:67:ALA:HB2	22:T:77:ALA:HB2	1.83	0.60
1:A:448:A:OP2	1:A:485:G:N2	2.35	0.60
1:A:1425:U:H2'	1:A:1426:C:C6	2.37	0.60
4:B:62:ALA:C	4:B:64:ARG:H	2.08	0.60
6:D:50:ARG:HD2	6:D:51:PRO:O	2.02	0.60
15:M:78:ILE:HA	15:M:81:LEU:CD2	2.31	0.60
1:A:748:C:O2'	1:A:749:C:C6	2.55	0.60
5:C:107:GLN:H	5:C:107:GLN:CD	2.10	0.60
9:G:113:GLU:HG2	9:G:119:ARG:HG2	1.83	0.60
9:G:144:MET:O	9:G:147:ALA:HB3	2.02	0.60
12:J:42:THR:HG23	12:J:67:THR:O	2.00	0.60
14:L:60:LEU:N	14:L:64:TYR:O	2.34	0.60
1:A:975:A:H4'	1:A:976:G:H5'	1.84	0.60
1:A:1178:G:N2	1:A:1180:A:H3'	2.17	0.60
5:C:119:ARG:HG2	5:C:140:ARG:NH1	2.15	0.60
8:F:10:LEU:CD1	8:F:59:TYR:HB3	2.31	0.60
12:J:49:VAL:HG22	16:N:41:ARG:HD2	1.84	0.60
1:A:397:A:H5'	1:A:398:C:OP1	2.01	0.60
1:A:580:U:H2'	1:A:581:G:O4'	2.02	0.60
1:A:839:U:O2	1:A:839:U:H2'	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1225:A:H2'	1:A:1225:A:N3	2.17	0.60
9:G:3:ARG:HH11	9:G:3:ARG:HG3	1.66	0.60
9:G:22:LEU:HG	9:G:62:PHE:HE2	1.67	0.60
1:A:112:G:N2	1:A:354:G:H5'	2.17	0.59
5:C:43:LEU:HD22	5:C:68:VAL:HG21	1.84	0.59
9:G:139:GLU:O	9:G:143:ARG:HG3	2.01	0.59
14:L:85:ILE:HG23	14:L:98:TYR:HB3	1.84	0.59
1:A:1124:G:H4'	12:J:38:ILE:HG12	1.83	0.59
1:A:130:A:OP2	1:A:190(E):U:H2'	2.01	0.59
1:A:478:A:O2'	1:A:479:C:H5'	2.02	0.59
1:A:948:C:O2'	1:A:949:A:H5'	2.03	0.59
1:A:1133:G:H2'	1:A:1134:G:H8	1.66	0.59
1:A:1497:G:C2'	1:A:1498:U:H5'	2.32	0.59
22:T:44:ALA:C	22:T:46:GLU:H	2.10	0.59
1:A:986:A:H1'	21:S:54:GLY:O	2.01	0.59
1:A:1115:C:H2'	1:A:1116:C:H6	1.67	0.59
1:A:1320:C:OP1	21:S:70:LYS:HE3	2.02	0.59
6:D:162:LEU:HD12	6:D:181:MET:CE	2.26	0.59
11:I:5:TYR:HA	11:I:17:VAL:O	2.01	0.59
20:R:43:PHE:C	20:R:51:LEU:HD12	2.28	0.59
1:A:620:C:N1	6:D:135:LEU:HD13	2.17	0.59
5:C:155:GLY:HA3	5:C:164:ARG:H	1.68	0.59
12:J:71:LEU:O	12:J:72:VAL:HB	2.03	0.59
18:P:20:VAL:CG1	18:P:32:TYR:HB2	2.32	0.59
1:A:130:A:C8	19:Q:63:ARG:HG3	2.38	0.59
1:A:975:A:H4'	1:A:976:G:C5'	2.32	0.59
1:A:975:A:H4'	1:A:976:G:O5'	2.03	0.59
1:A:1347:G:O2'	1:A:1348:U:P	2.60	0.59
7:E:144:THR:HG22	7:E:146:ALA:N	2.18	0.59
10:H:55:GLY:O	10:H:56:LYS:HD2	2.02	0.59
1:A:627:G:O2'	1:A:628:G:H5'	2.02	0.59
1:A:1206:G:H4'	5:C:192:THR:O	2.03	0.59
1:A:1369:C:H2'	1:A:1370:G:C8	2.37	0.59
11:I:23:ASN:HD22	11:I:23:ASN:C	2.10	0.59
18:P:21:VAL:HG21	18:P:59:TRP:CD1	2.38	0.59
4:B:80:ILE:HD13	4:B:212:GLN:HB2	1.84	0.59
4:B:209:ARG:HE	4:B:239:VAL:HG11	1.67	0.59
4:B:219:VAL:O	4:B:223:ILE:HG13	2.03	0.59
6:D:19:LEU:HD22	6:D:67:ILE:HG12	1.84	0.59
1:A:190(L):U:O2	22:T:105:SER:HB2	2.03	0.59
6:D:63:LYS:HD2	6:D:198:VAL:HG22	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:79:GLU:HG3	7:E:93:PRO:CD	2.32	0.59
1:A:991:U:O2'	1:A:992:U:H5'	2.02	0.59
1:A:1247:U:O2'	1:A:1248:A:H5'	2.02	0.59
4:B:7:VAL:HG11	4:B:221:LEU:HD23	1.84	0.59
4:B:141:GLU:O	4:B:145:LEU:HG	2.02	0.59
10:H:119:LEU:HB2	10:H:123:GLU:HB2	1.83	0.59
4:B:88:ALA:HB1	4:B:90:MET:HG2	1.85	0.58
7:E:24:ARG:HG2	7:E:24:ARG:HH11	1.68	0.58
15:M:37:THR:HG22	15:M:39:ILE:HG13	1.85	0.58
15:M:63:THR:CG2	15:M:64:TRP:N	2.66	0.58
23:V:3:LYS:HB3	23:V:14:TRP:CG	2.38	0.58
20:R:53:ARG:C	20:R:55:ARG:H	2.11	0.58
21:S:3:ARG:HH22	21:S:69:HIS:HE1	1.51	0.58
21:S:20:LEU:HD12	21:S:21:GLU:N	2.18	0.58
1:A:357:G:O2'	1:A:358:U:H5'	2.03	0.58
1:A:523:A:H61	14:L:92:ASP:HB2	1.67	0.58
1:A:760:G:H1	19:Q:105:ALA:HA	1.67	0.58
4:B:97:TRP:CZ2	4:B:101:MET:HB2	2.38	0.58
5:C:155:GLY:O	5:C:156:ARG:HB2	2.02	0.58
10:H:103:VAL:CG2	10:H:110:ALA:HB2	2.33	0.58
1:A:501:C:H2'	1:A:502:G:H8	1.67	0.58
1:A:977:A:H2'	1:A:978:A:H5''	1.86	0.58
23:V:24:ARG:HD3	23:V:24:ARG:H	1.69	0.58
5:C:108:ASN:ND2	5:C:111:LEU:HG	2.19	0.58
9:G:112:PRO:O	9:G:113:GLU:C	2.46	0.58
1:A:129(A):G:O2'	1:A:190(E):U:H2'	2.03	0.58
1:A:135:C:O2	18:P:1:MET:HB2	2.03	0.58
1:A:352:C:H4'	1:A:354:G:OP1	2.04	0.58
1:A:1201:A:O2'	1:A:1202:G:OP2	2.22	0.58
1:A:1397:C:H4'	1:A:1398:A:OP2	2.04	0.58
4:B:71:VAL:HG23	4:B:164:VAL:CA	2.32	0.58
4:B:188:ALA:HB1	4:B:192:SER:OG	2.03	0.58
5:C:107:GLN:O	5:C:108:ASN:HB3	2.03	0.58
12:J:82:ILE:O	12:J:86:MET:HB2	2.03	0.58
14:L:41:ARG:HH12	14:L:57:LYS:HZ3	1.52	0.58
20:R:18:ARG:C	20:R:19:LYS:HD2	2.28	0.58
20:R:37:VAL:O	20:R:41:LYS:HG3	2.03	0.58
1:A:353:A:H5'	1:A:353:A:H8	1.69	0.58
1:A:1095:U:H2'	1:A:1096:C:C6	2.38	0.58
1:A:1148:U:H2'	1:A:1149:C:O4'	2.04	0.58
22:T:73:HIS:O	22:T:74:LYS:HB2	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:706:A:O2'	13:K:29:ILE:HD11	2.03	0.58
1:A:959:A:H3'	1:A:960:U:H5''	1.85	0.58
1:A:1420:C:H2'	1:A:1421:G:H8	1.68	0.58
10:H:112:LEU:N	10:H:112:LEU:HD23	2.19	0.58
1:A:1057:G:H5''	5:C:154:SER:CB	2.34	0.58
4:B:84:GLU:HB3	4:B:219:VAL:CG2	2.23	0.58
5:C:22:TRP:CG	5:C:59:ARG:HD2	2.39	0.58
6:D:30:LYS:C	6:D:32:ALA:N	2.61	0.58
4:B:17:PHE:CD1	4:B:18:GLY:N	2.72	0.58
9:G:37:ASN:HD21	11:I:41:VAL:HG23	1.69	0.58
13:K:84:VAL:HG23	13:K:110:ASP:CA	2.29	0.58
15:M:5:ALA:HB2	15:M:22:ILE:HD13	1.85	0.58
22:T:50:GLU:HG3	22:T:100:ILE:HG13	1.84	0.58
1:A:1121:U:H2'	1:A:1122:U:C6	2.38	0.57
1:A:1392:G:O2'	1:A:1502:A:H5''	2.03	0.57
1:A:1443:G:H5''	1:A:1446:A:C5'	2.34	0.57
4:B:17:PHE:HD1	4:B:18:GLY:N	2.01	0.57
10:H:113:SER:HB2	10:H:134:ILE:HD11	1.85	0.57
15:M:78:ILE:O	15:M:81:LEU:HD23	2.03	0.57
1:A:405:U:H3'	1:A:406:G:H5'	1.86	0.57
1:A:1152:A:H5''	12:J:13:HIS:HD2	1.69	0.57
1:A:1312:G:O2'	1:A:1313:U:H5'	2.05	0.57
5:C:64:VAL:HB	5:C:99:VAL:HB	1.86	0.57
12:J:86:MET:HA	12:J:86:MET:HE3	1.85	0.57
14:L:41:ARG:NH1	14:L:41:ARG:HB3	2.19	0.57
1:A:1193:G:O2'	1:A:1194:U:H5'	2.04	0.57
5:C:87:LEU:C	5:C:89:GLU:H	2.12	0.57
11:I:24:GLY:HA2	11:I:59:PHE:O	2.05	0.57
12:J:24:VAL:O	12:J:28:ARG:HG3	2.04	0.57
19:Q:45:HIS:CD2	19:Q:47:PRO:HG3	2.38	0.57
1:A:287:U:O2'	1:A:288:A:H5'	2.04	0.57
1:A:1347:G:H2'	1:A:1373:G:H1	1.69	0.57
7:E:88:LYS:NZ	7:E:123:LEU:HD12	2.18	0.57
17:O:33:THR:HG23	17:O:63:ARG:HH12	1.70	0.57
19:Q:5:VAL:O	19:Q:6:LEU:HD23	2.04	0.57
1:A:262:A:H5'	22:T:74:LYS:HD3	1.86	0.57
1:A:1160:G:O2'	1:A:1161:C:H5'	2.04	0.57
1:A:1197:G:O2'	1:A:1198:G:H5'	2.04	0.57
1:A:1525:G:P	13:K:120:ARG:HH22	2.27	0.57
5:C:134:ILE:HG23	5:C:151:VAL:HB	1.87	0.57
12:J:4:ILE:HG13	12:J:74:ILE:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L:71:PRO:O	14:L:102:ARG:HD2	2.03	0.57
14:L:110:VAL:O	14:L:113:ARG:HB2	2.04	0.57
18:P:51:VAL:HG12	18:P:52:ASP:N	2.18	0.57
19:Q:76:LEU:C	19:Q:76:LEU:HD23	2.29	0.57
1:A:384:G:H2'	1:A:385:C:C6	2.39	0.57
1:A:653:A:C8	10:H:56:LYS:HG2	2.40	0.57
5:C:34:LEU:HD12	16:N:25:VAL:CG2	2.33	0.57
14:L:46:LYS:CD	14:L:47:LYS:H	2.17	0.57
1:A:17:U:H2'	1:A:18:C:C6	2.39	0.57
1:A:353:A:H8	1:A:353:A:C5'	2.17	0.57
1:A:1305:G:H5''	23:V:4:GLY:C	2.29	0.57
8:F:44:GLY:HA2	8:F:59:TYR:CE1	2.40	0.57
19:Q:68:ARG:O	19:Q:69:LYS:HB2	2.04	0.57
20:R:55:ARG:HB3	20:R:55:ARG:HH11	1.69	0.57
10:H:112:LEU:HD23	10:H:112:LEU:H	1.68	0.57
21:S:15:LEU:O	21:S:19:VAL:HG12	2.05	0.57
1:A:586:C:O2'	1:A:587:G:H5'	2.04	0.57
1:A:1056:U:H5'	5:C:163:ALA:HB2	1.87	0.57
9:G:155:ARG:HA	9:G:155:ARG:NH1	2.20	0.57
1:A:353:A:C8	1:A:353:A:C5'	2.88	0.57
1:A:528:C:H5'	1:A:535:A:C6	2.40	0.57
1:A:1128:C:H4'	11:I:16:ARG:HH12	1.69	0.57
11:I:11:LYS:O	11:I:11:LYS:HG2	2.05	0.57
12:J:5:ARG:HB3	12:J:99:LYS:C	2.29	0.57
12:J:30:SER:OG	12:J:81:THR:HA	2.05	0.57
16:N:14:PRO:O	16:N:15:LYS:CB	2.53	0.57
21:S:28:LYS:CG	21:S:29:ARG:H	2.09	0.57
1:A:190(F):G:H4'	1:A:190(G):G:OP2	2.03	0.56
4:B:14:GLY:O	4:B:15:VAL:HG13	2.04	0.56
5:C:44:GLU:C	5:C:46:GLU:H	2.12	0.56
5:C:91:LEU:HD21	5:C:99:VAL:HG12	1.86	0.56
6:D:24:GLU:HG2	6:D:25:ARG:H	1.70	0.56
9:G:26:PHE:CE2	9:G:30:ILE:HD11	2.39	0.56
11:I:8:GLY:CA	11:I:79:LEU:HB3	2.35	0.56
4:B:69:LEU:CD1	4:B:155:LEU:HD11	2.35	0.56
4:B:116:GLU:HG2	4:B:153:ARG:CZ	2.34	0.56
5:C:89:GLU:O	5:C:93:LYS:HB2	2.05	0.56
5:C:134:ILE:HG22	5:C:168:ALA:HB3	1.85	0.56
6:D:177:ASP:OD1	6:D:179:GLU:HB2	2.05	0.56
13:K:32:ILE:CG2	13:K:77:MET:HE2	2.35	0.56
21:S:5:LEU:O	21:S:6:LYS:CB	2.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:C:H2'	1:A:336:C:H6	1.70	0.56
4:B:14:GLY:C	4:B:15:VAL:HG22	2.30	0.56
4:B:15:VAL:HG11	4:B:209:ARG:CG	2.35	0.56
4:B:97:TRP:CH2	4:B:101:MET:HB2	2.40	0.56
4:B:139:LYS:O	4:B:139:LYS:HD3	2.05	0.56
4:B:181:PHE:HD2	10:H:70:GLN:HB3	1.70	0.56
10:H:4:ASP:OD2	10:H:85:ARG:NH1	2.38	0.56
10:H:28:ALA:HB2	10:H:59:LEU:HG	1.87	0.56
11:I:127:LYS:H	11:I:127:LYS:HE3	1.70	0.56
12:J:47:PHE:CZ	16:N:37:PHE:HE1	2.23	0.56
14:L:39:VAL:HG12	14:L:40:VAL:N	2.20	0.56
19:Q:40:LYS:HD3	19:Q:42:TYR:CZ	2.40	0.56
1:A:390:C:H2'	1:A:391:G:C8	2.40	0.56
5:C:18:TRP:HE3	5:C:18:TRP:H	1.54	0.56
5:C:70:VAL:HG12	5:C:72:LYS:H	1.70	0.56
12:J:9:ARG:HB3	12:J:9:ARG:NH1	2.21	0.56
19:Q:80:GLY:O	19:Q:81:ARG:HB3	2.05	0.56
21:S:30:LEU:HD23	21:S:31:ILE:H	1.67	0.56
21:S:31:ILE:O	21:S:32:LYS:HB3	2.04	0.56
1:A:67:C:H2'	1:A:68:G:C8	2.41	0.56
1:A:149:A:H2'	1:A:150:C:C6	2.40	0.56
1:A:750:G:N3	17:O:23:GLY:HA3	2.19	0.56
1:A:1066:C:O2'	1:A:1067:A:H5'	2.06	0.56
1:A:1292:U:P	9:G:41:ARG:HH22	2.28	0.56
4:B:121:LEU:O	4:B:127:ILE:HG23	2.05	0.56
9:G:79:ARG:NH1	9:G:82:GLY:H	2.03	0.56
1:A:974:A:OP2	16:N:41:ARG:NH1	2.38	0.56
1:A:1305:G:C8	1:A:1305:G:OP2	2.58	0.56
4:B:87:ARG:O	4:B:88:ALA:HB2	2.06	0.56
1:A:1154:G:H2'	1:A:1155:G:H8	1.70	0.56
1:A:1281:U:H4'	1:A:1282:C:OP2	2.06	0.56
1:A:1316:G:N2	1:A:1318:A:H3'	2.21	0.56
10:H:51:VAL:HG12	10:H:52:ASP:N	2.19	0.56
13:K:121:PRO:HG2	13:K:126:ARG:HG3	1.87	0.56
21:S:15:LEU:HD12	21:S:16:LEU:H	1.71	0.56
4:B:178:ARG:NH2	10:H:68:ARG:HH22	2.04	0.56
5:C:51:GLY:O	5:C:70:VAL:HG13	2.05	0.56
10:H:34:GLU:OE2	10:H:34:GLU:HA	2.06	0.56
1:A:370:C:O2'	1:A:371:G:H5'	2.05	0.56
1:A:954:G:H2'	1:A:955:U:H6	1.69	0.56
1:A:1392:G:N2	1:A:1502:A:H8	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1521:G:H2'	1:A:1522:U:C6	2.41	0.56
4:B:88:ALA:CB	4:B:90:MET:HG2	2.36	0.56
5:C:99:VAL:CG2	5:C:100:ALA:N	2.68	0.56
5:C:130:VAL:HG21	5:C:157:ILE:HG23	1.87	0.56
6:D:8:VAL:C	6:D:10:ARG:H	2.13	0.56
12:J:39:PRO:O	12:J:40:LEU:HB2	2.05	0.56
14:L:46:LYS:O	14:L:47:LYS:C	2.49	0.56
22:T:100:ILE:C	22:T:102:GLY:N	2.63	0.56
4:B:25:ASN:HD22	4:B:25:ASN:C	2.13	0.56
4:B:221:LEU:O	4:B:221:LEU:HD13	2.05	0.56
11:I:51:ARG:HG2	11:I:56:LEU:HD12	1.87	0.56
11:I:53:VAL:HG21	11:I:85:LEU:HD21	1.88	0.56
12:J:49:VAL:O	12:J:60:ARG:O	2.23	0.56
15:M:82:MET:HE3	15:M:92:HIS:HB2	1.87	0.56
1:A:157:G:O2'	1:A:158:G:H5'	2.06	0.55
1:A:1053:G:HO2'	1:A:1199:U:H5	1.54	0.55
1:A:1176:A:H2'	1:A:1177:G:C8	2.42	0.55
4:B:235:SER:C	4:B:237:ALA:H	2.14	0.55
6:D:32:ALA:C	6:D:34:GLU:H	2.15	0.55
1:A:269:C:H2'	1:A:270:A:C8	2.41	0.55
1:A:421:U:H5''	1:A:423:G:N2	2.20	0.55
1:A:1052:U:H2'	1:A:1055:A:OP1	2.07	0.55
5:C:14:ILE:HG22	5:C:15:THR:HG23	1.88	0.55
6:D:29:PRO:C	6:D:30:LYS:HG3	2.31	0.55
10:H:64:LYS:HG2	10:H:79:VAL:HG21	1.89	0.55
12:J:38:ILE:HB	12:J:71:LEU:HB3	1.89	0.55
14:L:34:ARG:O	14:L:61:THR:HG23	2.05	0.55
17:O:33:THR:HG23	17:O:63:ARG:NH1	2.21	0.55
1:A:1054:C:OP1	1:A:1197:G:OP1	2.24	0.55
1:A:1057:G:H5''	5:C:154:SER:HB2	1.87	0.55
1:A:1392:G:O2'	1:A:1393:U:H5'	2.06	0.55
1:A:1425:U:H3	1:A:1475:G:H1	1.53	0.55
4:B:78:GLN:HA	4:B:94:ASN:OD1	2.06	0.55
13:K:72:ALA:HB1	13:K:77:MET:HG3	1.87	0.55
21:S:36:ARG:HA	21:S:71:LEU:HB2	1.88	0.55
23:V:12:LYS:HB3	23:V:22:ARG:HD2	1.89	0.55
1:A:328:C:O2	1:A:328:C:C2'	2.53	0.55
11:I:20:ARG:O	11:I:60:ASP:N	2.39	0.55
5:C:40:ARG:HB3	5:C:44:GLU:OE2	2.06	0.55
16:N:29:ARG:HG2	16:N:29:ARG:NH1	2.22	0.55
16:N:29:ARG:HB3	16:N:40:CYS:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:R:43:PHE:HA	20:R:51:LEU:HD12	1.88	0.55
22:T:73:HIS:O	22:T:74:LYS:CB	2.54	0.55
1:A:559:A:P	7:E:126:ARG:HH22	2.30	0.55
1:A:683:G:H21	13:K:38:ASN:ND2	2.04	0.55
1:A:718:G:C8	13:K:116:HIS:HB3	2.41	0.55
1:A:738:C:OP2	8:F:92:LYS:HE3	2.07	0.55
1:A:1106:G:OP1	5:C:172:ARG:HD3	2.06	0.55
8:F:19:LEU:O	8:F:23:LYS:HG3	2.07	0.55
12:J:4:ILE:HA	12:J:100:THR:CA	2.37	0.55
12:J:8:LEU:HB2	12:J:70:ARG:HB2	1.87	0.55
15:M:85:GLY:O	15:M:86:CYS:O	2.24	0.55
18:P:20:VAL:HG11	18:P:32:TYR:HB3	1.87	0.55
1:A:683:G:H21	13:K:38:ASN:HD22	1.54	0.55
1:A:1116:C:H2'	1:A:1117:G:C5'	2.37	0.55
4:B:97:TRP:CZ2	4:B:102:LEU:HD13	2.39	0.55
8:F:2:ARG:NH1	8:F:69:GLU:HB3	2.21	0.55
10:H:45:ILE:HG13	10:H:47:GLY:H	1.70	0.55
11:I:118:LYS:O	11:I:119:ALA:CB	2.53	0.55
14:L:24:VAL:O	14:L:24:VAL:HG12	2.05	0.55
14:L:41:ARG:HB3	14:L:41:ARG:HH11	1.71	0.55
14:L:46:LYS:HE3	14:L:47:LYS:HB2	1.89	0.55
15:M:63:THR:CG2	15:M:64:TRP:H	2.20	0.55
17:O:17:ARG:HG3	17:O:17:ARG:NH1	2.20	0.55
20:R:87:ARG:HG2	20:R:87:ARG:HH11	1.72	0.55
4:B:16:HIS:NE2	4:B:214:ILE:HG12	2.22	0.55
8:F:101:ALA:HA	20:R:28:GLU:CD	2.31	0.55
11:I:117:HIS:C	11:I:118:LYS:HG3	2.32	0.55
18:P:67:THR:CG2	18:P:68:ASP:H	2.20	0.55
1:A:1218:C:H2'	1:A:1219:U:C6	2.42	0.55
1:A:1481:U:O2'	1:A:1482:G:H5'	2.06	0.55
4:B:16:HIS:HE2	4:B:214:ILE:HG13	1.72	0.55
7:E:43:LEU:HD11	7:E:132:ALA:HB1	1.88	0.55
8:F:19:LEU:C	8:F:19:LEU:HD23	2.31	0.55
9:G:78:ARG:HB2	9:G:156:TRP:HZ3	1.72	0.55
11:I:89:ASN:HD21	11:I:91:ASP:HB2	1.71	0.55
16:N:23:ARG:NH1	16:N:30:ALA:HB2	2.22	0.55
1:A:1151:A:O2'	1:A:1152:A:H8	1.89	0.55
1:A:1208:C:H2'	1:A:1209:C:C6	2.40	0.55
4:B:12:GLU:C	4:B:14:GLY:N	2.63	0.55
5:C:36:ASP:HB3	5:C:40:ARG:NH1	2.21	0.55
5:C:123:GLN:HE22	5:C:140:ARG:NH2	2.04	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:92:VAL:O	6:D:96:LEU:HD13	2.07	0.55
9:G:15:ASP:HB3	9:G:19:GLY:H	1.72	0.55
12:J:4:ILE:HA	12:J:100:THR:CB	2.37	0.55
14:L:126:LYS:H	14:L:126:LYS:CE	2.20	0.55
15:M:5:ALA:O	15:M:6:GLY:C	2.50	0.55
16:N:24:CYS:HB3	16:N:28:GLY:H	1.71	0.55
1:A:961:U:O2'	1:A:962:C:H5'	2.07	0.54
1:A:1343:G:H2'	1:A:1344:C:H6	1.70	0.54
5:C:33:LEU:HD11	16:N:53:LEU:HD23	1.89	0.54
6:D:162:LEU:CD1	6:D:181:MET:HE2	2.31	0.54
6:D:173:TRP:CD2	6:D:189:PRO:HB3	2.42	0.54
9:G:114:ARG:HG2	9:G:114:ARG:HH11	1.72	0.54
12:J:4:ILE:CD1	12:J:74:ILE:HB	2.29	0.54
1:A:1157:A:H4'	1:A:1158:C:O5'	2.07	0.54
1:A:1285:A:H8	1:A:1285:A:OP1	1.90	0.54
5:C:86:VAL:O	5:C:89:GLU:HB3	2.07	0.54
5:C:110:ASN:HD22	5:C:140:ARG:HB3	1.72	0.54
5:C:156:ARG:NH2	5:C:161:GLU:HA	2.22	0.54
6:D:64:LEU:HD12	6:D:75:PHE:HZ	1.71	0.54
18:P:45:THR:C	18:P:47:ASP:H	2.15	0.54
23:V:24:ARG:N	23:V:24:ARG:CD	2.69	0.54
1:A:556:C:O2'	1:A:557:G:H5'	2.07	0.54
1:A:722:A:H4'	1:A:723:U:C4	2.43	0.54
1:A:877:C:H1'	10:H:3:THR:CG2	2.38	0.54
1:A:1250:A:H2'	1:A:1251:A:C8	2.43	0.54
7:E:103:GLY:O	7:E:106:PRO:HD2	2.08	0.54
14:L:75:HIS:HD2	14:L:77:LEU:N	1.98	0.54
18:P:19:ILE:HG22	18:P:36:ILE:HG13	1.88	0.54
1:A:107:G:C2'	1:A:108:G:H5'	2.38	0.54
1:A:190(I):G:O2'	1:A:190(J):U:H5'	2.07	0.54
1:A:538:G:H5''	14:L:114:LYS:CG	2.37	0.54
1:A:639:G:O2'	1:A:640:A:H5'	2.07	0.54
1:A:740:U:O2'	1:A:741:G:H5'	2.07	0.54
1:A:1241:G:H2'	1:A:1242:C:H6	1.68	0.54
4:B:230:VAL:HG12	4:B:231:GLU:N	2.23	0.54
5:C:70:VAL:O	5:C:106:VAL:HG23	2.07	0.54
6:D:127:THR:HG22	6:D:147:ALA:HB3	1.88	0.54
7:E:72:GLN:O	7:E:73:ASN:HB3	2.08	0.54
19:Q:4:LYS:HE3	19:Q:6:LEU:HD21	1.89	0.54
1:A:151:A:H2'	1:A:152:A:O4'	2.08	0.54
1:A:653:A:OP1	10:H:56:LYS:NZ	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:15:ARG:O	7:E:27:ARG:O	2.26	0.54
14:L:55:VAL:HG12	14:L:56:ALA:H	1.71	0.54
15:M:84:ILE:HG21	21:S:65:ASN:HD22	1.72	0.54
17:O:70:LEU:HD12	17:O:78:TYR:CA	2.36	0.54
1:A:60:A:H4'	1:A:61:G:O5'	2.06	0.54
1:A:539:A:H2'	1:A:540:G:C8	2.42	0.54
1:A:743:U:H2'	1:A:744:C:C6	2.43	0.54
1:A:861:G:O2'	1:A:862:C:H5'	2.08	0.54
1:A:1223:C:OP1	1:A:1224:G:H3'	2.08	0.54
5:C:134:ILE:HD11	5:C:153:VAL:CG2	2.38	0.54
6:D:149:ALA:HB3	6:D:152:SER:HB2	1.90	0.54
7:E:87:SER:HB3	7:E:131:ILE:HD13	1.90	0.54
9:G:85:TYR:HD1	9:G:154:TYR:HE1	1.54	0.54
17:O:78:TYR:CZ	17:O:82:ILE:HD11	2.43	0.54
21:S:77:THR:HG22	21:S:78:ARG:N	2.21	0.54
1:A:1236:A:OP1	23:V:2:GLY:HA3	2.08	0.54
13:K:126:ARG:HB3	13:K:126:ARG:NH1	2.22	0.54
14:L:60:LEU:CD2	14:L:66:VAL:HG22	2.38	0.54
1:A:955:U:O2'	1:A:956:U:H5'	2.08	0.54
1:A:1118:C:H1'	1:A:1179:A:C4	2.43	0.54
1:A:1381:U:O2'	1:A:1382:C:H5'	2.08	0.54
4:B:25:ASN:HD22	4:B:27:LYS:H	1.55	0.54
5:C:87:LEU:C	5:C:89:GLU:N	2.63	0.54
7:E:13:ILE:HA	7:E:29:GLY:O	2.08	0.54
9:G:122:HIS:HD2	9:G:125:MET:CE	2.20	0.54
12:J:59:SER:O	12:J:60:ARG:HB2	2.07	0.54
16:N:9:LYS:HG3	16:N:21:TYR:O	2.08	0.54
1:A:191:G:N3	22:T:105:SER:HB3	2.23	0.54
1:A:346:G:C2'	1:A:347:G:H5'	2.38	0.54
1:A:1007:C:H2'	1:A:1008:C:H6	1.72	0.54
1:A:1101:A:H4'	1:A:1102:A:O5'	2.08	0.54
1:A:1250:A:H5''	11:I:68:GLY:N	2.23	0.54
6:D:5:ILE:HG22	6:D:5:ILE:O	2.06	0.54
8:F:2:ARG:NE	8:F:69:GLU:HG2	2.23	0.54
8:F:62:TRP:O	8:F:62:TRP:CE3	2.61	0.54
13:K:49:GLY:O	13:K:50:TYR:C	2.50	0.54
14:L:119:LYS:O	14:L:120:TYR:HB2	2.08	0.54
1:A:1064:G:H4'	1:A:1065:U:C5'	2.37	0.54
1:A:1453:G:H2'	1:A:1454:G:O4'	2.08	0.54
4:B:19:HIS:ND1	4:B:204:ASN:ND2	2.56	0.54
9:G:23:VAL:HG13	9:G:43:PHE:CE2	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:37:ASN:ND2	11:I:41:VAL:HG23	2.23	0.54
11:I:28:VAL:O	11:I:29:ASN:HB2	2.07	0.54
11:I:71:SER:HA	11:I:74:ILE:HD12	1.89	0.54
12:J:22:LYS:HE2	12:J:90:LEU:HB2	1.90	0.54
21:S:20:LEU:HA	21:S:23:ASN:ND2	2.22	0.54
1:A:112:G:H5'	1:A:389:A:H4'	1.90	0.53
1:A:190(L):U:C2	22:T:105:SER:HB2	2.43	0.53
1:A:542:G:H2'	1:A:543:C:H6	1.72	0.53
1:A:738:C:OP1	8:F:92:LYS:HE3	2.08	0.53
1:A:1314:C:OP2	21:S:6:LYS:HG2	2.08	0.53
1:A:1520:G:O2'	1:A:1521:G:H5'	2.08	0.53
8:F:4:TYR:CE2	8:F:72:VAL:CG2	2.91	0.53
13:K:91:ARG:O	13:K:95:ILE:HG13	2.08	0.53
18:P:26:ARG:HD3	18:P:31:LYS:N	2.22	0.53
1:A:19:C:H2'	1:A:20:U:C6	2.43	0.53
4:B:235:SER:C	4:B:237:ALA:N	2.65	0.53
6:D:61:LYS:HD3	6:D:206:PHE:CD2	2.44	0.53
7:E:60:TYR:HE1	7:E:64:ARG:NH2	2.03	0.53
9:G:3:ARG:HG3	9:G:3:ARG:NH1	2.23	0.53
18:P:42:ARG:O	18:P:43:LYS:C	2.50	0.53
21:S:31:ILE:O	21:S:32:LYS:CB	2.55	0.53
1:A:769:G:H4'	1:A:1513:A:H4'	1.91	0.53
1:A:1054:C:O2'	1:A:1055:A:H5''	2.09	0.53
1:A:1065:U:H4'	1:A:1066:C:O5'	2.07	0.53
10:H:121:ASP:HB2	10:H:125:ARG:NH2	2.23	0.53
14:L:47:LYS:CG	14:L:48:PRO:HD3	2.39	0.53
17:O:14:GLU:HG3	17:O:15:PHE:CD1	2.43	0.53
1:A:1495:U:H2'	1:A:1496:C:H6	1.73	0.53
10:H:86:ILE:HD12	10:H:133:LEU:CD2	2.39	0.53
15:M:40:ASN:C	15:M:40:ASN:HD22	2.15	0.53
15:M:40:ASN:HD22	15:M:41:PRO:CD	2.21	0.53
15:M:65:LYS:HE3	15:M:69:GLU:CG	2.37	0.53
20:R:86:VAL:O	20:R:87:ARG:CB	2.56	0.53
1:A:203:U:H5'	1:A:216:G:N2	2.24	0.53
1:A:1038:C:H2'	1:A:1039:C:H6	1.74	0.53
6:D:199:ASN:C	6:D:199:ASN:ND2	2.62	0.53
16:N:35:ARG:C	16:N:37:PHE:H	2.16	0.53
19:Q:94:ASN:O	19:Q:97:SER:HB3	2.09	0.53
1:A:881:G:P	14:L:12:ARG:HH22	2.32	0.53
1:A:1250:A:H5'	11:I:68:GLY:O	2.08	0.53
9:G:120:ILE:H	9:G:120:ILE:HD12	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L:24:VAL:HG13	14:L:98:TYR:CE2	2.41	0.53
14:L:110:VAL:H	14:L:122:THR:HG22	1.72	0.53
1:A:264:U:H4'	19:Q:63:ARG:HD3	1.89	0.53
1:A:502:G:H4'	1:A:550:G:H4'	1.90	0.53
1:A:810:C:H2'	1:A:811:C:H6	1.73	0.53
1:A:1424:C:O2'	1:A:1425:U:H5'	2.09	0.53
9:G:115:ARG:HB2	9:G:118:VAL:HG23	1.90	0.53
9:G:116:ALA:O	9:G:120:ILE:HD12	2.09	0.53
14:L:40:VAL:O	14:L:40:VAL:HG12	2.09	0.53
17:O:2:PRO:C	17:O:3:ILE:HD12	2.33	0.53
20:R:19:LYS:HD2	20:R:19:LYS:N	2.24	0.53
1:A:537:G:OP1	14:L:113:ARG:NH2	2.41	0.53
1:A:540:G:H21	6:D:42:GLN:NE2	2.07	0.53
1:A:1128:C:H4'	11:I:16:ARG:NH1	2.24	0.53
1:A:1501:C:OP2	1:A:1504:G:H2'	2.09	0.53
4:B:17:PHE:O	4:B:18:GLY:C	2.51	0.53
5:C:195:VAL:C	5:C:196:LEU:HD22	2.34	0.53
11:I:93:ARG:C	11:I:95:LYS:H	2.17	0.53
18:P:22:THR:HA	18:P:33:ILE:HD12	1.91	0.53
1:A:426:G:H2'	1:A:427:U:C6	2.43	0.53
4:B:16:HIS:NE2	4:B:214:ILE:CG1	2.71	0.53
4:B:75:LYS:HE3	4:B:78:GLN:NE2	2.24	0.53
4:B:134:GLU:HA	4:B:137:ARG:HG3	1.90	0.53
11:I:4:TYR:CE2	11:I:88:TYR:HA	2.44	0.53
11:I:108:VAL:HG12	11:I:109:VAL:N	2.23	0.53
19:Q:79:SER:O	19:Q:80:GLY:O	2.27	0.53
21:S:63:THR:HG22	21:S:64:GLU:N	2.23	0.53
1:A:530:G:O6	2:W:3:A:H1'	2.09	0.53
1:A:723:U:H5''	1:A:724:G:OP2	2.09	0.53
1:A:968:A:H4'	1:A:969:A:OP2	2.09	0.53
5:C:108:ASN:C	5:C:110:ASN:H	2.17	0.53
13:K:84:VAL:HG11	13:K:95:ILE:HD11	1.90	0.53
14:L:24:VAL:O	14:L:26:ALA:N	2.35	0.53
19:Q:66:SER:OG	19:Q:69:LYS:HB3	2.09	0.53
1:A:701:C:H5'	1:A:703:G:O4'	2.09	0.52
1:A:984:C:H2'	1:A:985:C:H6	1.74	0.52
1:A:1262:C:O2'	1:A:1263:C:H5'	2.09	0.52
1:A:1300:G:O2'	1:A:1301:U:P	2.67	0.52
5:C:14:ILE:O	5:C:16:ARG:N	2.42	0.52
7:E:147:ASP:OD1	7:E:147:ASP:N	2.41	0.52
16:N:57:ARG:HG2	16:N:58:LYS:N	2.20	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:G:H2'	1:A:267:C:H5	1.73	0.52
1:A:945:G:C2	1:A:946:A:C8	2.96	0.52
1:A:1278:U:H5''	1:A:1279:A:O4'	2.09	0.52
9:G:75:VAL:HG21	9:G:86:GLN:HB3	1.91	0.52
12:J:94:VAL:CG1	12:J:95:GLU:N	2.71	0.52
17:O:4:THR:OG1	17:O:7:GLU:HB2	2.10	0.52
1:A:401:C:H1'	1:A:622:A:H1'	1.92	0.52
4:B:51:LEU:CD2	4:B:55:PHE:HE1	2.23	0.52
4:B:178:ARG:NH2	10:H:68:ARG:NH2	2.57	0.52
5:C:205:GLY:O	5:C:206:GLU:HB2	2.09	0.52
6:D:64:LEU:HD12	6:D:75:PHE:CZ	2.45	0.52
7:E:32:VAL:HG23	7:E:58:ALA:HB1	1.92	0.52
9:G:79:ARG:HH12	9:G:82:GLY:HA2	1.75	0.52
14:L:111:LYS:O	14:L:112:ASP:HB2	2.08	0.52
1:A:337:C:H2'	1:A:338:A:C8	2.44	0.52
1:A:376:G:P	18:P:67:THR:HG21	2.49	0.52
1:A:1056:U:H5'	5:C:163:ALA:CB	2.40	0.52
6:D:70:ILE:HD11	6:D:100:ARG:HD2	1.90	0.52
9:G:78:ARG:HH11	9:G:154:TYR:HB3	1.75	0.52
9:G:79:ARG:HH11	9:G:82:GLY:H	1.57	0.52
19:Q:78:GLU:HG3	19:Q:78:GLU:O	2.09	0.52
1:A:428:G:OP2	6:D:7:PRO:HG3	2.09	0.52
4:B:45:GLN:O	4:B:49:GLU:HG3	2.09	0.52
5:C:22:TRP:CZ3	5:C:32:LEU:HB2	2.45	0.52
5:C:110:ASN:O	5:C:111:LEU:HD23	2.10	0.52
9:G:140:ASP:HA	9:G:143:ARG:HD2	1.91	0.52
11:I:36:TYR:CD2	11:I:37:PHE:CE2	2.98	0.52
11:I:48:GLU:HA	11:I:51:ARG:HD2	1.92	0.52
19:Q:81:ARG:HG3	19:Q:81:ARG:O	2.08	0.52
22:T:76:ALA:O	22:T:80:ARG:HG2	2.09	0.52
1:A:748:C:OP2	1:A:748:C:H6	1.92	0.52
1:A:1347:G:C6	11:I:107:ARG:NH2	2.78	0.52
7:E:43:LEU:N	7:E:136:MET:HE2	2.24	0.52
9:G:110:GLN:OE1	9:G:110:GLN:HA	2.09	0.52
12:J:49:VAL:O	12:J:60:ARG:CA	2.50	0.52
12:J:50:ILE:HB	16:N:41:ARG:NE	2.25	0.52
13:K:29:ILE:C	13:K:29:ILE:HD12	2.35	0.52
18:P:45:THR:HB	18:P:46:PRO:HD2	1.92	0.52
1:A:676:A:H1'	13:K:115:PRO:HB3	1.92	0.52
1:A:992:U:O2'	1:A:993:G:OP2	2.24	0.52
1:A:1333:A:H2'	1:A:1334:G:O4'	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1347:G:H2'	1:A:1373:G:N1	2.25	0.52
14:L:125:PRO:HA	14:L:126:LYS:HE3	1.92	0.52
18:P:67:THR:HG22	18:P:68:ASP:H	1.69	0.52
22:T:47:GLY:O	22:T:49:ALA:N	2.42	0.52
1:A:973:G:H3'	1:A:974:A:H5''	1.92	0.52
9:G:122:HIS:HD2	9:G:125:MET:HE3	1.75	0.52
1:A:131:C:H2'	1:A:132:C:H6	1.75	0.52
1:A:346:G:H2'	1:A:347:G:H5'	1.92	0.52
1:A:1108:G:H5'	1:A:1191:A:H4'	1.92	0.52
1:A:1343:G:H1'	11:I:121:ARG:NH1	2.25	0.52
1:A:1353:G:OP1	23:V:3:LYS:HE2	2.09	0.52
1:A:1372:U:O2'	1:A:1373:G:H5'	2.10	0.52
5:C:107:GLN:H	5:C:107:GLN:NE2	2.07	0.52
10:H:118:VAL:C	10:H:119:LEU:HD23	2.34	0.52
10:H:123:GLU:O	10:H:126:LYS:HB3	2.09	0.52
11:I:23:ASN:C	11:I:23:ASN:ND2	2.68	0.52
15:M:3:ARG:HA	15:M:8:GLU:O	2.09	0.52
15:M:80:ARG:C	15:M:82:MET:H	2.18	0.52
18:P:51:VAL:CG1	18:P:52:ASP:N	2.73	0.52
21:S:53:ASN:HD21	21:S:58:VAL:HG13	1.75	0.52
1:A:267:C:P	19:Q:67:LYS:HB2	2.50	0.52
1:A:1161:C:H2'	1:A:1162:C:C6	2.44	0.52
1:A:1347:G:C2'	1:A:1348:U:OP2	2.58	0.52
5:C:11:ARG:HG3	5:C:178:LEU:HD12	1.91	0.52
9:G:111:ARG:HB3	9:G:113:GLU:OE2	2.10	0.52
14:L:46:LYS:CG	14:L:47:LYS:H	2.23	0.52
15:M:97:PRO:HB2	15:M:101:GLN:OE1	2.10	0.52
21:S:39:THR:HG22	21:S:40:ILE:O	2.09	0.52
1:A:176:C:H2'	1:A:177:C:H6	1.74	0.51
1:A:1532:U:O2'	1:A:1533:C:H5'	2.10	0.51
3:X:30:G:H2'	3:X:30:G:N3	2.25	0.51
4:B:8:LYS:CD	4:B:9:GLU:N	2.71	0.51
4:B:54:THR:O	4:B:57:PHE:HB3	2.09	0.51
13:K:115:PRO:C	13:K:117:ASN:H	2.18	0.51
15:M:4:ILE:HG22	15:M:5:ALA:N	2.25	0.51
21:S:32:LYS:HA	21:S:50:ALA:O	2.09	0.51
21:S:40:ILE:HG21	21:S:62:ILE:HD13	1.91	0.51
22:T:57:ARG:HH11	22:T:102:GLY:HA3	1.75	0.51
1:A:131:C:H2'	1:A:132:C:C6	2.46	0.51
1:A:179:A:H2'	1:A:180:U:C6	2.46	0.51
1:A:657:G:H4'	17:O:28:GLN:HG2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1525:G:OP1	13:K:120:ARG:NH2	2.43	0.51
4:B:228:GLY:O	4:B:229:VAL:C	2.53	0.51
5:C:191:THR:CG2	5:C:192:THR:N	2.73	0.51
6:D:170:VAL:HG11	6:D:175:SER:HA	1.91	0.51
7:E:57:LYS:HG2	7:E:61:TYR:HE2	1.71	0.51
21:S:30:LEU:O	21:S:31:ILE:HD13	2.11	0.51
22:T:29:LYS:O	22:T:33:ILE:HG13	2.10	0.51
1:A:528:C:H5'	1:A:535:A:N6	2.26	0.51
1:A:975:A:C5'	1:A:976:G:H5'	2.40	0.51
1:A:1042:G:O2'	1:A:1043:C:H5'	2.09	0.51
1:A:1250:A:H4'	11:I:68:GLY:CA	2.40	0.51
4:B:12:GLU:CD	4:B:213:LEU:HD11	2.35	0.51
7:E:33:VAL:HG11	7:E:109:ILE:HA	1.92	0.51
8:F:4:TYR:CZ	8:F:72:VAL:HG21	2.45	0.51
1:A:748:C:O2'	1:A:749:C:H6	1.92	0.51
7:E:51:VAL:O	7:E:55:VAL:HG23	2.11	0.51
10:H:65:TYR:HA	10:H:79:VAL:HG23	1.92	0.51
10:H:103:VAL:HG21	10:H:110:ALA:HB2	1.91	0.51
12:J:19:SER:OG	12:J:91:PRO:HB3	2.11	0.51
15:M:110:ARG:HG2	15:M:110:ARG:HH11	1.76	0.51
17:O:66:LEU:O	17:O:69:TYR:HB3	2.10	0.51
1:A:258:G:O2'	1:A:259:G:H5'	2.11	0.51
1:A:920:U:H2'	1:A:921:U:C6	2.46	0.51
1:A:1320:C:H41	21:S:37:ARG:HH11	1.59	0.51
7:E:83:GLU:HG2	7:E:88:LYS:HD2	1.93	0.51
7:E:110:LEU:HD13	7:E:118:ILE:HG21	1.93	0.51
12:J:5:ARG:O	12:J:98:ILE:HA	2.10	0.51
13:K:77:MET:HE3	13:K:80:VAL:CG1	2.40	0.51
14:L:85:ILE:CG2	14:L:98:TYR:HB3	2.40	0.51
14:L:126:LYS:HD2	14:L:126:LYS:N	2.26	0.51
15:M:62:ASN:O	15:M:63:THR:CB	2.59	0.51
1:A:195:A:H4'	22:T:68:LYS:HE2	1.91	0.51
1:A:689:C:P	13:K:46:GLY:HA3	2.50	0.51
1:A:1206:G:H1'	5:C:193:TYR:O	2.11	0.51
4:B:118:LEU:CB	4:B:142:LEU:HD12	2.41	0.51
6:D:17:VAL:HG12	6:D:18:LYS:N	2.25	0.51
11:I:5:TYR:C	11:I:5:TYR:CD1	2.89	0.51
15:M:5:ALA:CB	15:M:22:ILE:HD13	2.41	0.51
15:M:82:MET:HE3	15:M:92:HIS:CB	2.41	0.51
16:N:27:CYS:SG	16:N:29:ARG:HB2	2.50	0.51
22:T:57:ARG:NH2	22:T:100:ILE:HG21	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:T:94:ALA:O	22:T:95:ALA:HB3	2.09	0.51
1:A:622:A:H2'	1:A:623:C:H5'	1.93	0.51
1:A:969:A:H61	15:M:126:LYS:HB3	1.74	0.51
1:A:1028:C:H2'	1:A:1029:C:C6	2.45	0.51
1:A:1140:C:H2'	1:A:1141:C:C6	2.46	0.51
1:A:1221:G:H4'	21:S:53:ASN:O	2.11	0.51
1:A:1327:C:O2'	1:A:1328:C:H5'	2.11	0.51
4:B:42:ILE:HD12	4:B:203:GLY:HA2	1.92	0.51
5:C:25:GLY:C	5:C:27:LYS:H	2.19	0.51
5:C:60:ALA:O	5:C:61:ALA:CB	2.57	0.51
11:I:55:ALA:O	11:I:56:LEU:HB3	2.10	0.51
1:A:620:C:C1'	6:D:135:LEU:HD13	2.41	0.51
1:A:818:G:C2'	1:A:819:A:H5''	2.40	0.51
4:B:21:ARG:HH11	4:B:21:ARG:HG3	1.75	0.51
4:B:84:GLU:OE1	4:B:216:SER:HA	2.11	0.51
5:C:10:PHE:O	5:C:178:LEU:HD11	2.11	0.51
6:D:61:LYS:HD2	6:D:207:TYR:OH	2.11	0.51
7:E:100:VAL:O	7:E:107:ARG:NH2	2.43	0.51
12:J:80:LYS:HA	12:J:83:GLU:OE2	2.10	0.51
14:L:46:LYS:CG	14:L:47:LYS:N	2.70	0.51
16:N:36:PHE:O	16:N:36:PHE:CD1	2.63	0.51
18:P:4:ILE:HG23	18:P:36:ILE:HD11	1.92	0.51
1:A:377:G:OP1	18:P:3:LYS:HD3	2.10	0.51
1:A:403:C:O3'	6:D:122:ARG:HD2	2.11	0.51
1:A:501:C:H2'	1:A:502:G:C8	2.45	0.51
1:A:1221:G:O3'	21:S:77:THR:HG21	2.10	0.51
1:A:1306:A:N6	1:A:1331:G:H1'	2.25	0.51
4:B:16:HIS:HE2	4:B:214:ILE:HG12	1.76	0.51
5:C:134:ILE:CG2	5:C:168:ALA:HB3	2.41	0.51
7:E:12:LEU:HD13	7:E:31:LEU:HB2	1.92	0.51
10:H:51:VAL:HG11	10:H:60:ARG:NH1	2.26	0.51
11:I:10:ARG:O	11:I:11:LYS:C	2.53	0.51
15:M:8:GLU:C	15:M:9:ILE:HD12	2.36	0.51
15:M:34:LEU:HD13	15:M:41:PRO:HA	1.93	0.51
22:T:10:LEU:O	22:T:12:ALA:N	2.43	0.51
23:V:5:ASP:O	23:V:11:GLY:HA3	2.10	0.51
1:A:883:C:O2'	1:A:884:U:H5'	2.11	0.51
1:A:1041:A:H2'	1:A:1042:G:H8	1.76	0.51
1:A:1256:A:O3'	1:A:1257:U:H4'	2.11	0.51
4:B:189:ASP:OD1	4:B:205:ASP:HB3	2.11	0.51
5:C:154:SER:O	5:C:165:THR:HA	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:539:A:H2'	1:A:540:G:H8	1.75	0.50
11:I:8:GLY:HA2	11:I:79:LEU:CD1	2.40	0.50
13:K:33:THR:HB	13:K:38:ASN:C	2.36	0.50
21:S:63:THR:CB	21:S:66:MET:HE3	2.41	0.50
1:A:1300:G:HO2'	1:A:1301:U:H6	1.54	0.50
4:B:23:ARG:HD3	4:B:24:TRP:N	2.26	0.50
4:B:211:ILE:O	4:B:215:LEU:HB2	2.10	0.50
11:I:46:ALA:HB2	11:I:74:ILE:CG2	2.38	0.50
11:I:75:ASP:O	11:I:78:LYS:HB3	2.11	0.50
12:J:31:GLY:HA2	12:J:78:ASN:HD22	1.70	0.50
22:T:67:ALA:O	22:T:73:HIS:ND1	2.44	0.50
1:A:244:U:O4	1:A:906:G:H1'	2.11	0.50
1:A:279:A:H5''	1:A:280:C:H3'	1.91	0.50
1:A:332:G:O2'	1:A:333:G:H5'	2.11	0.50
4:B:77:ALA:HB2	4:B:211:ILE:CD1	2.35	0.50
4:B:213:LEU:HD23	4:B:213:LEU:C	2.36	0.50
5:C:179:ARG:HD3	5:C:206:GLU:HG2	1.92	0.50
7:E:41:VAL:HG21	7:E:113:ALA:CB	2.42	0.50
7:E:81:GLU:HG2	7:E:90:VAL:HG22	1.92	0.50
12:J:5:ARG:HB3	12:J:99:LYS:O	2.12	0.50
14:L:50:SER:O	14:L:51:ALA:HB2	2.10	0.50
1:A:384:G:H2'	1:A:385:C:H6	1.75	0.50
1:A:392:G:H2'	1:A:393:A:C8	2.46	0.50
1:A:407:G:H2'	1:A:408:A:C8	2.46	0.50
1:A:665:A:N3	1:A:732:C:H2'	2.27	0.50
1:A:1053:G:H4'	1:A:1054:C:H5'	1.94	0.50
4:B:80:ILE:HD11	4:B:208:ILE:CG2	2.41	0.50
9:G:23:VAL:O	9:G:27:ILE:HG13	2.11	0.50
11:I:93:ARG:O	11:I:95:LYS:N	2.45	0.50
12:J:89:ASP:HB2	12:J:91:PRO:HD2	1.91	0.50
1:A:474:G:H2'	1:A:475:G:H8	1.76	0.50
1:A:560:U:H5'	1:A:566:G:N2	2.27	0.50
1:A:1128:C:H5'	11:I:16:ARG:NH2	2.27	0.50
7:E:121:LYS:HE3	7:E:123:LEU:CD2	2.42	0.50
9:G:122:HIS:HA	9:G:125:MET:HE3	1.93	0.50
12:J:16:LEU:O	12:J:17:ASP:C	2.55	0.50
19:Q:66:SER:O	19:Q:70:ARG:NH1	2.45	0.50
1:A:547:A:H4'	1:A:548:G:O5'	2.11	0.50
1:A:624:C:H2'	1:A:625:G:H8	1.77	0.50
1:A:1222:G:P	21:S:77:THR:HG21	2.52	0.50
4:B:13:ALA:HA	4:B:17:PHE:HD2	1.74	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:70:ILE:HD11	6:D:100:ARG:CD	2.42	0.50
6:D:70:ILE:HG22	6:D:71:SER:O	2.12	0.50
8:F:30:LEU:HD23	8:F:75:LEU:HD21	1.92	0.50
14:L:27:LEU:HG	14:L:28:LYS:H	1.77	0.50
17:O:87:ILE:HG22	17:O:88:ARG:N	2.26	0.50
1:A:560:U:O2'	1:A:561:U:OP2	2.24	0.50
1:A:1386:G:O2'	1:A:1387:G:H5'	2.12	0.50
4:B:80:ILE:HD11	4:B:208:ILE:HG22	1.94	0.50
5:C:70:VAL:CG1	5:C:71:ALA:N	2.74	0.50
11:I:26:VAL:HG13	11:I:61:ALA:HB3	1.93	0.50
14:L:114:LYS:NZ	14:L:125:PRO:HG3	2.26	0.50
1:A:532:A:H2	1:A:1207:G:H4'	1.76	0.50
5:C:55:VAL:O	5:C:55:VAL:HG12	2.11	0.50
5:C:84:ILE:O	5:C:88:ARG:HG3	2.11	0.50
5:C:148:GLY:O	5:C:149:ALA:HB2	2.09	0.50
8:F:73:ASN:O	8:F:77:ARG:HG3	2.11	0.50
9:G:32:ARG:O	9:G:33:ASP:HB2	2.11	0.50
12:J:55:LYS:HG3	12:J:56:HIS:N	2.27	0.50
12:J:79:ARG:HG2	12:J:79:ARG:HH11	1.75	0.50
21:S:17:GLU:HA	21:S:20:LEU:CG	2.40	0.50
1:A:586:C:O3'	10:H:89:PRO:HB2	2.12	0.50
5:C:61:ALA:C	5:C:63:ASN:H	2.19	0.50
7:E:37:ARG:HG2	7:E:37:ARG:HH11	1.77	0.50
7:E:41:VAL:CG2	7:E:113:ALA:HA	2.38	0.50
7:E:53:LEU:O	7:E:57:LYS:HB2	2.12	0.50
15:M:3:ARG:HG2	15:M:9:ILE:CG1	2.37	0.50
15:M:84:ILE:O	15:M:85:GLY:C	2.55	0.50
1:A:1316:G:H5''	16:N:17:LYS:HD2	1.94	0.49
1:A:1404:C:H2'	1:A:1405:G:C8	2.47	0.49
10:H:60:ARG:NH1	10:H:60:ARG:HG3	2.27	0.49
12:J:80:LYS:O	12:J:83:GLU:HB2	2.12	0.49
1:A:141:A:O2'	1:A:142:G:H5'	2.12	0.49
1:A:552:U:O2	14:L:31:PRO:HB3	2.12	0.49
6:D:187:ARG:HG3	6:D:188:LEU:N	2.27	0.49
6:D:199:ASN:ND2	6:D:201:GLN:H	2.09	0.49
8:F:22:GLU:OE1	8:F:25:ILE:HD12	2.12	0.49
10:H:6:ILE:HD12	10:H:35:ILE:HD12	1.93	0.49
10:H:68:ARG:HG2	10:H:68:ARG:HH11	1.76	0.49
13:K:77:MET:HE3	13:K:80:VAL:HG12	1.94	0.49
15:M:44:ARG:HB3	15:M:46:LYS:HG3	1.94	0.49
19:Q:86:GLU:O	19:Q:87:LYS:C	2.54	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:G:H2'	1:A:42:G:C8	2.47	0.49
1:A:407:G:H2'	1:A:408:A:H8	1.77	0.49
1:A:1143:G:H2'	1:A:1144:G:C8	2.48	0.49
7:E:6:PHE:HE2	7:E:36:ASP:HB3	1.77	0.49
17:O:82:ILE:HD13	17:O:88:ARG:HG3	1.94	0.49
18:P:8:ARG:HB2	18:P:28:ARG:NH1	2.27	0.49
18:P:31:LYS:NZ	18:P:31:LYS:HB3	2.27	0.49
1:A:57:G:H2'	1:A:58:C:C6	2.46	0.49
1:A:782:A:H2'	1:A:783:C:O4'	2.12	0.49
1:A:1412:C:H2'	1:A:1413:A:C8	2.48	0.49
6:D:6:GLY:O	6:D:8:VAL:HG23	2.11	0.49
9:G:136:LYS:O	9:G:139:GLU:N	2.45	0.49
10:H:20:TYR:CE2	10:H:75:ARG:HD2	2.48	0.49
14:L:115:LYS:C	14:L:117:ARG:H	2.20	0.49
16:N:9:LYS:HE2	16:N:22:THR:O	2.12	0.49
19:Q:45:HIS:HB3	19:Q:72:ARG:HG2	1.93	0.49
21:S:53:ASN:HD22	21:S:53:ASN:N	2.07	0.49
1:A:375:U:O2	18:P:28:ARG:NE	2.39	0.49
1:A:530:G:H1'	3:X:35:U:O2'	2.12	0.49
1:A:794:A:H2'	1:A:795:C:C6	2.47	0.49
1:A:1080:A:O3'	7:E:16:THR:OG1	2.30	0.49
1:A:1196:U:H5''	1:A:1197:G:C5'	2.40	0.49
1:A:1296:C:H5''	15:M:14:ARG:HD2	1.94	0.49
1:A:1317:C:OP1	16:N:17:LYS:HG2	2.12	0.49
4:B:18:GLY:CA	4:B:41:ILE:HA	2.32	0.49
5:C:58:GLU:O	5:C:64:VAL:HA	2.12	0.49
5:C:70:VAL:CG1	5:C:71:ALA:H	2.26	0.49
6:D:196:LEU:CD2	6:D:197:PRO:HD2	2.43	0.49
11:I:10:ARG:HD2	11:I:105:ASP:HB3	1.95	0.49
12:J:45:ARG:O	12:J:64:GLU:HA	2.13	0.49
1:A:302:G:H5''	14:L:17:LYS:HZ1	1.78	0.49
1:A:518:C:H2'	1:A:530:G:C2	2.47	0.49
1:A:1027:C:H3'	1:A:1028:C:H5''	1.92	0.49
4:B:178:ARG:O	10:H:71:GLY:HA2	2.11	0.49
11:I:10:ARG:HG2	11:I:75:ASP:HB2	1.94	0.49
18:P:20:VAL:CG1	18:P:21:VAL:N	2.76	0.49
20:R:47:THR:HG23	20:R:83:GLU:O	2.12	0.49
1:A:8:A:N6	6:D:209:ARG:HB2	2.27	0.49
1:A:26:A:N6	1:A:558:G:H1'	2.27	0.49
1:A:513:C:H2'	1:A:514:C:H6	1.78	0.49
1:A:838:G:C2'	1:A:839:U:H5''	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:77:ILE:CD1	5:C:84:ILE:HD12	2.43	0.49
6:D:55:ALA:O	6:D:59:ARG:HG2	2.12	0.49
8:F:19:LEU:O	8:F:19:LEU:HD23	2.12	0.49
10:H:119:LEU:HD12	10:H:124:ALA:N	2.27	0.49
11:I:28:VAL:HG22	11:I:63:ILE:HB	1.95	0.49
14:L:41:ARG:CG	14:L:42:THR:H	2.11	0.49
1:A:1360:A:H2'	1:A:1361:G:C8	2.48	0.49
5:C:52:LEU:H	5:C:52:LEU:CD2	2.23	0.49
5:C:139:GLN:O	5:C:143:GLU:N	2.46	0.49
7:E:12:LEU:HD22	7:E:12:LEU:C	2.37	0.49
7:E:80:ILE:CD1	7:E:91:LEU:HD12	2.41	0.49
8:F:99:ALA:O	8:F:100:ASN:HB3	2.11	0.49
15:M:36:LYS:HD2	15:M:59:TYR:OH	2.12	0.49
17:O:22:THR:O	17:O:27:VAL:HG11	2.13	0.49
19:Q:68:ARG:O	19:Q:68:ARG:CG	2.61	0.49
1:A:83:U:H2'	1:A:84:U:C6	2.48	0.49
1:A:707:C:H4'	13:K:20:TYR:CD1	2.48	0.49
1:A:1019:C:H2'	1:A:1020:U:C6	2.48	0.49
4:B:73:THR:HG23	4:B:95:GLN:O	2.13	0.49
5:C:191:THR:HG21	5:C:193:TYR:CE2	2.46	0.49
7:E:93:PRO:HG2	10:H:105:ARG:HH21	1.78	0.49
9:G:58:PRO:HG2	9:G:59:LEU:H	1.78	0.49
12:J:51:ARG:HG3	12:J:59:SER:HB3	1.94	0.49
13:K:91:ARG:HH11	20:R:88:LYS:NZ	2.08	0.49
15:M:40:ASN:HD22	15:M:41:PRO:N	2.11	0.49
1:A:972:C:C4'	12:J:57:LYS:HG2	2.23	0.49
2:W:3:A:C2'	2:W:4:A:H5'	2.42	0.49
4:B:137:ARG:HB3	4:B:137:ARG:HH11	1.78	0.49
5:C:30:ARG:HG2	5:C:30:ARG:NH1	2.26	0.49
6:D:8:VAL:C	6:D:10:ARG:N	2.70	0.49
11:I:42:ARG:O	11:I:43:ALA:C	2.56	0.49
15:M:98:VAL:O	15:M:98:VAL:HG12	2.13	0.49
16:N:9:LYS:HD3	16:N:9:LYS:O	2.12	0.49
19:Q:67:LYS:CA	19:Q:70:ARG:HH12	2.24	0.49
21:S:13:ASP:O	21:S:14:HIS:C	2.56	0.49
21:S:15:LEU:O	21:S:19:VAL:N	2.45	0.49
1:A:191:G:N2	22:T:85:MET:HE1	2.28	0.48
1:A:532:A:H5''	5:C:161:GLU:OE1	2.13	0.48
1:A:935:A:O2'	1:A:1383:C:N3	2.45	0.48
1:A:1130:A:OP2	1:A:1130:A:H3'	2.12	0.48
1:A:1342:C:O2'	1:A:1343:G:H5'	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:164:VAL:HG21	4:B:170:GLU:HB3	1.94	0.48
5:C:99:VAL:HG22	5:C:100:ALA:N	2.28	0.48
7:E:72:GLN:O	7:E:73:ASN:CB	2.61	0.48
11:I:19:LEU:HB3	11:I:59:PHE:CD2	2.48	0.48
1:A:163:C:O2'	1:A:164:U:H5'	2.13	0.48
1:A:662:G:O2'	1:A:836:G:H5'	2.13	0.48
1:A:865:A:H2'	1:A:866:C:C6	2.48	0.48
1:A:996:A:H2'	1:A:997:U:C6	2.48	0.48
1:A:1291:G:O2'	11:I:38:GLN:HB3	2.13	0.48
1:A:1460:A:H2'	1:A:1461:G:O4'	2.13	0.48
4:B:23:ARG:O	4:B:24:TRP:O	2.31	0.48
5:C:34:LEU:HD11	5:C:38:ARG:NH2	2.29	0.48
9:G:78:ARG:HB2	9:G:156:TRP:CZ3	2.48	0.48
9:G:125:MET:O	9:G:129:GLU:HG2	2.13	0.48
12:J:14:LYS:C	12:J:16:LEU:N	2.68	0.48
21:S:20:LEU:HA	21:S:23:ASN:HD22	1.79	0.48
1:A:84:U:H2'	1:A:88:A:C8	2.49	0.48
1:A:924:C:H5'	1:A:1399:C:OP2	2.13	0.48
6:D:7:PRO:HG2	6:D:10:ARG:HD2	1.94	0.48
6:D:148:VAL:HG11	6:D:158:ILE:HD13	1.95	0.48
7:E:37:ARG:HG2	7:E:37:ARG:NH1	2.28	0.48
10:H:10:LEU:CD2	10:H:83:ILE:HD11	2.37	0.48
13:K:51:LYS:C	13:K:51:LYS:HD3	2.38	0.48
18:P:39:TYR:CE2	18:P:41:PRO:HG3	2.47	0.48
20:R:87:ARG:O	20:R:88:LYS:HB3	2.13	0.48
21:S:4:SER:O	21:S:5:LEU:HG	2.13	0.48
1:A:41:G:H2'	1:A:42:G:H8	1.77	0.48
1:A:399:G:H2'	1:A:400:C:C6	2.48	0.48
1:A:403:C:O2'	1:A:404:U:H5'	2.12	0.48
1:A:498:U:O2'	1:A:499:A:H5'	2.13	0.48
1:A:542:G:OP1	6:D:10:ARG:NH2	2.46	0.48
1:A:942:G:H2'	1:A:943:U:H6	1.77	0.48
1:A:1194:U:H2'	1:A:1195:C:C6	2.48	0.48
1:A:1347:G:HO2'	1:A:1348:U:H6	1.58	0.48
1:A:1425:U:H2'	1:A:1426:C:H6	1.76	0.48
4:B:118:LEU:C	4:B:120:ALA:N	2.70	0.48
5:C:150:LYS:HB2	5:C:169:ALA:HB2	1.95	0.48
7:E:13:ILE:O	7:E:13:ILE:HG13	2.13	0.48
7:E:15:ARG:O	7:E:15:ARG:HD2	2.14	0.48
17:O:14:GLU:HG3	17:O:15:PHE:CE1	2.48	0.48
17:O:25:THR:CG2	17:O:70:LEU:HD23	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:G:H21	1:A:354:G:C5'	2.24	0.48
1:A:192:U:H1'	22:T:103:GLY:HA2	1.95	0.48
1:A:337:C:H2'	1:A:338:A:H8	1.78	0.48
1:A:575:G:OP1	1:A:575:G:H4'	2.13	0.48
1:A:840:C:H4'	1:A:841:U:O5'	2.13	0.48
1:A:1060:C:O2'	1:A:1061:G:H5'	2.14	0.48
1:A:1137:C:H4'	1:A:1138:G:N1	2.27	0.48
4:B:100:GLY:O	4:B:104:ASN:N	2.41	0.48
7:E:11:ILE:HG12	7:E:33:VAL:HG23	1.95	0.48
10:H:4:ASP:C	10:H:4:ASP:OD1	2.55	0.48
16:N:14:PRO:O	16:N:15:LYS:HB2	2.14	0.48
20:R:25:THR:O	20:R:26:LEU:HB2	2.13	0.48
1:A:1343:G:O2'	1:A:1344:C:H5'	2.14	0.48
14:L:53:ARG:CG	14:L:69:TYR:HE1	2.26	0.48
15:M:2:ALA:HB3	15:M:53:VAL:HG11	1.95	0.48
23:V:2:GLY:O	23:V:4:GLY:N	2.47	0.48
1:A:74:C:C2'	1:A:75:G:H5'	2.42	0.48
1:A:481:G:O2'	1:A:482:A:N7	2.34	0.48
1:A:1053:G:O2'	1:A:1199:U:H5	1.96	0.48
1:A:1238:A:H5'	1:A:1336:C:N4	2.26	0.48
5:C:39:ILE:HG22	5:C:40:ARG:N	2.28	0.48
9:G:135:VAL:O	9:G:139:GLU:HG3	2.13	0.48
10:H:60:ARG:HG3	10:H:60:ARG:HH11	1.79	0.48
14:L:117:ARG:NH2	14:L:124:LYS:HA	2.29	0.48
17:O:3:ILE:HD11	17:O:38:ARG:HG3	1.96	0.48
17:O:87:ILE:HG22	17:O:88:ARG:HG2	1.95	0.48
21:S:19:VAL:HG13	21:S:20:LEU:N	2.29	0.48
22:T:72:LEU:HD13	22:T:77:ALA:HA	1.96	0.48
1:A:107:G:H2'	1:A:108:G:H5'	1.96	0.48
1:A:136:C:H2'	1:A:137:C:H6	1.79	0.48
1:A:975:A:C4'	1:A:976:G:H5'	2.42	0.48
4:B:124:SER:HB2	4:B:125:PRO:CD	2.40	0.48
5:C:50:ALA:HB1	5:C:70:VAL:HG11	1.96	0.48
5:C:150:LYS:HB3	5:C:169:ALA:CB	2.44	0.48
12:J:64:GLU:HG2	16:N:59:ALA:HB2	1.95	0.48
15:M:14:ARG:NH1	15:M:16:ASP:OD1	2.47	0.48
15:M:78:ILE:HA	15:M:81:LEU:HD21	1.95	0.48
21:S:71:LEU:HD12	21:S:71:LEU:N	2.29	0.48
1:A:255:G:H1'	19:Q:16:GLN:NE2	2.28	0.48
1:A:939:G:H5''	9:G:102:ARG:HH22	1.74	0.48
1:A:1152:A:H2'	1:A:1153:C:C6	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1251:A:H2'	1:A:1252:A:H8	1.79	0.48
4:B:15:VAL:HG21	4:B:213:LEU:HD13	1.95	0.48
4:B:30:ARG:HG2	4:B:31:TYR:CD1	2.48	0.48
6:D:72:GLU:OE2	6:D:72:GLU:HA	2.13	0.48
9:G:92:SER:O	9:G:96:GLN:HB2	2.14	0.48
10:H:53:VAL:C	10:H:55:GLY:N	2.70	0.48
13:K:51:LYS:HD3	13:K:51:LYS:O	2.14	0.48
1:A:262:A:C6	1:A:263:A:C6	3.01	0.48
1:A:393:A:O2'	1:A:394:G:H5'	2.14	0.48
1:A:485:G:O2'	1:A:486:U:H5	1.95	0.48
1:A:828:A:H2'	1:A:829:G:O4'	2.13	0.48
1:A:1195:C:H2'	1:A:1197:G:H5'	1.96	0.48
5:C:30:ARG:HG2	5:C:30:ARG:HH11	1.78	0.48
6:D:30:LYS:O	6:D:32:ALA:N	2.47	0.48
6:D:31:CYS:C	6:D:33:MET:H	2.21	0.48
6:D:80:GLU:O	6:D:84:LYS:HG3	2.14	0.48
6:D:126:ILE:HG22	6:D:127:THR:N	2.28	0.48
10:H:86:ILE:HD12	10:H:133:LEU:HD22	1.96	0.48
12:J:72:VAL:HG12	12:J:73:ASP:N	2.29	0.48
13:K:36:ASP:C	13:K:36:ASP:OD2	2.57	0.48
18:P:20:VAL:CG1	18:P:32:TYR:CB	2.85	0.48
21:S:80:TYR:O	21:S:81:ARG:HB3	2.14	0.48
1:A:849:C:O2'	1:A:850:U:H5'	2.13	0.47
1:A:895:G:H2'	1:A:896:C:C6	2.48	0.47
1:A:1010:G:H2'	1:A:1011:G:H8	1.79	0.47
1:A:1326:C:OP1	23:V:12:LYS:NZ	2.45	0.47
4:B:178:ARG:HH22	10:H:74:PRO:HB3	1.79	0.47
12:J:5:ARG:CD	12:J:99:LYS:HB2	2.43	0.47
12:J:61:GLU:OE1	16:N:45:ARG:NH1	2.40	0.47
14:L:8:ASN:O	14:L:12:ARG:HG3	2.14	0.47
22:T:50:GLU:HB2	22:T:99:LEU:HD12	1.96	0.47
1:A:102:G:N3	1:A:151:A:H2	2.12	0.47
1:A:339:C:H2'	1:A:340:U:H6	1.80	0.47
1:A:339:C:H2'	1:A:340:U:C6	2.49	0.47
1:A:448:A:H2'	1:A:449:C:C6	2.48	0.47
1:A:953:G:O2'	1:A:954:G:H5'	2.13	0.47
1:A:1007:C:H2'	1:A:1008:C:C6	2.48	0.47
1:A:1041:A:H2'	1:A:1042:G:C8	2.49	0.47
1:A:1470:G:O2'	1:A:1471:G:H5'	2.14	0.47
4:B:23:ARG:HD3	4:B:23:ARG:C	2.39	0.47
6:D:6:GLY:O	6:D:7:PRO:C	2.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:157:LEU:HD23	6:D:157:LEU:O	2.14	0.47
8:F:91:VAL:HG13	20:R:72:ARG:HH22	1.79	0.47
10:H:111:ILE:O	10:H:134:ILE:HB	2.14	0.47
1:A:180:U:C2'	1:A:181:G:H5'	2.43	0.47
1:A:485:G:O2'	1:A:486:U:C5	2.68	0.47
1:A:895:G:H2'	1:A:896:C:H6	1.79	0.47
1:A:913:A:OP2	14:L:91:LYS:HE3	2.14	0.47
1:A:1363:A:H1'	1:A:1365:G:N7	2.28	0.47
6:D:36:ARG:N	6:D:37:PRO:CD	2.66	0.47
13:K:46:GLY:C	13:K:48:ILE:H	2.22	0.47
14:L:33:ARG:HD2	14:L:33:ARG:HA	1.51	0.47
17:O:70:LEU:HD12	17:O:78:TYR:CB	2.41	0.47
17:O:87:ILE:O	17:O:88:ARG:HB2	2.13	0.47
1:A:67:C:O2'	1:A:171:A:H1'	2.14	0.47
1:A:186:C:H2'	1:A:187:C:C6	2.48	0.47
1:A:864:A:H2'	1:A:865:A:C8	2.50	0.47
1:A:974:A:OP2	16:N:29:ARG:NH2	2.47	0.47
1:A:1285:A:OP1	1:A:1285:A:C8	2.67	0.47
1:A:1372:U:H2'	1:A:1373:G:O4'	2.14	0.47
4:B:82:ARG:O	4:B:86:GLU:HG3	2.15	0.47
9:G:115:ARG:HB2	9:G:118:VAL:CG2	2.43	0.47
12:J:20:ALA:C	12:J:22:LYS:H	2.21	0.47
19:Q:59:ILE:CG2	19:Q:71:PHE:CD1	2.94	0.47
20:R:22:VAL:O	20:R:22:VAL:HG12	2.14	0.47
21:S:33:THR:CG2	21:S:35:SER:H	2.07	0.47
1:A:818:G:C3'	1:A:819:A:H5''	2.44	0.47
4:B:16:HIS:CE1	4:B:214:ILE:HG12	2.49	0.47
5:C:123:GLN:HE22	5:C:140:ARG:HH22	1.57	0.47
5:C:131:ARG:O	5:C:135:LYS:HB2	2.14	0.47
6:D:149:ALA:O	6:D:152:SER:N	2.37	0.47
8:F:50:TYR:CE1	20:R:77:GLY:HA2	2.49	0.47
9:G:121:ALA:HB1	9:G:125:MET:HE2	1.95	0.47
10:H:119:LEU:HD12	10:H:124:ALA:CA	2.45	0.47
11:I:10:ARG:HE	11:I:105:ASP:HB3	1.80	0.47
13:K:13:GLN:HA	13:K:75:TYR:O	2.15	0.47
13:K:15:ALA:O	13:K:77:MET:HA	2.14	0.47
13:K:103:LEU:HD23	13:K:104:GLN:N	2.30	0.47
14:L:28:LYS:O	14:L:29:GLY:C	2.58	0.47
14:L:56:ALA:O	14:L:67:THR:HA	2.15	0.47
1:A:270:A:H2'	1:A:271:C:C6	2.50	0.47
1:A:302:G:H5''	14:L:17:LYS:NZ	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:820:U:H4'	1:A:821:G:OP2	2.15	0.47
1:A:900:A:H2'	1:A:901:A:C8	2.50	0.47
1:A:946:A:H2'	1:A:947:G:H8	1.76	0.47
1:A:1289:A:H2'	1:A:1290:G:H5'	1.97	0.47
1:A:1320:C:C2	21:S:72:GLY:HA3	2.49	0.47
1:A:1392:G:N2	1:A:1502:A:C8	2.81	0.47
1:A:1405:G:P	24:A:1545:PAR:O34	2.73	0.47
4:B:23:ARG:HH11	4:B:24:TRP:CA	2.27	0.47
4:B:206:ASP:CG	4:B:207:ALA:H	2.22	0.47
5:C:3:ASN:C	5:C:4:LYS:HG2	2.38	0.47
5:C:180:ALA:O	5:C:181:ASN:C	2.56	0.47
8:F:2:ARG:CD	8:F:69:GLU:HG2	2.45	0.47
9:G:126:ASP:OD1	9:G:131:LYS:HE3	2.15	0.47
10:H:119:LEU:HD12	10:H:124:ALA:HA	1.97	0.47
12:J:60:ARG:O	12:J:61:GLU:O	2.33	0.47
15:M:40:ASN:HD22	15:M:41:PRO:HD2	1.78	0.47
15:M:118:ALA:HB1	15:M:121:LYS:NZ	2.30	0.47
18:P:17:TYR:HE1	18:P:41:PRO:HG2	1.79	0.47
20:R:53:ARG:HG2	20:R:63:GLN:OE1	2.14	0.47
1:A:383:A:H2'	1:A:384:G:H5'	1.97	0.47
1:A:961:U:C2'	1:A:962:C:H5'	2.44	0.47
1:A:975:A:O2'	1:A:976:G:OP2	2.25	0.47
1:A:1133:G:H2'	1:A:1134:G:C8	2.47	0.47
1:A:1229:A:N6	15:M:105:THR:HG22	2.29	0.47
1:A:1305:G:H22	1:A:1331:G:H2'	1.79	0.47
4:B:23:ARG:NH1	4:B:24:TRP:HA	2.30	0.47
4:B:164:VAL:HG12	4:B:186:ALA:CB	2.44	0.47
5:C:147:LYS:HE2	5:C:205:GLY:N	2.30	0.47
5:C:150:LYS:CB	5:C:169:ALA:HB2	2.45	0.47
6:D:64:LEU:HB2	6:D:198:VAL:HG11	1.95	0.47
8:F:23:LYS:O	8:F:27:GLN:HG2	2.14	0.47
8:F:33:TYR:HB2	8:F:75:LEU:HD23	1.96	0.47
11:I:82:ALA:O	11:I:86:VAL:HG23	2.15	0.47
11:I:112:LYS:HD3	11:I:112:LYS:C	2.40	0.47
12:J:94:VAL:HG12	12:J:95:GLU:H	1.79	0.47
17:O:21:ASP:OD2	17:O:24:SER:HB3	2.15	0.47
18:P:71:ARG:HD3	18:P:75:ARG:HH21	1.80	0.47
21:S:12:ASP:HB3	21:S:14:HIS:CD2	2.49	0.47
21:S:64:GLU:OE2	21:S:67:VAL:HG21	2.15	0.47
22:T:77:ALA:O	22:T:80:ARG:HB2	2.14	0.47
1:A:32:A:H2'	1:A:33:A:C8	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:C:O2'	1:A:292:G:H5'	2.15	0.47
1:A:344:A:O2'	1:A:345:C:OP1	2.31	0.47
1:A:611:A:H2	1:A:630:G:N2	2.13	0.47
1:A:1109:C:OP2	5:C:176:HIS:CD2	2.68	0.47
9:G:145:ALA:O	9:G:146:GLU:C	2.55	0.47
11:I:44:VAL:HG12	11:I:51:ARG:HH22	1.80	0.47
19:Q:82:MET:O	19:Q:83:ASP:C	2.57	0.47
22:T:91:LEU:C	22:T:93:GLU:H	2.22	0.47
23:V:2:GLY:C	23:V:4:GLY:N	2.72	0.47
1:A:190:C:O2	1:A:190:C:O4'	2.33	0.47
1:A:335:C:H2'	1:A:336:C:C6	2.49	0.47
1:A:1011:G:C2'	1:A:1012:U:H5'	2.44	0.47
4:B:101:MET:CA	4:B:108:ILE:HD12	2.44	0.47
4:B:142:LEU:HD23	4:B:142:LEU:C	2.40	0.47
4:B:178:ARG:NH2	10:H:74:PRO:HG3	2.30	0.47
5:C:47:LEU:N	5:C:47:LEU:HD12	2.29	0.47
7:E:149:GLU:O	7:E:153:LYS:HG2	2.15	0.47
9:G:138:LYS:HE2	9:G:142:GLU:OE1	2.14	0.47
12:J:30:SER:HB2	12:J:81:THR:N	2.30	0.47
13:K:82:VAL:HG23	13:K:105:VAL:HG13	1.97	0.47
14:L:26:ALA:O	14:L:27:LEU:O	2.33	0.47
1:A:405:U:O4	6:D:2:GLY:HA3	2.15	0.47
1:A:521:G:OP1	14:L:73:GLU:O	2.33	0.47
1:A:1066:C:C2'	1:A:1067:A:H5'	2.45	0.47
1:A:1505:G:H2'	1:A:1541:U:OP2	2.14	0.47
15:M:67:GLU:HB3	15:M:68:GLY:H	1.52	0.47
1:A:485:G:HO2'	1:A:486:U:H5	1.60	0.46
1:A:674:G:H2'	1:A:675:A:H8	1.79	0.46
1:A:1069:C:O2'	1:A:1192:C:H1'	2.15	0.46
1:A:1176:A:H2'	1:A:1177:G:H8	1.78	0.46
4:B:187:LEU:HD12	4:B:201:ILE:O	2.15	0.46
7:E:11:ILE:CG2	7:E:12:LEU:HD12	2.44	0.46
8:F:40:VAL:CG2	8:F:41:GLU:N	2.79	0.46
8:F:44:GLY:O	8:F:59:TYR:HA	2.16	0.46
11:I:48:GLU:N	11:I:49:PRO:CD	2.78	0.46
22:T:100:ILE:O	22:T:102:GLY:N	2.48	0.46
1:A:722:A:H3'	1:A:722:A:N3	2.29	0.46
1:A:921:U:O2	7:E:19:MET:HB2	2.14	0.46
1:A:1038:C:H2'	1:A:1039:C:C5	2.50	0.46
1:A:1499:A:O2'	1:A:1500:A:H5'	2.14	0.46
4:B:88:ALA:C	4:B:90:MET:H	2.23	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:43:LEU:CD2	5:C:68:VAL:HG21	2.45	0.46
8:F:26:ILE:HG21	8:F:63:TYR:HE2	1.79	0.46
11:I:44:VAL:HG12	11:I:51:ARG:NH2	2.29	0.46
21:S:42:PRO:C	21:S:44:MET:H	2.23	0.46
1:A:8:A:H5'	7:E:101:ILE:HG22	1.96	0.46
1:A:1128:C:H42	1:A:1143:G:H1	1.64	0.46
1:A:1313:U:O4	21:S:4:SER:HB2	2.15	0.46
1:A:1521:G:H2'	1:A:1522:U:H6	1.79	0.46
5:C:43:LEU:O	5:C:47:LEU:HB2	2.16	0.46
15:M:33:ALA:HA	15:M:59:TYR:CE2	2.51	0.46
1:A:190(J):U:O2'	1:A:190(K):G:H5'	2.16	0.46
1:A:200:G:H2'	1:A:201:C:O4'	2.15	0.46
1:A:252:U:H2'	1:A:253:U:C6	2.50	0.46
1:A:647:C:O2'	1:A:648:A:H5'	2.14	0.46
1:A:833:U:H2'	1:A:834:C:C6	2.50	0.46
1:A:1124:G:H3'	1:A:1145:C:C4	2.49	0.46
1:A:1141:C:H2'	1:A:1142:G:H8	1.81	0.46
5:C:155:GLY:HA2	5:C:164:ARG:H	1.80	0.46
8:F:4:TYR:HD1	8:F:92:LYS:HA	1.80	0.46
11:I:40:LEU:O	11:I:41:VAL:C	2.58	0.46
12:J:26:ALA:HB1	12:J:84:GLN:CB	2.45	0.46
1:A:692:U:H2'	1:A:694:A:OP2	2.16	0.46
1:A:1203:C:O2'	1:A:1204:A:H5'	2.16	0.46
1:A:1544:U:O3'	2:W:1:A:O5'	2.31	0.46
5:C:18:TRP:HB3	16:N:51:GLY:O	2.16	0.46
5:C:84:ILE:O	5:C:84:ILE:HG12	2.15	0.46
5:C:111:LEU:HD21	5:C:144:SER:O	2.15	0.46
6:D:32:ALA:C	6:D:34:GLU:N	2.72	0.46
6:D:91:SER:O	6:D:94:LEU:N	2.49	0.46
7:E:48:ALA:HB1	7:E:49:PRO:HD2	1.97	0.46
8:F:9:VAL:HB	8:F:87:ARG:HB2	1.96	0.46
11:I:27:THR:HG23	11:I:30:GLY:O	2.15	0.46
12:J:8:LEU:HD23	12:J:96:ILE:HG12	1.97	0.46
12:J:12:ASP:HB3	12:J:15:THR:CG2	2.45	0.46
12:J:26:ALA:HB1	12:J:84:GLN:HB3	1.97	0.46
15:M:20:THR:C	15:M:22:ILE:H	2.24	0.46
15:M:107:ALA:O	15:M:111:LYS:HG3	2.15	0.46
16:N:23:ARG:HG3	16:N:23:ARG:HH11	1.80	0.46
22:T:50:GLU:HB2	22:T:99:LEU:CD1	2.46	0.46
1:A:97:G:H2'	1:A:98:U:O4'	2.16	0.46
1:A:333:G:H4'	22:T:16:HIS:CD2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:G:H2'	1:A:393:A:H8	1.81	0.46
1:A:1365:G:C6	1:A:1366:C:C4	3.04	0.46
4:B:136:VAL:HG12	4:B:140:HIS:CD2	2.50	0.46
5:C:103:VAL:HG12	5:C:104:GLN:N	2.29	0.46
9:G:15:ASP:OD2	9:G:16:LEU:N	2.48	0.46
15:M:65:LYS:HE3	15:M:69:GLU:OE2	2.15	0.46
15:M:121:LYS:O	15:M:122:LYS:HB2	2.16	0.46
15:M:124:PRO:HB3	15:M:126:LYS:HE3	1.97	0.46
1:A:204:U:H5'	1:A:216:G:OP1	2.15	0.46
1:A:939:G:H5''	9:G:102:ARG:CZ	2.45	0.46
1:A:1263:C:H2'	1:A:1264:C:C6	2.50	0.46
1:A:1287:A:H2'	1:A:1288:A:C8	2.51	0.46
1:A:1307:U:H2'	1:A:1308:U:C6	2.51	0.46
1:A:1451:A:O2'	1:A:1452:C:OP1	2.30	0.46
4:B:7:VAL:CG1	4:B:221:LEU:HD23	2.46	0.46
4:B:16:HIS:HA	4:B:204:ASN:OD1	2.16	0.46
4:B:60:ASP:O	4:B:64:ARG:HB2	2.15	0.46
5:C:134:ILE:O	5:C:138:VAL:HG23	2.16	0.46
6:D:65:ARG:HG3	6:D:75:PHE:CD1	2.51	0.46
7:E:18:ARG:HE	7:E:25:ARG:HB2	1.81	0.46
15:M:125:ARG:HD2	15:M:125:ARG:C	2.41	0.46
16:N:26:ARG:NH1	16:N:47:LEU:HG	2.31	0.46
18:P:53:VAL:HG23	18:P:54:GLU:N	2.30	0.46
19:Q:48:GLU:O	19:Q:50:LYS:N	2.49	0.46
22:T:67:ALA:HA	22:T:73:HIS:H	1.80	0.46
22:T:96:GLY:O	22:T:97:ALA:HB3	2.16	0.46
1:A:415:A:H3'	1:A:416:G:H5''	1.97	0.46
1:A:1260:C:O5'	1:A:1284:C:H4'	2.15	0.46
1:A:1305:G:N2	1:A:1331:G:C2'	2.78	0.46
1:A:1376:U:H2'	1:A:1377:A:C8	2.50	0.46
7:E:32:VAL:HG23	7:E:58:ALA:CB	2.45	0.46
9:G:126:ASP:CG	9:G:131:LYS:HE3	2.40	0.46
10:H:53:VAL:C	10:H:55:GLY:H	2.22	0.46
11:I:28:VAL:HA	11:I:63:ILE:O	2.15	0.46
11:I:93:ARG:C	11:I:95:LYS:N	2.74	0.46
12:J:32:ALA:C	12:J:34:VAL:H	2.23	0.46
13:K:15:ALA:O	13:K:78:GLN:N	2.48	0.46
15:M:40:ASN:C	15:M:40:ASN:ND2	2.74	0.46
21:S:63:THR:HB	21:S:66:MET:HE3	1.97	0.46
1:A:555:C:H2'	1:A:556:C:C6	2.51	0.46
1:A:1054:C:C2'	1:A:1055:A:H5''	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1422:G:O2'	1:A:1423:G:H5'	2.16	0.46
4:B:17:PHE:CB	4:B:44:LEU:HD21	2.41	0.46
4:B:25:ASN:ND2	4:B:27:LYS:H	2.14	0.46
4:B:126:GLU:HA	4:B:129:GLU:OE1	2.16	0.46
6:D:191:ARG:O	6:D:191:ARG:HD2	2.16	0.46
7:E:11:ILE:HG21	7:E:31:LEU:HD12	1.97	0.46
9:G:62:PHE:O	9:G:63:LYS:C	2.58	0.46
10:H:20:TYR:HE2	10:H:75:ARG:HD2	1.79	0.46
10:H:97:VAL:HG21	10:H:128:GLY:HA2	1.98	0.46
13:K:126:ARG:HB3	13:K:126:ARG:HH11	1.80	0.46
15:M:37:THR:O	15:M:55:ARG:NH1	2.43	0.46
18:P:82:GLN:O	18:P:83:GLU:C	2.59	0.46
1:A:960:U:O2	1:A:960:U:H2'	2.16	0.46
1:A:1202:G:C2'	1:A:1203:C:H5'	2.45	0.46
1:A:1248:A:H1'	11:I:70:LYS:NZ	2.30	0.46
4:B:88:ALA:C	4:B:90:MET:N	2.72	0.46
5:C:191:THR:HG22	5:C:193:TYR:H	1.81	0.46
7:E:89:ILE:HD13	7:E:90:VAL:H	1.81	0.46
10:H:107:LEU:HD23	10:H:107:LEU:N	2.30	0.46
13:K:12:ARG:O	13:K:13:GLN:O	2.32	0.46
13:K:74:ALA:C	13:K:76:GLY:H	2.24	0.46
21:S:22:LEU:HD22	21:S:28:LYS:HB2	1.98	0.46
1:A:190(K):G:HO2'	1:A:190(L):U:H6	1.59	0.45
1:A:959:A:H2'	1:A:960:U:O4'	2.16	0.45
1:A:1399:C:C2	1:A:1502:A:N6	2.84	0.45
4:B:76:GLN:OE1	4:B:76:GLN:HA	2.15	0.45
5:C:172:ARG:NH2	5:C:203:PHE:HE2	2.14	0.45
5:C:175:LEU:HD23	5:C:182:ILE:HD13	1.99	0.45
6:D:7:PRO:CB	6:D:10:ARG:HD2	2.46	0.45
6:D:52:SER:C	6:D:54:TYR:N	2.71	0.45
7:E:69:VAL:HG22	7:E:139:LEU:HB3	1.97	0.45
7:E:93:PRO:HG2	10:H:105:ARG:NH2	2.31	0.45
9:G:16:LEU:N	9:G:16:LEU:HD22	2.31	0.45
10:H:90:GLY:O	10:H:91:ARG:HB2	2.15	0.45
12:J:21:GLN:HG2	12:J:21:GLN:O	2.16	0.45
12:J:26:ALA:O	12:J:27:ALA:HB2	2.16	0.45
13:K:110:ASP:HB2	20:R:88:LYS:HZ2	1.81	0.45
13:K:124:LYS:HD3	13:K:125:PHE:CE1	2.51	0.45
18:P:7:ALA:O	18:P:17:TYR:HA	2.16	0.45
1:A:7:G:H21	7:E:121:LYS:HG2	1.82	0.45
1:A:363:A:H62	14:L:28:LYS:HE3	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:G:H2'	1:A:407:G:H8	1.81	0.45
1:A:686:U:O2'	1:A:687:A:C8	2.57	0.45
1:A:840:C:H5'	1:A:848:C:O2	2.16	0.45
1:A:1305:G:O2'	1:A:1306:A:C8	2.47	0.45
4:B:9:GLU:OE2	4:B:12:GLU:HA	2.16	0.45
4:B:95:GLN:HG3	4:B:147:LYS:O	2.16	0.45
5:C:113:ALA:HB3	5:C:114:PRO:HD3	1.98	0.45
5:C:155:GLY:O	5:C:156:ARG:CB	2.64	0.45
6:D:4:TYR:O	6:D:5:ILE:HB	2.15	0.45
7:E:7:GLU:OE2	7:E:37:ARG:NE	2.47	0.45
8:F:40:VAL:HG22	8:F:41:GLU:N	2.31	0.45
8:F:41:GLU:O	8:F:43:LEU:N	2.49	0.45
15:M:80:ARG:C	15:M:82:MET:N	2.73	0.45
21:S:62:ILE:HD12	21:S:66:MET:CG	2.45	0.45
22:T:38:LYS:O	22:T:39:LYS:C	2.59	0.45
1:A:149:A:H2'	1:A:150:C:H6	1.82	0.45
1:A:178:C:O2'	1:A:179:A:H5'	2.16	0.45
1:A:1071:C:H2'	1:A:1072:G:H8	1.82	0.45
1:A:1142:G:H2'	1:A:1143:G:O4'	2.15	0.45
1:A:1305:G:OP2	1:A:1305:G:H8	2.00	0.45
1:A:1323:G:H2'	1:A:1324:A:C8	2.51	0.45
5:C:23:TYR:CG	5:C:24:ALA:N	2.84	0.45
5:C:64:VAL:HG12	5:C:65:ALA:N	2.28	0.45
7:E:11:ILE:HD11	7:E:33:VAL:HG21	1.98	0.45
12:J:60:ARG:HG2	12:J:60:ARG:HH11	1.81	0.45
12:J:71:LEU:O	12:J:72:VAL:CB	2.64	0.45
13:K:51:LYS:O	13:K:55:LYS:HE2	2.16	0.45
20:R:55:ARG:HB3	20:R:55:ARG:CZ	2.45	0.45
21:S:62:ILE:CD1	21:S:66:MET:HG3	2.46	0.45
1:A:105:G:H2'	1:A:106:C:C6	2.51	0.45
1:A:830:G:O2'	1:A:831:U:H5'	2.16	0.45
1:A:1061:G:C2'	1:A:1062:U:H5'	2.47	0.45
1:A:1182:G:C2'	1:A:1183:A:OP2	2.64	0.45
1:A:1407:C:O2'	1:A:1408:A:H5'	2.16	0.45
5:C:6:HIS:HD2	5:C:8:ILE:H	1.65	0.45
6:D:3:ARG:NH1	6:D:70:ILE:HA	2.31	0.45
13:K:33:THR:HB	13:K:38:ASN:O	2.17	0.45
13:K:89:ALA:C	13:K:91:ARG:H	2.24	0.45
21:S:71:LEU:HD12	21:S:71:LEU:H	1.82	0.45
1:A:860:A:H2'	1:A:861:G:O4'	2.17	0.45
1:A:1072:G:H2'	1:A:1073:U:H6	1.77	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1117:G:O3'	11:I:104:ARG:HD2	2.16	0.45
6:D:149:ALA:O	6:D:150:GLU:C	2.59	0.45
6:D:187:ARG:HG3	6:D:188:LEU:H	1.81	0.45
7:E:5:ASP:CG	7:E:6:PHE:N	2.73	0.45
14:L:83:VAL:HG11	14:L:100:ILE:HD13	1.98	0.45
17:O:3:ILE:O	17:O:3:ILE:HG22	2.15	0.45
1:A:671:G:H2'	1:A:672:U:C6	2.52	0.45
1:A:810:C:H2'	1:A:811:C:C6	2.50	0.45
1:A:942:G:H2'	1:A:943:U:C6	2.51	0.45
1:A:1439:C:P	22:T:38:LYS:HZ3	2.39	0.45
4:B:204:ASN:HB2	4:B:210:SER:OG	2.15	0.45
4:B:215:LEU:O	4:B:219:VAL:HG23	2.17	0.45
9:G:78:ARG:NH1	9:G:154:TYR:HB3	2.31	0.45
11:I:13:ALA:CB	11:I:67:GLY:O	2.65	0.45
12:J:9:ARG:NH1	12:J:9:ARG:CB	2.80	0.45
17:O:26:GLU:HA	17:O:81:LEU:HD11	1.98	0.45
18:P:18:ARG:NH1	18:P:32:TYR:OH	2.49	0.45
20:R:38:GLU:OE1	20:R:38:GLU:N	2.38	0.45
20:R:87:ARG:O	20:R:88:LYS:CB	2.64	0.45
22:T:26:ASN:OD1	22:T:71:THR:HA	2.16	0.45
1:A:457:C:H2'	1:A:458:C:H6	1.81	0.45
1:A:474:G:H2'	1:A:475:G:C8	2.52	0.45
1:A:791:G:H2'	1:A:792:A:C5'	2.47	0.45
1:A:953:G:H1'	15:M:125:ARG:HA	1.99	0.45
1:A:1127:G:N2	1:A:1146:A:H62	2.14	0.45
1:A:1251:A:H1'	1:A:1369:C:O2'	2.17	0.45
1:A:1296:C:H5'	1:A:1302:U:O4	2.16	0.45
1:A:1370:G:O2'	1:A:1371:G:H5'	2.16	0.45
1:A:1413:A:C2	1:A:1488:G:C2	3.05	0.45
3:X:34:U:H2'	3:X:35:U:C6	2.51	0.45
4:B:36:ARG:HD2	4:B:41:ILE:CD1	2.47	0.45
9:G:120:ILE:HD12	9:G:120:ILE:N	2.31	0.45
12:J:45:ARG:HH11	12:J:45:ARG:CB	2.18	0.45
14:L:114:LYS:HE2	14:L:114:LYS:HA	1.98	0.45
18:P:43:LYS:HA	18:P:48:TRP:HB3	1.99	0.45
19:Q:98:LEU:H	19:Q:98:LEU:CD1	2.00	0.45
22:T:48:LYS:O	22:T:52:ALA:HB2	2.17	0.45
1:A:176:C:O2'	1:A:177:C:H5'	2.17	0.45
1:A:692:U:O2	1:A:695:A:H8	1.99	0.45
1:A:1183:A:O2'	1:A:1184:G:P	2.75	0.45
4:B:27:LYS:HD3	4:B:195:ASP:OD2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:219:VAL:C	4:B:221:LEU:N	2.74	0.45
5:C:108:ASN:OD1	5:C:110:ASN:HB2	2.17	0.45
7:E:69:VAL:HG21	7:E:139:LEU:HD13	1.99	0.45
8:F:97:PHE:O	8:F:98:LEU:C	2.59	0.45
10:H:117:GLY:O	10:H:119:LEU:HD23	2.17	0.45
13:K:101:SER:C	13:K:103:LEU:N	2.70	0.45
18:P:20:VAL:HG12	18:P:21:VAL:N	2.31	0.45
21:S:15:LEU:HD12	21:S:16:LEU:N	2.32	0.45
1:A:28:G:O2'	1:A:296:U:OP1	2.35	0.45
1:A:255:G:O6	1:A:266:G:O6	2.35	0.45
1:A:701:C:H5''	1:A:702:A:H3'	1.99	0.45
1:A:706:A:H1'	13:K:29:ILE:HD11	1.99	0.45
4:B:54:THR:O	4:B:58:ILE:HG13	2.16	0.45
5:C:167:TRP:O	5:C:168:ALA:HB3	2.17	0.45
9:G:22:LEU:O	9:G:25:ALA:HB3	2.17	0.45
9:G:122:HIS:O	9:G:126:ASP:HB2	2.17	0.45
11:I:9:ARG:HD3	11:I:14:VAL:HG22	1.98	0.45
1:A:248:C:O2'	1:A:249:U:H5'	2.15	0.45
1:A:412:A:H1'	1:A:413:G:C2	2.52	0.45
1:A:1108:G:H4'	1:A:1191:A:O4'	2.16	0.45
4:B:51:LEU:O	4:B:55:PHE:HD1	2.00	0.45
4:B:213:LEU:O	4:B:217:ARG:HG2	2.16	0.45
5:C:6:HIS:CD2	5:C:8:ILE:HB	2.52	0.45
5:C:136:GLN:O	5:C:139:GLN:N	2.50	0.45
6:D:3:ARG:HH22	6:D:74:GLN:CD	2.25	0.45
8:F:91:VAL:CG1	20:R:72:ARG:NH2	2.79	0.45
9:G:85:TYR:CD1	9:G:154:TYR:HE1	2.33	0.45
10:H:8:ASP:O	10:H:12:ARG:HG3	2.17	0.45
11:I:44:VAL:O	11:I:51:ARG:NH2	2.49	0.45
12:J:49:VAL:HG21	16:N:41:ARG:O	2.17	0.45
13:K:121:PRO:HG2	13:K:126:ARG:CG	2.47	0.45
14:L:110:VAL:O	14:L:122:THR:HG21	2.17	0.45
19:Q:24:GLU:OE1	19:Q:39:SER:HB3	2.16	0.45
22:T:74:LYS:HB3	22:T:74:LYS:HE3	1.61	0.45
1:A:251:G:H4'	1:A:252:U:O5'	2.17	0.44
1:A:1423:G:H2'	1:A:1424:C:C6	2.53	0.44
4:B:71:VAL:HG21	4:B:164:VAL:HG23	1.96	0.44
5:C:157:ILE:HG21	5:C:164:ARG:NH2	2.31	0.44
6:D:24:GLU:HG2	6:D:25:ARG:N	2.31	0.44
8:F:67:MET:HB2	8:F:68:PRO:CD	2.47	0.44
11:I:10:ARG:HH11	11:I:10:ARG:CG	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:I:13:ALA:HB1	11:I:67:GLY:O	2.17	0.44
11:I:44:VAL:C	11:I:51:ARG:HH22	2.25	0.44
12:J:15:THR:O	12:J:16:LEU:HD23	2.17	0.44
14:L:102:ARG:HB2	14:L:120:TYR:HA	1.99	0.44
14:L:119:LYS:O	14:L:120:TYR:CB	2.65	0.44
19:Q:27:PHE:CE1	19:Q:36:ILE:HD11	2.52	0.44
1:A:21:G:H2'	1:A:22:G:C8	2.53	0.44
1:A:716:A:N3	13:K:117:ASN:O	2.50	0.44
1:A:738:C:OP2	8:F:92:LYS:CE	2.65	0.44
1:A:925:G:C6	1:A:927:G:N7	2.85	0.44
1:A:1056:U:C5'	5:C:163:ALA:HB2	2.46	0.44
1:A:1125:U:P	1:A:1145:C:H42	2.40	0.44
1:A:1154:G:O2'	1:A:1155:G:H5'	2.17	0.44
1:A:1420:C:H2'	1:A:1421:G:C8	2.50	0.44
6:D:39:PRO:O	6:D:44:GLY:HA3	2.16	0.44
8:F:28:ARG:HG3	8:F:28:ARG:NH1	2.33	0.44
9:G:65:ALA:HB1	9:G:127:ALA:HB3	1.99	0.44
10:H:10:LEU:HD12	10:H:85:ARG:HG2	1.99	0.44
11:I:69:GLY:O	11:I:73:GLN:HG3	2.17	0.44
16:N:36:PHE:HD1	16:N:37:PHE:CE1	2.36	0.44
17:O:62:GLN:OE1	17:O:65:ARG:NH2	2.50	0.44
18:P:43:LYS:HB3	18:P:48:TRP:CD1	2.52	0.44
19:Q:97:SER:HA	19:Q:103:GLY:H	1.82	0.44
21:S:62:ILE:HD12	21:S:63:THR:H	1.82	0.44
1:A:113:G:C1'	1:A:354:G:H5'	2.47	0.44
1:A:190(K):G:O2'	1:A:190(L):U:P	2.75	0.44
1:A:222:U:H2'	1:A:223:U:C6	2.52	0.44
1:A:586:C:C2'	1:A:587:G:H5'	2.47	0.44
1:A:1174:G:O2'	1:A:1175:G:H5'	2.18	0.44
1:A:1197:G:OP1	1:A:1197:G:H3'	2.18	0.44
5:C:134:ILE:HG22	5:C:168:ALA:CB	2.48	0.44
7:E:152:ARG:NH2	10:H:107:LEU:O	2.50	0.44
9:G:45:ASP:O	9:G:49:ILE:HG13	2.17	0.44
9:G:52:GLU:C	9:G:54:THR:N	2.75	0.44
10:H:104:ARG:NH2	10:H:138:TRP:CH2	2.85	0.44
14:L:83:VAL:HG13	14:L:84:LEU:N	2.32	0.44
15:M:5:ALA:O	15:M:7:VAL:N	2.50	0.44
15:M:77:ASN:O	15:M:80:ARG:HB3	2.17	0.44
16:N:41:ARG:HG3	16:N:42:ILE:N	2.32	0.44
19:Q:59:ILE:HG23	19:Q:71:PHE:HB3	1.99	0.44
1:A:1128:C:C4'	11:I:16:ARG:HH12	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1172:C:H2'	1:A:1173:G:C8	2.52	0.44
1:A:1477:C:H2'	1:A:1478:C:C6	2.53	0.44
5:C:33:LEU:CD1	16:N:53:LEU:HD23	2.47	0.44
6:D:8:VAL:HG13	6:D:21:LEU:CD1	2.47	0.44
6:D:31:CYS:O	6:D:32:ALA:HB3	2.18	0.44
12:J:29:ARG:NH1	12:J:84:GLN:OE1	2.50	0.44
12:J:75:ILE:O	12:J:76:ASN:HB2	2.17	0.44
19:Q:15:MET:HE1	19:Q:43:LEU:HD22	1.99	0.44
20:R:87:ARG:HG2	20:R:87:ARG:NH1	2.32	0.44
1:A:56:U:H2'	1:A:57:G:C8	2.53	0.44
1:A:217:C:H2'	1:A:218:C:C6	2.52	0.44
1:A:652:U:C4	1:A:752:G:N3	2.85	0.44
1:A:934:C:C4	1:A:1345:U:C5	3.05	0.44
1:A:1091:U:O2	1:A:1093:A:C8	2.70	0.44
1:A:1141:C:O2'	1:A:1142:G:H5'	2.17	0.44
7:E:43:LEU:H	7:E:136:MET:HE2	1.81	0.44
8:F:91:VAL:CG1	20:R:72:ARG:HH22	2.30	0.44
9:G:52:GLU:C	9:G:54:THR:H	2.24	0.44
11:I:10:ARG:HG2	11:I:10:ARG:HH11	1.83	0.44
13:K:77:MET:CE	13:K:80:VAL:HG12	2.48	0.44
19:Q:67:LYS:O	19:Q:68:ARG:HB3	2.17	0.44
21:S:32:LYS:HG3	21:S:32:LYS:O	2.17	0.44
21:S:33:THR:CG2	21:S:34:TRP:H	2.28	0.44
21:S:64:GLU:O	21:S:67:VAL:HG23	2.17	0.44
1:A:242:C:H2'	1:A:243:A:H5'	2.00	0.44
1:A:390:C:H2'	1:A:391:G:H8	1.78	0.44
1:A:839:U:O2	1:A:839:U:C2'	2.64	0.44
1:A:1454:G:H2'	1:A:1455:G:H8	1.82	0.44
4:B:53:ARG:NH1	4:B:199:TYR:CD2	2.85	0.44
5:C:19:GLU:O	5:C:40:ARG:NH2	2.51	0.44
14:L:28:LYS:O	14:L:28:LYS:HG2	2.17	0.44
15:M:33:ALA:O	15:M:37:THR:HB	2.18	0.44
20:R:59:SER:O	20:R:60:GLY:C	2.59	0.44
21:S:10:PHE:C	21:S:11:VAL:HG23	2.43	0.44
21:S:80:TYR:CD2	21:S:81:ARG:HB2	2.53	0.44
1:A:1014:A:H2'	1:A:1015:A:C8	2.53	0.44
4:B:122:PHE:O	4:B:123:ALA:HB2	2.18	0.44
5:C:180:ALA:CB	5:C:182:ILE:HG13	2.48	0.44
6:D:127:THR:HG21	6:D:147:ALA:HB3	2.00	0.44
8:F:15:ASP:OD1	8:F:17:SER:HB2	2.18	0.44
8:F:75:LEU:C	8:F:75:LEU:HD13	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:141:VAL:O	9:G:144:MET:N	2.50	0.44
13:K:74:ALA:C	13:K:76:GLY:N	2.75	0.44
14:L:41:ARG:HG2	14:L:42:THR:O	2.17	0.44
14:L:76:ASN:O	14:L:76:ASN:CG	2.60	0.44
16:N:11:LYS:HE3	16:N:11:LYS:HB2	1.83	0.44
17:O:17:ARG:NH1	17:O:77:ARG:NH1	2.66	0.44
17:O:45:VAL:HG12	17:O:46:HIS:H	1.82	0.44
20:R:20:ALA:O	20:R:21:LYS:C	2.60	0.44
21:S:53:ASN:N	21:S:53:ASN:ND2	2.66	0.44
22:T:100:ILE:O	22:T:101:GLY:C	2.60	0.44
1:A:674:G:H2'	1:A:675:A:C8	2.53	0.44
1:A:832:C:O2'	1:A:833:U:H5'	2.17	0.44
1:A:1451:A:HO2'	1:A:1452:C:P	2.39	0.44
5:C:107:GLN:O	5:C:108:ASN:CB	2.66	0.44
8:F:99:ALA:C	8:F:101:ALA:H	2.25	0.44
9:G:8:GLU:OE1	9:G:8:GLU:O	2.36	0.44
10:H:51:VAL:HG21	10:H:60:ARG:HH11	1.83	0.44
12:J:23:ILE:HG21	12:J:72:VAL:HG11	1.99	0.44
12:J:60:ARG:O	12:J:61:GLU:HB3	2.18	0.44
13:K:69:ALA:O	13:K:73:MET:HG2	2.17	0.44
14:L:6:THR:OG1	14:L:9:GLN:HG3	2.18	0.44
14:L:41:ARG:HH22	14:L:57:LYS:NZ	2.15	0.44
15:M:84:ILE:CG2	21:S:65:ASN:HD22	2.29	0.44
19:Q:95:TYR:HA	19:Q:98:LEU:HD13	1.98	0.44
22:T:50:GLU:O	22:T:54:LYS:HG3	2.18	0.44
1:A:865:A:O2'	1:A:866:C:H5'	2.17	0.44
1:A:1053:G:C3'	1:A:1054:C:C5'	2.94	0.44
1:A:1202:G:H2'	1:A:1203:C:H5'	1.99	0.44
1:A:1234:C:O2'	1:A:1235:U:H5'	2.18	0.44
1:A:1354:C:O2'	1:A:1355:G:H5'	2.17	0.44
1:A:1375:A:P	9:G:28:ASN:HD22	2.40	0.44
4:B:107:THR:C	4:B:109:SER:N	2.74	0.44
4:B:162:ILE:HD12	4:B:177:ALA:HB2	2.00	0.44
5:C:61:ALA:O	5:C:62:ASP:HB2	2.17	0.44
5:C:139:GLN:O	5:C:140:ARG:C	2.60	0.44
6:D:7:PRO:CG	6:D:10:ARG:HD2	2.48	0.44
8:F:82:ARG:HA	8:F:82:ARG:HE	1.83	0.44
11:I:19:LEU:HB3	11:I:59:PHE:HD2	1.83	0.44
18:P:55:ARG:O	18:P:56:ALA:C	2.59	0.44
19:Q:95:TYR:HA	19:Q:98:LEU:CD1	2.48	0.44
1:A:328:C:O2'	1:A:329:A:OP2	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:584:G:H2'	1:A:585:G:C8	2.53	0.43
1:A:609:A:C2'	1:A:610:G:H5'	2.48	0.43
2:W:3:A:O2'	2:W:4:A:H5'	2.18	0.43
4:B:70:PHE:CD2	4:B:215:LEU:HD21	2.53	0.43
4:B:102:LEU:N	4:B:102:LEU:CD1	2.81	0.43
4:B:200:ILE:HG22	4:B:202:PRO:HD3	1.99	0.43
5:C:136:GLN:O	5:C:137:ALA:C	2.61	0.43
8:F:82:ARG:HB2	8:F:85:VAL:CG2	2.48	0.43
12:J:85:LEU:O	12:J:87:THR:N	2.50	0.43
14:L:53:ARG:HG3	14:L:69:TYR:HE1	1.82	0.43
14:L:89:ARG:NH2	14:L:97:ARG:HD2	2.33	0.43
18:P:26:ARG:O	18:P:27:LYS:C	2.60	0.43
20:R:53:ARG:C	20:R:55:ARG:N	2.74	0.43
20:R:53:ARG:NH1	20:R:60:GLY:N	2.65	0.43
1:A:334:C:H2'	1:A:335:C:C6	2.53	0.43
1:A:1061:G:H1'	12:J:56:HIS:CE1	2.53	0.43
1:A:1152:A:O2'	1:A:1153:C:H5'	2.18	0.43
1:A:1313:U:O4	21:S:4:SER:CB	2.67	0.43
4:B:19:HIS:CD2	4:B:204:ASN:HA	2.53	0.43
4:B:62:ALA:C	4:B:64:ARG:N	2.71	0.43
4:B:132:LYS:O	4:B:136:VAL:HG23	2.17	0.43
7:E:28:PHE:O	7:E:47:LYS:HA	2.18	0.43
10:H:104:ARG:O	10:H:105:ARG:C	2.60	0.43
11:I:112:LYS:HD3	11:I:112:LYS:O	2.17	0.43
12:J:94:VAL:HG12	12:J:95:GLU:O	2.18	0.43
15:M:13:LYS:O	15:M:14:ARG:C	2.61	0.43
19:Q:27:PHE:HB2	19:Q:28:PRO:CD	2.44	0.43
20:R:34:TYR:HA	20:R:69:THR:HG23	1.99	0.43
1:A:22:G:H2'	1:A:23:C:C6	2.53	0.43
1:A:528:C:H41	14:L:49:ASN:ND2	2.17	0.43
1:A:757:U:H2'	1:A:758:G:O4'	2.17	0.43
1:A:1300:G:O2'	1:A:1301:U:H6	2.01	0.43
1:A:1330:U:OP1	15:M:23:TYR:O	2.35	0.43
3:X:36:U:H2'	3:X:37:T6A:H5'	2.00	0.43
4:B:8:LYS:HD2	4:B:9:GLU:N	2.34	0.43
4:B:206:ASP:O	4:B:207:ALA:HB3	2.17	0.43
5:C:4:LYS:HE2	5:C:4:LYS:HB3	1.85	0.43
5:C:23:TYR:CD2	5:C:23:TYR:C	2.96	0.43
5:C:172:ARG:NH2	5:C:203:PHE:CE2	2.86	0.43
7:E:144:THR:CG2	7:E:146:ALA:H	2.31	0.43
8:F:10:LEU:HD12	8:F:59:TYR:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:M:58:GLU:HA	15:M:58:GLU:OE2	2.17	0.43
19:Q:26:GLN:O	19:Q:27:PHE:HB3	2.18	0.43
22:T:63:ILE:HD13	22:T:80:ARG:HB3	2.01	0.43
1:A:1320:C:O2'	1:A:1321:C:H5'	2.18	0.43
1:A:1320:C:N4	21:S:37:ARG:HD3	2.33	0.43
3:X:31:A:H2'	3:X:32:C:C6	2.53	0.43
5:C:91:LEU:CD2	5:C:92:ALA:N	2.76	0.43
6:D:196:LEU:HD23	6:D:197:PRO:HD2	2.00	0.43
11:I:53:VAL:O	11:I:54:ASP:HB2	2.18	0.43
15:M:110:ARG:HH11	15:M:110:ARG:CG	2.30	0.43
15:M:121:LYS:N	15:M:121:LYS:HD2	2.32	0.43
18:P:73:LEU:O	18:P:74:LEU:C	2.62	0.43
19:Q:6:LEU:O	19:Q:59:ILE:N	2.47	0.43
19:Q:80:GLY:O	19:Q:81:ARG:CB	2.66	0.43
1:A:513:C:H2'	1:A:514:C:C6	2.54	0.43
1:A:662:G:O2'	1:A:836:G:C5'	2.67	0.43
1:A:780:A:O2'	1:A:781:A:H5''	2.19	0.43
1:A:1301:U:O2'	1:A:1302:U:OP1	2.34	0.43
1:A:1318:A:O2'	21:S:37:ARG:HB3	2.19	0.43
5:C:178:LEU:O	5:C:179:ARG:CB	2.63	0.43
8:F:2:ARG:NH1	8:F:69:GLU:HG2	2.32	0.43
15:M:105:THR:O	15:M:106:ASN:C	2.61	0.43
16:N:8:GLU:O	16:N:11:LYS:HB3	2.19	0.43
16:N:11:LYS:C	16:N:13:THR:H	2.27	0.43
17:O:14:GLU:OE1	17:O:84:LYS:HE2	2.19	0.43
20:R:37:VAL:HG22	20:R:78:LEU:HB3	1.99	0.43
1:A:74:C:H2'	1:A:75:G:H5'	2.01	0.43
1:A:562:C:H1'	14:L:15:ARG:HB3	1.99	0.43
1:A:824:C:H2'	1:A:825:G:H8	1.82	0.43
1:A:1182:G:H5'	1:A:1184:G:H5'	2.00	0.43
1:A:1236:A:H2'	1:A:1237:C:C6	2.53	0.43
1:A:1286:A:H2'	1:A:1287:A:O5'	2.19	0.43
4:B:212:GLN:NE2	4:B:216:SER:HB3	2.33	0.43
5:C:5:ILE:O	5:C:5:ILE:HD12	2.19	0.43
7:E:79:GLU:O	10:H:104:ARG:CZ	2.67	0.43
7:E:96:PRO:HA	7:E:117:ASP:CG	2.43	0.43
8:F:64:GLN:O	8:F:64:GLN:HG2	2.17	0.43
11:I:44:VAL:HG12	11:I:51:ARG:CZ	2.49	0.43
11:I:56:LEU:HD23	11:I:56:LEU:C	2.44	0.43
12:J:60:ARG:HD2	12:J:60:ARG:N	2.34	0.43
1:A:272:C:O2'	1:A:273:A:H5'	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1305:G:H22	1:A:1331:G:C2'	2.30	0.43
4:B:134:GLU:C	4:B:136:VAL:N	2.76	0.43
6:D:58:LEU:HD13	6:D:58:LEU:C	2.44	0.43
9:G:3:ARG:HH11	9:G:3:ARG:CG	2.31	0.43
11:I:49:PRO:O	11:I:52:ALA:HB3	2.19	0.43
12:J:42:THR:HG22	12:J:43:ARG:N	2.34	0.43
15:M:11:ARG:HG2	15:M:12:ASN:N	2.33	0.43
18:P:67:THR:N	18:P:70:ALA:HB3	2.34	0.43
19:Q:100:LYS:O	19:Q:101:ARG:NE	2.52	0.43
21:S:15:LEU:O	21:S:16:LEU:C	2.61	0.43
23:V:15:ARG:O	23:V:17:THR:HG23	2.19	0.43
1:A:136:C:H2'	1:A:137:C:C6	2.54	0.43
1:A:232:G:H1'	1:A:262:A:N1	2.34	0.43
1:A:999:C:H2'	1:A:1000:U:C6	2.53	0.43
1:A:1201:A:H4'	1:A:1202:G:C5'	2.48	0.43
1:A:1273:G:H2'	1:A:1274:G:O4'	2.19	0.43
5:C:167:TRP:HB3	5:C:168:ALA:H	1.37	0.43
7:E:51:VAL:CB	7:E:52:PRO:HD3	2.43	0.43
9:G:151:TYR:CD1	9:G:151:TYR:N	2.87	0.43
10:H:38:ILE:CD1	10:H:118:VAL:HG12	2.48	0.43
12:J:30:SER:HB2	12:J:80:LYS:C	2.44	0.43
13:K:126:ARG:O	13:K:127:LYS:CB	2.65	0.43
14:L:126:LYS:H	14:L:126:LYS:HE3	1.84	0.43
20:R:55:ARG:HH11	20:R:55:ARG:CB	2.29	0.43
20:R:73:ALA:HB3	20:R:79:LEU:HD12	2.01	0.43
22:T:45:GLN:HB2	22:T:91:LEU:HD13	2.01	0.43
1:A:119:A:H4'	1:A:120:A:O5'	2.19	0.43
1:A:123:C:OP1	1:A:312:C:H5'	2.18	0.43
1:A:285:G:O2'	1:A:286:G:H5'	2.18	0.43
1:A:1054:C:N4	3:X:34:U:C1'	2.82	0.43
1:A:1489:G:C2'	1:A:1490:C:C5'	2.85	0.43
5:C:91:LEU:HD21	5:C:99:VAL:HG13	1.99	0.43
6:D:89:THR:O	6:D:90:GLY:C	2.62	0.43
7:E:6:PHE:CE2	7:E:36:ASP:HB3	2.53	0.43
11:I:114:TYR:CE1	12:J:59:SER:O	2.72	0.43
15:M:108:ARG:O	15:M:109:THR:C	2.61	0.43
17:O:26:GLU:OE2	17:O:26:GLU:N	2.51	0.43
1:A:265:G:H2'	1:A:267:C:C5	2.53	0.43
1:A:343:U:H2'	1:A:345:C:C5	2.54	0.43
1:A:598:U:H4'	10:H:94:TYR:CD1	2.54	0.43
1:A:603:U:H2'	1:A:604:G:H8	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:939:G:H2'	1:A:940:C:H6	1.81	0.43
1:A:1167:A:H2'	1:A:1168:A:C8	2.54	0.43
1:A:1399:C:C2	1:A:1401:G:C5	3.07	0.43
1:A:1424:C:C2'	1:A:1425:U:H5'	2.49	0.43
4:B:55:PHE:O	4:B:56:ARG:C	2.60	0.43
4:B:160:ASP:O	4:B:183:PRO:HD2	2.19	0.43
5:C:139:GLN:CA	5:C:139:GLN:HE21	2.30	0.43
8:F:10:LEU:HD11	8:F:59:TYR:HD2	1.84	0.43
9:G:26:PHE:O	9:G:30:ILE:HG13	2.19	0.43
11:I:127:LYS:HE3	11:I:127:LYS:HA	2.01	0.43
12:J:94:VAL:CG1	12:J:95:GLU:H	2.32	0.43
15:M:35:GLU:C	15:M:37:THR:H	2.27	0.43
17:O:57:LEU:HD12	17:O:57:LEU:HA	1.73	0.43
21:S:42:PRO:O	21:S:45:VAL:HG23	2.19	0.43
1:A:113:G:H1'	1:A:354:G:C5'	2.46	0.42
1:A:261:U:O2	1:A:263:A:C8	2.72	0.42
1:A:463:A:O2'	1:A:474:G:H5'	2.18	0.42
1:A:731:G:H5'	1:A:766:A:H4'	2.00	0.42
1:A:951:G:O2'	1:A:952:U:H5'	2.19	0.42
1:A:1128:C:HO2'	1:A:1130:A:H8	1.62	0.42
1:A:1269:A:N1	1:A:1312:G:O2'	2.49	0.42
1:A:1495:U:H2'	1:A:1496:C:C6	2.53	0.42
1:A:1499:A:H1'	1:A:1520:G:H5'	2.01	0.42
7:E:143:ARG:NH1	10:H:77:GLU:OE2	2.52	0.42
10:H:31:PHE:HZ	10:H:134:ILE:CD1	2.32	0.42
10:H:56:LYS:O	10:H:58:TYR:HD1	2.02	0.42
12:J:23:ILE:N	12:J:23:ILE:HD12	2.34	0.42
13:K:59:TYR:O	13:K:62:GLN:HB3	2.18	0.42
14:L:25:PRO:C	14:L:27:LEU:N	2.68	0.42
15:M:32:GLU:OE1	15:M:64:TRP:HZ2	2.01	0.42
15:M:114:ARG:C	15:M:115:LYS:HD3	2.44	0.42
21:S:41:VAL:HB	21:S:43:GLU:OE2	2.19	0.42
21:S:58:VAL:O	21:S:58:VAL:HG23	2.19	0.42
22:T:50:GLU:H	22:T:99:LEU:HD12	1.83	0.42
22:T:54:LYS:HG3	22:T:100:ILE:HD12	2.01	0.42
1:A:129(A):G:O2'	1:A:130:A:OP2	2.36	0.42
1:A:327:A:O3'	1:A:328:C:H4'	2.19	0.42
1:A:1153:C:H2'	1:A:1154:G:H8	1.84	0.42
1:A:1202:G:H2'	1:A:1203:C:C5'	2.49	0.42
1:A:1206:G:C6	1:A:1207:G:C5	3.08	0.42
1:A:1226:C:OP2	15:M:103:THR:HG21	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1246:C:O2'	1:A:1247:U:H5'	2.19	0.42
1:A:1250:A:C5'	11:I:68:GLY:N	2.82	0.42
4:B:209:ARG:NH2	4:B:236:TYR:HE2	2.17	0.42
5:C:123:GLN:NE2	5:C:140:ARG:NH2	2.59	0.42
7:E:15:ARG:C	7:E:16:THR:HG22	2.44	0.42
9:G:52:GLU:O	9:G:54:THR:N	2.52	0.42
12:J:9:ARG:CB	12:J:9:ARG:HH11	2.32	0.42
14:L:41:ARG:NH1	14:L:41:ARG:CB	2.82	0.42
21:S:30:LEU:C	21:S:31:ILE:HD13	2.45	0.42
1:A:106:C:O2	1:A:379:C:H4'	2.20	0.42
1:A:413:G:O2'	1:A:416:G:O6	2.36	0.42
1:A:437:U:C2'	1:A:438:G:H5'	2.49	0.42
1:A:1250:A:C4'	11:I:68:GLY:H	2.24	0.42
1:A:1367:C:H4'	12:J:48:THR:HG21	2.01	0.42
1:A:1380:U:O2'	1:A:1381:U:P	2.77	0.42
4:B:223:ILE:HG21	4:B:230:VAL:HG21	2.02	0.42
5:C:31:HIS:C	5:C:33:LEU:N	2.77	0.42
6:D:52:SER:O	6:D:53:ASP:C	2.59	0.42
9:G:38:LEU:O	9:G:39:ALA:C	2.62	0.42
14:L:38:THR:HG22	14:L:39:VAL:HG23	2.01	0.42
15:M:49:THR:CG2	15:M:51:ALA:HB3	2.49	0.42
16:N:23:ARG:NH1	16:N:23:ARG:HG3	2.34	0.42
17:O:43:LEU:C	17:O:45:VAL:O	2.63	0.42
18:P:10:GLY:HA3	18:P:14:ASN:O	2.20	0.42
21:S:9:VAL:O	21:S:9:VAL:HG12	2.18	0.42
1:A:416:G:C8	1:A:418:C:N4	2.87	0.42
1:A:528:C:H41	14:L:49:ASN:CG	2.27	0.42
1:A:635:G:O2'	1:A:636:U:H5'	2.19	0.42
1:A:957:U:H3	1:A:960:U:C5'	2.32	0.42
1:A:1009:G:N1	1:A:1021:G:N2	2.67	0.42
1:A:1011:G:H2'	1:A:1012:U:H5'	2.01	0.42
4:B:7:VAL:C	4:B:8:LYS:HG3	2.44	0.42
4:B:27:LYS:C	4:B:29:ALA:H	2.27	0.42
5:C:119:ARG:O	5:C:122:GLU:HB2	2.18	0.42
5:C:133:ALA:O	5:C:136:GLN:HB2	2.20	0.42
5:C:139:GLN:O	5:C:143:GLU:HB2	2.20	0.42
6:D:60:GLU:OE1	6:D:60:GLU:HA	2.20	0.42
6:D:70:ILE:HG22	6:D:71:SER:N	2.34	0.42
7:E:69:VAL:HA	7:E:70:PRO:HD3	1.75	0.42
10:H:86:ILE:HD11	10:H:136:GLU:HB2	2.00	0.42
11:I:10:ARG:CD	11:I:105:ASP:HB3	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:I:128:ARG:HG2	11:I:128:ARG:OXT	2.18	0.42
19:Q:27:PHE:CZ	19:Q:36:ILE:HD11	2.54	0.42
21:S:36:ARG:NH2	21:S:75:ALA:HB3	2.34	0.42
1:A:51:A:H4'	1:A:52:G:C5'	2.50	0.42
1:A:191:G:C4	22:T:105:SER:HB3	2.53	0.42
1:A:731:G:OP1	1:A:766:A:H1'	2.20	0.42
1:A:818:G:H3'	1:A:819:A:C5'	2.50	0.42
1:A:976:G:C8	1:A:1358:U:O2	2.73	0.42
1:A:1027:C:N4	1:A:1029:C:H41	2.17	0.42
1:A:1230:C:O2'	1:A:1231:G:H5'	2.20	0.42
1:A:1441:G:H4'	1:A:1442:G:C5	2.55	0.42
4:B:69:LEU:HD23	4:B:69:LEU:C	2.44	0.42
4:B:71:VAL:HG23	4:B:164:VAL:HG23	2.00	0.42
5:C:44:GLU:C	5:C:46:GLU:N	2.78	0.42
6:D:8:VAL:HG11	6:D:21:LEU:CB	2.50	0.42
6:D:8:VAL:HG11	6:D:21:LEU:HB3	2.01	0.42
9:G:78:ARG:HD2	9:G:156:TRP:HE3	1.84	0.42
12:J:26:ALA:HA	12:J:84:GLN:OE1	2.19	0.42
13:K:47:VAL:O	13:K:47:VAL:CG1	2.62	0.42
13:K:123:LYS:O	13:K:124:LYS:C	2.63	0.42
22:T:93:GLU:HA	22:T:93:GLU:OE2	2.19	0.42
1:A:1222:G:OP1	21:S:77:THR:HG21	2.19	0.42
1:A:1522:U:O2'	1:A:1523:G:H5'	2.19	0.42
4:B:53:ARG:NH1	4:B:199:TYR:HD2	2.18	0.42
5:C:23:TYR:OH	12:J:9:ARG:HD3	2.20	0.42
5:C:51:GLY:C	5:C:70:VAL:HG13	2.44	0.42
5:C:83:ARG:C	5:C:85:ARG:N	2.76	0.42
5:C:172:ARG:HB3	5:C:172:ARG:HH11	1.84	0.42
14:L:89:ARG:HG2	14:L:97:ARG:CA	2.47	0.42
15:M:71:ARG:HG2	15:M:71:ARG:HH11	1.84	0.42
1:A:287:U:C2'	1:A:288:A:H5'	2.50	0.42
1:A:614:A:C2	1:A:627:G:C2	3.08	0.42
1:A:1070:U:O2'	1:A:1071:C:H5'	2.19	0.42
1:A:1227:A:H8	1:A:1227:A:H3'	1.85	0.42
1:A:1527:C:O2'	1:A:1528:U:H5'	2.19	0.42
4:B:144:ARG:HA	4:B:147:LYS:CD	2.49	0.42
4:B:223:ILE:CD1	4:B:230:VAL:HG21	2.50	0.42
6:D:162:LEU:HD12	6:D:181:MET:SD	2.58	0.42
7:E:15:ARG:O	7:E:16:THR:HG22	2.20	0.42
7:E:144:THR:CG2	7:E:145:LYS:N	2.80	0.42
11:I:17:VAL:HG11	11:I:81:ILE:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:J:22:LYS:HE2	12:J:90:LEU:HD12	2.00	0.42
21:S:13:ASP:O	21:S:17:GLU:HG2	2.20	0.42
21:S:63:THR:HG22	21:S:64:GLU:H	1.84	0.42
22:T:36:LEU:HA	22:T:39:LYS:HB2	2.02	0.42
22:T:53:LEU:O	22:T:54:LYS:C	2.61	0.42
22:T:100:ILE:C	22:T:102:GLY:H	2.27	0.42
1:A:61:G:H2'	1:A:62:U:O4'	2.19	0.42
1:A:280:C:O2	19:Q:38:ARG:HG3	2.20	0.42
1:A:502:G:H2'	1:A:503:C:C6	2.55	0.42
5:C:14:ILE:CG2	5:C:15:THR:H	2.09	0.42
5:C:125:GLU:HG2	5:C:190:ARG:O	2.19	0.42
6:D:25:ARG:C	6:D:27:TYR:N	2.68	0.42
9:G:21:VAL:HG23	9:G:22:LEU:N	2.35	0.42
9:G:116:ALA:HA	9:G:119:ARG:CZ	2.50	0.42
11:I:44:VAL:CG1	11:I:51:ARG:HH22	2.32	0.42
11:I:50:LEU:O	11:I:53:VAL:HG22	2.20	0.42
11:I:58:ARG:HH11	11:I:58:ARG:HG3	1.84	0.42
12:J:51:ARG:CZ	12:J:61:GLU:HB2	2.49	0.42
13:K:78:GLN:O	13:K:103:LEU:HD23	2.20	0.42
16:N:34:TYR:HD1	16:N:34:TYR:H	1.66	0.42
18:P:4:ILE:HA	18:P:20:VAL:O	2.20	0.42
18:P:28:ARG:NH1	18:P:29:ASP:OD2	2.49	0.42
1:A:559:A:OP1	7:E:126:ARG:NH2	2.52	0.42
1:A:818:G:C3'	1:A:819:A:C5'	2.97	0.42
1:A:882:C:O2'	1:A:883:C:H5'	2.20	0.42
1:A:959:A:C2	1:A:1222:G:O4'	2.73	0.42
1:A:1196:U:OP1	1:A:1197:G:H5'	2.20	0.42
1:A:1296:C:H4'	1:A:1302:U:C5	2.55	0.42
5:C:17:ASP:O	5:C:54:ARG:NH2	2.53	0.42
5:C:20:SER:HB3	5:C:22:TRP:NE1	2.35	0.42
5:C:25:GLY:O	5:C:27:LYS:N	2.53	0.42
6:D:12:CYS:SG	6:D:19:LEU:O	2.78	0.42
12:J:99:LYS:O	12:J:100:THR:O	2.38	0.42
13:K:49:GLY:O	13:K:50:TYR:O	2.38	0.42
13:K:69:ALA:O	13:K:72:ALA:HB3	2.20	0.42
22:T:44:ALA:C	22:T:46:GLU:N	2.75	0.42
1:A:58:C:O2'	1:A:59:A:H5'	2.20	0.42
1:A:406:G:H2'	1:A:407:G:C8	2.55	0.42
1:A:940:C:H2'	1:A:941:G:C8	2.55	0.42
1:A:1058:G:O2'	1:A:1059:C:H5'	2.20	0.42
1:A:1109:C:P	5:C:176:HIS:CD2	3.12	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1237:C:H4'	1:A:1334:G:N2	2.35	0.42
1:A:1298:C:H4'	1:A:1299:A:O4'	2.20	0.42
1:A:1454:G:O2'	1:A:1455:G:H5'	2.20	0.42
10:H:116:LYS:HD2	10:H:129:VAL:HG21	2.02	0.42
11:I:4:TYR:CZ	11:I:88:TYR:HD1	2.38	0.42
11:I:10:ARG:NE	11:I:105:ASP:HB3	2.35	0.42
11:I:18:PHE:O	11:I:61:ALA:HA	2.20	0.42
11:I:127:LYS:HE3	11:I:127:LYS:N	2.33	0.42
14:L:47:LYS:HG2	14:L:48:PRO:HD3	2.02	0.42
15:M:117:VAL:HG12	15:M:118:ALA:N	2.34	0.42
1:A:193:C:H2'	1:A:194:C:C6	2.55	0.41
1:A:373:A:H1'	1:A:481:G:O2'	2.20	0.41
1:A:375:U:O2'	18:P:28:ARG:HD2	2.20	0.41
1:A:382:A:C2	1:A:383:A:C4	3.08	0.41
1:A:463:A:C2'	1:A:474:G:H5'	2.50	0.41
1:A:664:G:OP1	20:R:64:ARG:HD2	2.20	0.41
1:A:834:C:H2'	1:A:835:U:H6	1.84	0.41
1:A:976:G:N7	1:A:1358:U:C2	2.88	0.41
1:A:1117:G:H5'	1:A:1117:G:C8	2.50	0.41
1:A:1229:A:H2'	1:A:1230:C:C6	2.55	0.41
5:C:36:ASP:O	5:C:39:ILE:HB	2.20	0.41
7:E:12:LEU:CD1	7:E:31:LEU:HB2	2.50	0.41
7:E:78:HIS:CD2	10:H:107:LEU:HD12	2.49	0.41
10:H:31:PHE:CZ	10:H:134:ILE:HD13	2.55	0.41
12:J:9:ARG:HB3	12:J:9:ARG:CZ	2.50	0.41
14:L:47:LYS:HB3	14:L:48:PRO:HD2	1.92	0.41
16:N:47:LEU:O	16:N:48:ALA:C	2.62	0.41
22:T:76:ALA:HA	22:T:79:ARG:NH1	2.34	0.41
1:A:490:G:O2'	1:A:491:G:H5'	2.20	0.41
1:A:653:A:P	10:H:56:LYS:NZ	2.93	0.41
1:A:692:U:O2	1:A:695:A:C8	2.73	0.41
1:A:779:C:H2'	1:A:780:A:O4'	2.20	0.41
1:A:1163:C:H2'	1:A:1164:G:H8	1.85	0.41
1:A:1423:G:H2'	1:A:1424:C:H6	1.85	0.41
1:A:1531:A:O5'	1:A:1531:A:H8	2.02	0.41
4:B:92:TYR:CD1	4:B:92:TYR:C	2.99	0.41
4:B:141:GLU:O	4:B:144:ARG:HG3	2.20	0.41
5:C:18:TRP:C	5:C:20:SER:H	2.27	0.41
5:C:137:ALA:O	5:C:138:VAL:C	2.63	0.41
5:C:193:TYR:CE1	5:C:196:LEU:HD21	2.42	0.41
6:D:60:GLU:OE2	6:D:199:ASN:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:199:ASN:HD22	6:D:201:GLN:H	1.68	0.41
9:G:141:VAL:O	9:G:144:MET:HB2	2.20	0.41
10:H:104:ARG:HG2	10:H:104:ARG:HH11	1.85	0.41
13:K:91:ARG:NH1	20:R:88:LYS:NZ	2.67	0.41
15:M:9:ILE:N	15:M:9:ILE:CD1	2.77	0.41
15:M:59:TYR:O	15:M:63:THR:CG2	2.69	0.41
18:P:20:VAL:HG11	18:P:32:TYR:CG	2.55	0.41
20:R:16:PRO:O	20:R:17:SER:HB3	2.19	0.41
20:R:34:TYR:HA	20:R:69:THR:CG2	2.50	0.41
20:R:36:ASN:O	20:R:40:LEU:HG	2.20	0.41
20:R:43:PHE:CA	20:R:51:LEU:HD12	2.50	0.41
1:A:640:A:O2'	1:A:641:U:H5'	2.20	0.41
1:A:866:C:H2'	1:A:867:G:O5'	2.20	0.41
1:A:1060:C:H5	5:C:2:GLY:HA3	1.84	0.41
1:A:1127:G:H21	1:A:1146:A:H62	1.69	0.41
1:A:1229:A:C2	1:A:1230:C:C4	3.08	0.41
4:B:20:GLU:HB2	4:B:190:THR:HB	2.02	0.41
6:D:196:LEU:C	6:D:198:VAL:H	2.29	0.41
9:G:26:PHE:HB2	9:G:62:PHE:HZ	1.85	0.41
12:J:32:ALA:C	12:J:34:VAL:N	2.77	0.41
13:K:79:SER:OG	13:K:106:LYS:HG2	2.20	0.41
13:K:82:VAL:C	13:K:83:ILE:HG13	2.44	0.41
17:O:2:PRO:O	17:O:3:ILE:HD12	2.19	0.41
17:O:87:ILE:CG2	17:O:88:ARG:N	2.83	0.41
19:Q:63:ARG:HG2	19:Q:64:PRO:HD2	2.02	0.41
22:T:74:LYS:HB3	22:T:75:ASN:H	1.56	0.41
1:A:53:A:N6	1:A:54:C:C4	2.87	0.41
1:A:217:C:H2'	1:A:218:C:H6	1.86	0.41
1:A:269:C:H2'	1:A:270:A:H8	1.84	0.41
1:A:556:C:C2'	1:A:557:G:H5'	2.51	0.41
1:A:609:A:H2'	1:A:610:G:H5'	2.03	0.41
1:A:791:G:H2'	1:A:792:A:H5'	2.01	0.41
1:A:959:A:H5''	1:A:960:U:OP2	2.20	0.41
1:A:1055:A:C2	1:A:1056:U:H1'	2.55	0.41
1:A:1172:C:H2'	1:A:1173:G:H8	1.84	0.41
1:A:1370:G:H5''	11:I:12:GLU:OE1	2.20	0.41
7:E:18:ARG:NH2	7:E:25:ARG:HB3	2.33	0.41
10:H:127:LEU:N	10:H:127:LEU:HD23	2.34	0.41
11:I:97:LYS:HG2	11:I:102:LEU:CD1	2.44	0.41
13:K:40:ILE:O	13:K:41:THR:HG23	2.21	0.41
16:N:17:LYS:HG3	16:N:18:VAL:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:T:42:GLN:OE1	22:T:42:GLN:HA	2.21	0.41
1:A:57:G:H2'	1:A:58:C:H6	1.85	0.41
1:A:109:A:H2'	1:A:326:G:H21	1.84	0.41
1:A:112:G:H4'	1:A:389:A:C5'	2.46	0.41
1:A:518:C:HO2'	14:L:50:SER:CB	2.30	0.41
1:A:877:C:H1'	10:H:3:THR:HG23	2.02	0.41
1:A:976:G:C8	1:A:1358:U:C2	3.09	0.41
1:A:1107:C:C4	1:A:1108:G:C8	3.07	0.41
4:B:67:THR:N	4:B:160:ASP:OD2	2.48	0.41
4:B:228:GLY:O	4:B:229:VAL:O	2.39	0.41
5:C:38:ARG:HG3	5:C:38:ARG:HH11	1.86	0.41
5:C:65:ALA:O	5:C:66:VAL:HB	2.20	0.41
5:C:73:PRO:O	5:C:74:GLY:C	2.63	0.41
5:C:139:GLN:CA	5:C:139:GLN:NE2	2.84	0.41
6:D:121:VAL:O	6:D:134:ASP:HA	2.21	0.41
6:D:146:ILE:N	6:D:146:ILE:CD1	2.77	0.41
7:E:15:ARG:HG2	7:E:28:PHE:CE2	2.56	0.41
7:E:40:ARG:HG2	7:E:40:ARG:HH11	1.84	0.41
8:F:15:ASP:C	8:F:17:SER:H	2.29	0.41
9:G:51:GLN:OE1	9:G:51:GLN:HA	2.21	0.41
11:I:50:LEU:HG	11:I:81:ILE:HG21	2.02	0.41
16:N:16:PHE:O	16:N:17:LYS:C	2.62	0.41
19:Q:5:VAL:HA	19:Q:59:ILE:O	2.20	0.41
22:T:43:LEU:CD1	22:T:55:ILE:HD12	2.50	0.41
1:A:250:A:O2'	1:A:251:G:OP2	2.38	0.41
1:A:559:A:P	7:E:126:ARG:NH2	2.94	0.41
1:A:967:C:O3'	11:I:128:ARG:CZ	2.68	0.41
1:A:1347:G:N7	11:I:10:ARG:NH2	2.69	0.41
1:A:1355:G:O2'	1:A:1356:G:H5'	2.20	0.41
5:C:132:ARG:O	5:C:133:ALA:C	2.64	0.41
8:F:99:ALA:C	8:F:101:ALA:N	2.79	0.41
9:G:6:ARG:O	9:G:7:ALA:C	2.64	0.41
10:H:10:LEU:HD12	10:H:85:ARG:CG	2.50	0.41
11:I:127:LYS:HE3	11:I:127:LYS:CA	2.51	0.41
13:K:26:ASN:O	13:K:27:ASN:HB2	2.20	0.41
15:M:15:VAL:HG21	15:M:48:LEU:HD21	2.01	0.41
20:R:54:ARG:H	20:R:54:ARG:HG3	1.71	0.41
21:S:31:ILE:O	21:S:32:LYS:HG2	2.21	0.41
1:A:404:U:H2'	1:A:405:U:C6	2.56	0.41
1:A:824:C:H2'	1:A:825:G:C8	2.56	0.41
1:A:911:U:H2'	1:A:912:C:C6	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:979:C:OP2	1:A:980:C:H5	2.03	0.41
1:A:994:A:N7	1:A:1216:G:H4'	2.36	0.41
1:A:1300:G:C2'	1:A:1301:U:OP2	2.69	0.41
1:A:1315:U:H2'	1:A:1316:G:O4'	2.20	0.41
4:B:19:HIS:CG	4:B:204:ASN:HA	2.55	0.41
9:G:115:ARG:O	9:G:116:ALA:C	2.63	0.41
9:G:141:VAL:O	9:G:142:GLU:C	2.63	0.41
10:H:126:LYS:HG2	10:H:127:LEU:HD23	2.02	0.41
15:M:11:ARG:HA	15:M:45:VAL:HB	2.02	0.41
20:R:37:VAL:CG2	20:R:78:LEU:HB3	2.51	0.41
22:T:84:LEU:C	22:T:86:ARG:N	2.77	0.41
1:A:437:U:O2'	1:A:438:G:H5'	2.19	0.41
1:A:443:C:H2'	1:A:444:C:H6	1.86	0.41
1:A:1194:U:H4'	7:E:22:GLY:HA2	2.03	0.41
1:A:1249:C:O2'	11:I:73:GLN:NE2	2.53	0.41
1:A:1320:C:O2	21:S:36:ARG:NH1	2.54	0.41
1:A:1435:G:H2'	1:A:1436:U:H6	1.82	0.41
1:A:1497:G:H2'	1:A:1498:U:H5'	2.03	0.41
1:A:1521:G:O2'	1:A:1522:U:H5'	2.20	0.41
4:B:239:VAL:HG12	4:B:240:GLN:NE2	2.35	0.41
6:D:76:ARG:HG2	6:D:76:ARG:NH1	2.31	0.41
6:D:112:VAL:HG22	6:D:116:GLN:OE1	2.20	0.41
8:F:26:ILE:O	8:F:30:LEU:HG	2.20	0.41
11:I:78:LYS:HB3	11:I:78:LYS:HE2	1.92	0.41
14:L:58:VAL:N	14:L:66:VAL:O	2.52	0.41
14:L:83:VAL:HG13	14:L:100:ILE:HG23	2.02	0.41
15:M:15:VAL:O	15:M:19:LEU:HG	2.20	0.41
15:M:24:GLY:HA3	15:M:66:LEU:HD22	2.03	0.41
18:P:69:THR:O	18:P:70:ALA:C	2.64	0.41
22:T:10:LEU:C	22:T:12:ALA:N	2.77	0.41
22:T:16:HIS:CE1	22:T:20:LEU:HD11	2.55	0.41
1:A:6:G:H4'	1:A:298:A:H4'	2.01	0.41
1:A:104:G:N7	22:T:14:LYS:NZ	2.61	0.41
1:A:185:A:N3	22:T:81:LYS:NZ	2.62	0.41
1:A:240:C:H2'	1:A:241:C:H6	1.85	0.41
1:A:279:A:C5'	1:A:280:C:H3'	2.51	0.41
1:A:286:G:O2'	1:A:287:U:H5'	2.21	0.41
1:A:558:G:H2'	1:A:559:A:C2	2.55	0.41
1:A:623:C:O2'	1:A:624:C:H5'	2.21	0.41
1:A:708:C:O2'	1:A:709:G:H5'	2.20	0.41
1:A:832:C:H2'	1:A:833:U:O4'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1194:U:O2'	1:A:1195:C:H5'	2.20	0.41
1:A:1202:G:O2'	1:A:1203:C:H5'	2.21	0.41
1:A:1216:G:O2'	1:A:1217:C:H5'	2.20	0.41
1:A:1264:C:O2'	1:A:1265:G:H5'	2.21	0.41
1:A:1347:G:O2'	1:A:1348:U:OP2	2.38	0.41
1:A:1419:G:O2'	1:A:1420:C:H5'	2.21	0.41
4:B:22:LYS:C	4:B:23:ARG:HG3	2.45	0.41
4:B:98:LEU:HG	4:B:101:MET:HE3	2.02	0.41
5:C:35:GLU:OE1	5:C:97:LYS:HE3	2.20	0.41
5:C:83:ARG:O	5:C:85:ARG:N	2.53	0.41
6:D:17:VAL:CG1	6:D:18:LYS:N	2.84	0.41
6:D:101:LEU:O	6:D:102:ASP:C	2.64	0.41
7:E:87:SER:HB3	7:E:131:ILE:CD1	2.50	0.41
8:F:48:LEU:CD1	8:F:52:ILE:HB	2.51	0.41
10:H:88:LYS:O	10:H:89:PRO:C	2.64	0.41
10:H:104:ARG:O	10:H:106:GLY:N	2.54	0.41
11:I:11:LYS:O	11:I:12:GLU:HB3	2.21	0.41
12:J:42:THR:HG23	12:J:67:THR:C	2.46	0.41
14:L:45:PRO:HD3	14:L:51:ALA:O	2.20	0.41
15:M:44:ARG:HB3	15:M:46:LYS:CG	2.51	0.41
15:M:118:ALA:HB1	15:M:121:LYS:HZ1	1.84	0.41
15:M:125:ARG:O	15:M:126:LYS:C	2.64	0.41
18:P:12:LYS:O	18:P:13:HIS:HB2	2.20	0.41
20:R:19:LYS:O	20:R:20:ALA:HB2	2.19	0.41
20:R:47:THR:CG2	20:R:83:GLU:H	2.34	0.41
21:S:30:LEU:HA	21:S:48:THR:O	2.20	0.41
1:A:502:G:H2'	1:A:503:C:O4'	2.21	0.41
1:A:744:C:H2'	1:A:745:C:C6	2.55	0.41
1:A:834:C:H2'	1:A:835:U:C6	2.56	0.41
1:A:839:U:H5'	1:A:840:C:H5	1.86	0.41
1:A:918:A:H2'	1:A:919:A:O4'	2.21	0.41
1:A:1014:A:C2	1:A:1219:U:H1'	2.56	0.41
1:A:1184:G:OP1	1:A:1184:G:H3'	2.21	0.41
1:A:1403:C:O5'	1:A:1403:C:H6	2.03	0.41
4:B:7:VAL:HG23	4:B:7:VAL:O	2.21	0.41
4:B:178:ARG:HH22	10:H:74:PRO:CB	2.33	0.41
5:C:8:ILE:O	5:C:9:GLY:C	2.64	0.41
5:C:145:GLY:O	5:C:146:ALA:HB3	2.20	0.41
7:E:76:ILE:CG2	7:E:77:PRO:HD2	2.45	0.41
9:G:37:ASN:O	9:G:41:ARG:HG3	2.21	0.41
10:H:4:ASP:CG	10:H:85:ARG:HH11	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:M:13:LYS:O	15:M:45:VAL:HG23	2.21	0.41
19:Q:18:THR:HG23	19:Q:69:LYS:HE3	2.02	0.41
22:T:8:ARG:O	22:T:9:ASN:C	2.64	0.41
1:A:158:G:N2	1:A:164:U:H1'	2.36	0.40
1:A:509:A:H2'	1:A:510:A:C8	2.56	0.40
1:A:532:A:C2'	1:A:533:A:OP1	2.69	0.40
1:A:1152:A:H5''	12:J:13:HIS:HB2	2.03	0.40
1:A:1347:G:H2'	1:A:1373:G:C6	2.56	0.40
1:A:1427:U:O2'	1:A:1428:A:H5'	2.21	0.40
4:B:80:ILE:CD1	4:B:212:GLN:HB2	2.51	0.40
4:B:144:ARG:HD2	4:B:145:LEU:HD23	2.02	0.40
9:G:155:ARG:HA	9:G:155:ARG:NE	2.33	0.40
10:H:80:ILE:O	10:H:80:ILE:HG22	2.19	0.40
19:Q:13:ASP:O	19:Q:13:ASP:OD2	2.38	0.40
21:S:36:ARG:NH2	21:S:75:ALA:O	2.48	0.40
1:A:173:U:H5''	1:A:197:A:O4'	2.22	0.40
1:A:938:A:C6	1:A:939:G:C5	3.09	0.40
1:A:1053:G:O6	1:A:1199:U:H2'	2.22	0.40
1:A:1094:G:OP2	1:A:1095:U:H5	2.04	0.40
1:A:1286:A:H2	23:V:18:TYR:HH	1.66	0.40
1:A:1329:A:O2'	1:A:1330:U:H5'	2.20	0.40
4:B:89:GLY:O	4:B:154:LEU:HD13	2.21	0.40
5:C:34:LEU:C	5:C:34:LEU:CD2	2.92	0.40
5:C:100:ALA:O	5:C:101:LEU:HB2	2.21	0.40
5:C:179:ARG:HG2	5:C:180:ALA:N	2.29	0.40
6:D:50:ARG:HA	6:D:51:PRO:HD3	1.89	0.40
9:G:15:ASP:OD1	9:G:18:TYR:HD1	2.03	0.40
11:I:32:ASP:O	11:I:33:PHE:C	2.65	0.40
12:J:47:PHE:HB2	12:J:63:PHE:HB2	2.04	0.40
18:P:43:LYS:HA	18:P:48:TRP:CB	2.51	0.40
1:A:142:G:O2'	1:A:196:A:N1	2.52	0.40
1:A:450:G:N7	1:A:481:G:C6	2.90	0.40
1:A:713:G:H2'	1:A:714:G:C8	2.56	0.40
1:A:947:G:H2'	1:A:948:C:O4'	2.21	0.40
1:A:1068:G:N7	1:A:1094:G:O2'	2.49	0.40
4:B:107:THR:C	4:B:109:SER:H	2.29	0.40
6:D:165:MET:SD	6:D:168:ARG:HD2	2.61	0.40
9:G:121:ALA:O	9:G:125:MET:HG3	2.21	0.40
11:I:83:ARG:O	11:I:84:ALA:C	2.64	0.40
12:J:22:LYS:CE	12:J:90:LEU:HD12	2.51	0.40
15:M:120:LYS:C	15:M:121:LYS:HD2	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:S:44:MET:O	21:S:62:ILE:HG21	2.21	0.40
21:S:47:HIS:O	21:S:62:ILE:HG22	2.21	0.40
22:T:37:SER:O	22:T:38:LYS:C	2.64	0.40
1:A:463:A:O4'	18:P:82:GLN:NE2	2.55	0.40
1:A:836:G:C6	1:A:851:G:C6	3.10	0.40
1:A:855:G:C6	1:A:856:C:C4	3.09	0.40
1:A:962:C:H2'	1:A:963:G:O4'	2.21	0.40
1:A:1029:C:H2'	1:A:1030:C:C6	2.56	0.40
1:A:1216:G:H5''	16:N:5:ALA:HB2	2.02	0.40
4:B:117:GLU:O	4:B:117:GLU:HG2	2.21	0.40
4:B:118:LEU:O	4:B:119:GLU:C	2.64	0.40
5:C:91:LEU:HD23	5:C:91:LEU:C	2.47	0.40
5:C:113:ALA:HB2	5:C:202:ILE:HG13	2.04	0.40
6:D:152:SER:O	6:D:158:ILE:HD12	2.22	0.40
8:F:28:ARG:HG3	8:F:28:ARG:HH11	1.85	0.40
10:H:24:THR:HG23	10:H:61:VAL:HB	2.03	0.40
10:H:35:ILE:O	10:H:39:LEU:HD23	2.20	0.40
10:H:94:TYR:CE2	10:H:132:GLU:HG3	2.57	0.40
13:K:11:LYS:O	13:K:12:ARG:HB2	2.22	0.40
14:L:24:VAL:HG12	14:L:26:ALA:HB2	2.03	0.40
14:L:89:ARG:NE	14:L:97:ARG:HD2	2.36	0.40
17:O:61:GLY:O	17:O:64:ARG:HG2	2.22	0.40
20:R:51:LEU:HA	20:R:52:PRO:HD3	1.84	0.40
1:A:109:A:H5'	1:A:110:C:C5	2.56	0.40
1:A:321:A:O2'	1:A:322:C:H5'	2.21	0.40
1:A:434:U:H2'	1:A:435:C:C6	2.56	0.40
1:A:1061:G:H1'	12:J:56:HIS:HE1	1.87	0.40
1:A:1079:G:O3'	7:E:14:ARG:NH2	2.55	0.40
4:B:24:TRP:N	4:B:24:TRP:CD1	2.89	0.40
4:B:57:PHE:CZ	4:B:61:LEU:HD11	2.57	0.40
5:C:31:HIS:C	5:C:33:LEU:H	2.30	0.40
9:G:69:VAL:O	9:G:69:VAL:HG12	2.20	0.40
9:G:72:ARG:HA	9:G:96:GLN:HE21	1.87	0.40
12:J:75:ILE:HG22	12:J:76:ASN:ND2	2.36	0.40
13:K:91:ARG:NH1	20:R:88:LYS:HZ3	2.16	0.40
19:Q:92:ARG:O	19:Q:95:TYR:HB2	2.22	0.40
22:T:58:LYS:O	22:T:59:ALA:C	2.64	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	
4	B	232/256 (91%)	176 (76%)	40 (17%)	16 (7%)	1	5
5	C	204/239 (85%)	131 (64%)	46 (22%)	27 (13%)	0	1
6	D	206/209 (99%)	168 (82%)	28 (14%)	10 (5%)	1	10
7	E	148/162 (91%)	140 (95%)	5 (3%)	3 (2%)	6	28
8	F	99/101 (98%)	80 (81%)	18 (18%)	1 (1%)	12	45
9	G	153/156 (98%)	122 (80%)	24 (16%)	7 (5%)	2	11
10	H	136/138 (99%)	116 (85%)	15 (11%)	5 (4%)	2	15
11	I	125/128 (98%)	94 (75%)	19 (15%)	12 (10%)	0	2
12	J	96/105 (91%)	60 (62%)	25 (26%)	11 (12%)	0	1
13	K	117/129 (91%)	88 (75%)	23 (20%)	6 (5%)	1	10
14	L	122/135 (90%)	97 (80%)	16 (13%)	9 (7%)	1	4
15	M	123/126 (98%)	88 (72%)	22 (18%)	13 (11%)	0	2
16	N	58/61 (95%)	44 (76%)	10 (17%)	4 (7%)	1	5
17	O	86/89 (97%)	77 (90%)	8 (9%)	1 (1%)	10	40
18	P	81/88 (92%)	69 (85%)	11 (14%)	1 (1%)	10	40
19	Q	102/105 (97%)	85 (83%)	9 (9%)	8 (8%)	1	4
20	R	71/88 (81%)	53 (75%)	16 (22%)	2 (3%)	4	21
21	S	78/93 (84%)	60 (77%)	12 (15%)	6 (8%)	1	4
22	T	97/106 (92%)	68 (70%)	20 (21%)	9 (9%)	0	2
23	V	22/27 (82%)	16 (73%)	5 (23%)	1 (4%)	2	12
All	All	2356/2541 (93%)	1832 (78%)	372 (16%)	152 (6%)	1	5

All (152) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	B	8	LYS

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Mol	Chain	Res	Type
4	B	15	VAL
4	B	16	HIS
4	B	24	TRP
4	B	123	ALA
4	B	229	VAL
4	B	232	PRO
5	C	4	LYS
5	C	15	THR
5	C	61	ALA
5	C	100	ALA
5	C	101	LEU
5	C	156	ARG
5	C	179	ARG
5	C	206	GLU
6	D	3	ARG
6	D	29	PRO
6	D	36	ARG
6	D	88	VAL
7	E	16	THR
10	H	91	ARG
11	I	23	ASN
11	I	41	VAL
11	I	55	ALA
11	I	127	LYS
12	J	27	ALA
12	J	72	VAL
12	J	90	LEU
13	K	12	ARG
13	K	13	GLN
13	K	50	TYR
14	L	27	LEU
14	L	28	LYS
14	L	47	LYS
15	M	63	THR
15	M	86	CYS
15	M	122	LYS
16	N	22	THR
19	Q	69	LYS
19	Q	80	GLY
19	Q	81	ARG
20	R	87	ARG
21	S	5	LEU

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Mol	Chain	Res	Type
21	S	6	LYS
21	S	32	LYS
22	T	74	LYS
22	T	99	LEU
4	B	18	GLY
4	B	21	ARG
4	B	23	ARG
4	B	88	ALA
5	C	16	ARG
5	C	26	LYS
5	C	154	SER
5	C	171	GLY
5	C	180	ALA
6	D	42	GLN
6	D	179	GLU
8	F	42	GLU
9	G	147	ALA
10	H	24	THR
10	H	105	ARG
11	I	38	GLN
11	I	94	ALA
12	J	34	VAL
12	J	61	GLU
12	J	73	ASP
13	K	128	ALA
14	L	41	ARG
14	L	80	HIS
15	M	6	GLY
15	M	106	ASN
16	N	15	LYS
16	N	36	PHE
18	P	10	GLY
19	Q	49	GLU
19	Q	97	SER
19	Q	99	SER
20	R	20	ALA
21	S	9	VAL
22	T	9	ASN
22	T	11	SER
4	B	17	PHE
4	B	20	GLU
4	B	131	PRO

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Mol	Chain	Res	Type
5	C	14	ILE
5	C	45	LYS
5	C	81	GLY
5	C	98	ASN
5	C	102	ASN
5	C	189	ALA
7	E	153	LYS
9	G	7	ALA
9	G	62	PHE
11	I	11	LYS
11	I	45	ALA
11	I	46	ALA
11	I	105	ASP
12	J	89	ASP
13	K	15	ALA
14	L	48	PRO
15	M	67	GLU
15	M	116	THR
22	T	48	LYS
22	T	73	HIS
22	T	98	PRO
22	T	102	GLY
23	V	3	LYS
4	B	77	ALA
5	C	55	VAL
5	C	64	VAL
5	C	108	ASN
6	D	4	TYR
6	D	46	LYS
10	H	83	ILE
11	I	24	GLY
12	J	17	ASP
12	J	57	LYS
15	M	37	THR
19	Q	14	LYS
19	Q	98	LEU
21	S	31	ILE
22	T	45	GLN
5	C	29	TYR
5	C	66	VAL
6	D	23	GLY
7	E	73	ASN

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Mol	Chain	Res	Type
9	G	53	LYS
9	G	112	PRO
9	G	155	ARG
12	J	40	LEU
14	L	51	ALA
14	L	116	SER
4	B	95	GLN
5	C	168	ALA
9	G	113	GLU
14	L	79	GLU
15	M	21	TYR
15	M	36	LYS
16	N	23	ARG
5	C	77	ILE
10	H	103	VAL
13	K	47	VAL
15	M	4	ILE
15	M	117	VAL
6	D	5	ILE
11	I	44	VAL
12	J	39	PRO
15	M	85	GLY
21	S	11	VAL
17	O	86	GLY
5	C	130	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	B	202/220 (92%)	181 (90%)	21 (10%)	7	28
5	C	160/188 (85%)	145 (91%)	15 (9%)	8	32
6	D	180/181 (99%)	170 (94%)	10 (6%)	19	52
7	E	115/123 (94%)	99 (86%)	16 (14%)	3	17
8	F	90/90 (100%)	87 (97%)	3 (3%)	33	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	G	126/127 (99%)	120 (95%)	6 (5%)	23	57
10	H	119/119 (100%)	109 (92%)	10 (8%)	10	37
11	I	98/99 (99%)	91 (93%)	7 (7%)	13	43
12	J	87/92 (95%)	82 (94%)	5 (6%)	18	52
13	K	90/99 (91%)	84 (93%)	6 (7%)	15	46
14	L	104/111 (94%)	92 (88%)	12 (12%)	5	24
15	M	100/101 (99%)	93 (93%)	7 (7%)	14	44
16	N	49/50 (98%)	46 (94%)	3 (6%)	17	49
17	O	79/80 (99%)	71 (90%)	8 (10%)	7	29
18	P	72/74 (97%)	68 (94%)	4 (6%)	19	52
19	Q	96/97 (99%)	86 (90%)	10 (10%)	7	28
20	R	64/77 (83%)	62 (97%)	2 (3%)	35	68
21	S	71/80 (89%)	69 (97%)	2 (3%)	38	70
22	T	75/82 (92%)	68 (91%)	7 (9%)	8	32
23	V	19/22 (86%)	18 (95%)	1 (5%)	20	54
All	All	1996/2112 (94%)	1841 (92%)	155 (8%)	11	39

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

Mol	Chain	Res	Type
4	B	8	LYS
4	B	9	GLU
4	B	15	VAL
4	B	23	ARG
4	B	25	ASN
4	B	71	VAL
4	B	74	LYS
4	B	75	LYS
4	B	98	LEU
4	B	144	ARG
4	B	156	LYS
4	B	157	ARG
4	B	162	ILE
4	B	164	VAL
4	B	170	GLU
4	B	178	ARG
4	B	190	THR

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Mol	Chain	Res	Type
4	B	215	LEU
4	B	221	LEU
4	B	231	GLU
4	B	232	PRO
5	C	3	ASN
5	C	5	ILE
5	C	18	TRP
5	C	26	LYS
5	C	34	LEU
5	C	37	GLN
5	C	99	VAL
5	C	139	GLN
5	C	166	GLU
5	C	167	TRP
5	C	179	ARG
5	C	188	LEU
5	C	190	ARG
5	C	192	THR
5	C	204	LEU
6	D	9	CYS
6	D	15	GLU
6	D	29	PRO
6	D	57	ARG
6	D	58	LEU
6	D	122	ARG
6	D	131	ARG
6	D	146	ILE
6	D	199	ASN
6	D	201	GLN
7	E	6	PHE
7	E	12	LEU
7	E	31	LEU
7	E	32	VAL
7	E	41	VAL
7	E	43	LEU
7	E	47	LYS
7	E	56	GLN
7	E	80	ILE
7	E	89	ILE
7	E	116	THR
7	E	120	THR
7	E	137	GLU

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Mol	Chain	Res	Type
7	E	144	THR
7	E	147	ASP
7	E	150	ARG
8	F	10	LEU
8	F	43	LEU
8	F	69	GLU
9	G	8	GLU
9	G	38	LEU
9	G	113	GLU
9	G	126	ASP
9	G	140	ASP
9	G	155	ARG
10	H	24	THR
10	H	26	VAL
10	H	60	ARG
10	H	63	LEU
10	H	85	ARG
10	H	91	ARG
10	H	92	ARG
10	H	105	ARG
10	H	112	LEU
10	H	119	LEU
11	I	5	TYR
11	I	10	ARG
11	I	60	ASP
11	I	79	LEU
11	I	111	ARG
11	I	118	LYS
11	I	127	LYS
12	J	6	ILE
12	J	29	ARG
12	J	45	ARG
12	J	71	LEU
12	J	83	GLU
13	K	24	SER
13	K	29	ILE
13	K	54	ARG
13	K	84	VAL
13	K	92	GLU
13	K	114	VAL
14	L	33	ARG
14	L	42	THR

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Mol	Chain	Res	Type
14	L	48	PRO
14	L	53	ARG
14	L	60	LEU
14	L	80	HIS
14	L	81	SER
14	L	83	VAL
14	L	86	ARG
14	L	96	VAL
14	L	113	ARG
14	L	126	LYS
15	M	9	ILE
15	M	20	THR
15	M	56	LEU
15	M	70	LEU
15	M	81	LEU
15	M	110	ARG
15	M	115	LYS
16	N	22	THR
16	N	33	VAL
16	N	41	ARG
17	O	6	GLU
17	O	7	GLU
17	O	31	LEU
17	O	34	LEU
17	O	39	LEU
17	O	57	LEU
17	O	70	LEU
17	O	81	LEU
18	P	2	VAL
18	P	8	ARG
18	P	28	ARG
18	P	31	LYS
19	Q	9	VAL
19	Q	34	LYS
19	Q	38	ARG
19	Q	53	LEU
19	Q	60	ILE
19	Q	68	ARG
19	Q	73	VAL
19	Q	74	LEU
19	Q	76	LEU
19	Q	98	LEU

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Mol	Chain	Res	Type
20	R	28	GLU
20	R	54	ARG
21	S	15	LEU
21	S	65	ASN
22	T	10	LEU
22	T	39	LYS
22	T	42	GLN
22	T	56	MET
22	T	73	HIS
22	T	75	ASN
22	T	84	LEU
23	V	24	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
4	B	25	ASN
4	B	40	HIS
4	B	78	GLN
4	B	110	GLN
4	B	240	GLN
5	C	3	ASN
5	C	69	HIS
5	C	108	ASN
5	C	110	ASN
5	C	123	GLN
5	C	139	GLN
5	C	176	HIS
5	C	181	ASN
6	D	42	GLN
6	D	62	GLN
6	D	119	GLN
6	D	199	ASN
7	E	73	ASN
7	E	141	GLN
8	F	16	GLN
8	F	18	GLN
8	F	27	GLN
8	F	32	ASN
8	F	57	GLN
8	F	64	GLN
8	F	84	ASN

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Mol	Chain	Res	Type
8	F	100	ASN
9	G	13	GLN
9	G	37	ASN
9	G	84	ASN
9	G	96	GLN
9	G	97	GLN
9	G	106	GLN
11	I	3	GLN
11	I	23	ASN
11	I	73	GLN
11	I	87	GLN
11	I	89	ASN
12	J	56	HIS
12	J	62	HIS
12	J	76	ASN
12	J	78	ASN
13	K	38	ASN
13	K	62	GLN
13	K	104	GLN
13	K	116	HIS
13	K	117	ASN
14	L	49	ASN
14	L	75	HIS
15	M	40	ASN
15	M	62	ASN
15	M	106	ASN
16	N	49	HIS
17	O	13	GLN
17	O	37	ASN
17	O	71	GLN
18	P	82	GLN
19	Q	16	GLN
20	R	36	ASN
21	S	14	HIS
21	S	23	ASN
21	S	53	ASN
21	S	56	GLN
21	S	69	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1506/1522 (98%)	243 (16%)	69 (4%)
2	W	3/4 (75%)	0	0
3	X	10/11 (90%)	2 (20%)	1 (10%)
All	All	1519/1537 (98%)	245 (16%)	70 (4%)

All (245) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	8	A
1	A	9	G
1	A	31	G
1	A	32	A
1	A	39	G
1	A	47	C
1	A	49	U
1	A	50	A
1	A	51	A
1	A	52	G
1	A	60	A
1	A	61	G
1	A	101	A
1	A	116	A
1	A	120	A
1	A	121	C
1	A	129(A)	G
1	A	130	A
1	A	131	C
1	A	144	G
1	A	163	C
1	A	182	U
1	A	189	G
1	A	190	C
1	A	190(A)	C
1	A	190(D)	U
1	A	190(E)	U
1	A	190(F)	G
1	A	190(L)	U
1	A	195	A
1	A	197	A
1	A	201	C
1	A	202	U
1	A	204	U
1	A	216	G

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Mol	Chain	Res	Type
1	A	244	U
1	A	247	G
1	A	251	G
1	A	252	U
1	A	266	G
1	A	267	C
1	A	280	C
1	A	282	A
1	A	289	G
1	A	328	C
1	A	329	A
1	A	332	G
1	A	344	A
1	A	345	C
1	A	351	G
1	A	352	C
1	A	353	A
1	A	354	G
1	A	367	U
1	A	373	A
1	A	397	A
1	A	398	C
1	A	411	A
1	A	413	G
1	A	414	A
1	A	416	G
1	A	417	C
1	A	420	U
1	A	421	U
1	A	422	C
1	A	423	G
1	A	424	G
1	A	425	G
1	A	429	U
1	A	430	A
1	A	439	A
1	A	448	A
1	A	452	A
1	A	461	C
1	A	462	G
1	A	481	G
1	A	482	A

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Mol	Chain	Res	Type
1	A	484	G
1	A	485	G
1	A	497	A
1	A	498	U
1	A	509	A
1	A	510	A
1	A	511	C
1	A	518	C
1	A	519	C
1	A	527	G
1	A	531	U
1	A	532	A
1	A	533	A
1	A	534	U
1	A	547	A
1	A	559	A
1	A	560	U
1	A	561	U
1	A	562	C
1	A	572	A
1	A	573	A
1	A	575	G
1	A	576	G
1	A	577	G
1	A	596	C
1	A	653	A
1	A	665	A
1	A	666	G
1	A	686	U
1	A	687	A
1	A	688	G
1	A	695	A
1	A	702	A
1	A	703	G
1	A	718	G
1	A	723	U
1	A	731	G
1	A	733	A
1	A	748	C
1	A	755	G
1	A	777	A
1	A	781	A

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Mol	Chain	Res	Type
1	A	782	A
1	A	793	U
1	A	794	A
1	A	813	U
1	A	817	C
1	A	819	A
1	A	820	U
1	A	828	A
1	A	839	U
1	A	840	C
1	A	841	U
1	A	848	C
1	A	902	G
1	A	913	A
1	A	914	A
1	A	922	G
1	A	926	G
1	A	927	G
1	A	934	C
1	A	935	A
1	A	945	G
1	A	960	U
1	A	961	U
1	A	966	G
1	A	969	A
1	A	971	G
1	A	974	A
1	A	975	A
1	A	976	G
1	A	977	A
1	A	991	U
1	A	992	U
1	A	993	G
1	A	994	A
1	A	1005	A
1	A	1021	G
1	A	1027	C
1	A	1028	C
1	A	1029	C
1	A	1032	G
1	A	1036	G
1	A	1045	C

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Mol	Chain	Res	Type
1	A	1050	G
1	A	1053	G
1	A	1054	C
1	A	1055	A
1	A	1065	U
1	A	1066	C
1	A	1068	G
1	A	1094	G
1	A	1095	U
1	A	1101	A
1	A	1117	G
1	A	1125	U
1	A	1129	C
1	A	1130	A
1	A	1137	C
1	A	1138	G
1	A	1139	G
1	A	1146	A
1	A	1152	A
1	A	1159	U
1	A	1160	G
1	A	1183	A
1	A	1184	G
1	A	1196	U
1	A	1197	G
1	A	1200	C
1	A	1201	A
1	A	1202	G
1	A	1212	U
1	A	1214	C
1	A	1224	G
1	A	1225	A
1	A	1226	C
1	A	1227	A
1	A	1257	U
1	A	1280	A
1	A	1281	U
1	A	1282	C
1	A	1285	A
1	A	1286	A
1	A	1287	A
1	A	1300	G

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Mol	Chain	Res	Type
1	A	1301	U
1	A	1302	U
1	A	1303	C
1	A	1305	G
1	A	1320	C
1	A	1338	G
1	A	1346	A
1	A	1347	G
1	A	1348	U
1	A	1353	G
1	A	1361	G
1	A	1362	C
1	A	1363	A
1	A	1379	G
1	A	1381	U
1	A	1398	A
1	A	1401	G
1	A	1442	G
1	A	1443	G
1	A	1446	A
1	A	1447	G
1	A	1452	C
1	A	1487	G
1	A	1490	C
1	A	1492	A
1	A	1494	G
1	A	1499	A
1	A	1502	A
1	A	1503	A
1	A	1504	G
1	A	1505	G
1	A	1506	U
1	A	1517	G
1	A	1520	G
1	A	1529	G
1	A	1530	G
1	A	1533	C
1	A	1534	A
1	A	1539	C
1	A	1541	U
3	X	37	T6A
3	X	38	A

All (70) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	7	G
1	A	30	U
1	A	48	C
1	A	51	A
1	A	60	A
1	A	115	G
1	A	119	A
1	A	129(A)	G
1	A	181	G
1	A	243	A
1	A	250	A
1	A	251	G
1	A	266	G
1	A	279	A
1	A	281	G
1	A	328	C
1	A	344	A
1	A	353	A
1	A	366	C
1	A	372	C
1	A	428	G
1	A	429	U
1	A	484	G
1	A	496	A
1	A	497	A
1	A	509	A
1	A	518	C
1	A	533	A
1	A	559	A
1	A	560	U
1	A	575	G
1	A	687	A
1	A	701	C
1	A	792	A
1	A	812	C
1	A	819	A
1	A	840	C
1	A	913	A
1	A	945	G
1	A	960	U
1	A	965	A
1	A	975	A

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Mol	Chain	Res	Type
1	A	992	U
1	A	993	G
1	A	1049	U
1	A	1065	U
1	A	1067	A
1	A	1117	G
1	A	1183	A
1	A	1196	U
1	A	1201	A
1	A	1224	G
1	A	1226	C
1	A	1281	U
1	A	1285	A
1	A	1300	G
1	A	1301	U
1	A	1302	U
1	A	1346	A
1	A	1347	G
1	A	1380	U
1	A	1397	C
1	A	1451	A
1	A	1490	C
1	A	1498	U
1	A	1503	A
1	A	1504	G
1	A	1505	G
1	A	1528	U
3	X	37	T6A

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

1 non-standard protein/DNA/RNA residue is 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
3	T6A	X	37	3	31,34,35	1.31	6 (19%)	43,49,52	3.22	11 (25%)

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
3	T6A	X	37	3	1/1/9/11	5/23/41/42	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	X	37	T6A	C15-C14	-3.24	1.42	1.51
3	X	37	T6A	ODA-C13	3.16	1.31	1.22
3	X	37	T6A	O14-C14	-2.96	1.35	1.43
3	X	37	T6A	ODB-C13	-2.79	1.21	1.30
3	X	37	T6A	C6-N6	-2.28	1.34	1.39
3	X	37	T6A	C12-N11	-2.05	1.41	1.45

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	X	37	T6A	O14-C14-C15	11.98	145.52	109.68
3	X	37	T6A	C12-N11-C10	7.93	135.18	121.99
3	X	37	T6A	O14-C14-C12	-7.08	94.80	109.07
3	X	37	T6A	ODA-C13-C12	-6.88	99.03	121.86
3	X	37	T6A	N6-C10-N11	6.27	122.40	113.77
3	X	37	T6A	ODB-C13-C12	5.67	133.83	114.15
3	X	37	T6A	C13-C12-N11	4.53	120.13	110.17
3	X	37	T6A	O10-C10-N6	-4.21	116.16	123.64
3	X	37	T6A	C15-C14-C12	3.71	119.62	112.29
3	X	37	T6A	C5-C6-N6	2.34	124.91	118.94
3	X	37	T6A	O4'-C4'-C5'	-2.26	102.10	109.33

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	X	37	T6A	C14

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	X	37	T6A	N11-C12-C14-O14
3	X	37	T6A	C13-C12-C14-O14
3	X	37	T6A	C13-C12-N11-C10
3	X	37	T6A	C13-C12-C14-C15
3	X	37	T6A	C14-C12-N11-C10

There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	X	37	T6A	8	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 110 ligands modelled in this entry, 109 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
24	PAR	A	1545	1	44,45,45	1.46	6 (13%)	63,67,67	1.26	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
24	PAR	A	1545	1	-	4/18/94/94	0/4/4/4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	1545	PAR	C24-N24	4.16	1.53	1.47
24	A	1545	PAR	O54-C14	3.76	1.51	1.41
24	A	1545	PAR	C11-C21	3.13	1.58	1.52
24	A	1545	PAR	C44-C34	2.18	1.58	1.52
24	A	1545	PAR	O51-C11	2.15	1.47	1.41
24	A	1545	PAR	O51-C51	2.13	1.49	1.44

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	1545	PAR	C14-O54-C54	3.72	120.99	113.72
24	A	1545	PAR	O33-C14-C24	3.41	113.65	108.08
24	A	1545	PAR	O11-C11-C21	3.03	113.04	108.08
24	A	1545	PAR	O54-C54-C64	2.74	111.33	106.07
24	A	1545	PAR	O52-C13-O43	-2.29	109.03	111.37
24	A	1545	PAR	C22-C12-C62	-2.03	107.04	110.08
24	A	1545	PAR	C22-C32-C42	2.02	114.45	109.50

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	A	1545	PAR	C33-C43-C53-O53
24	A	1545	PAR	O43-C43-C53-O53
24	A	1545	PAR	C24-C14-O33-C33
24	A	1545	PAR	C52-C42-O11-C11

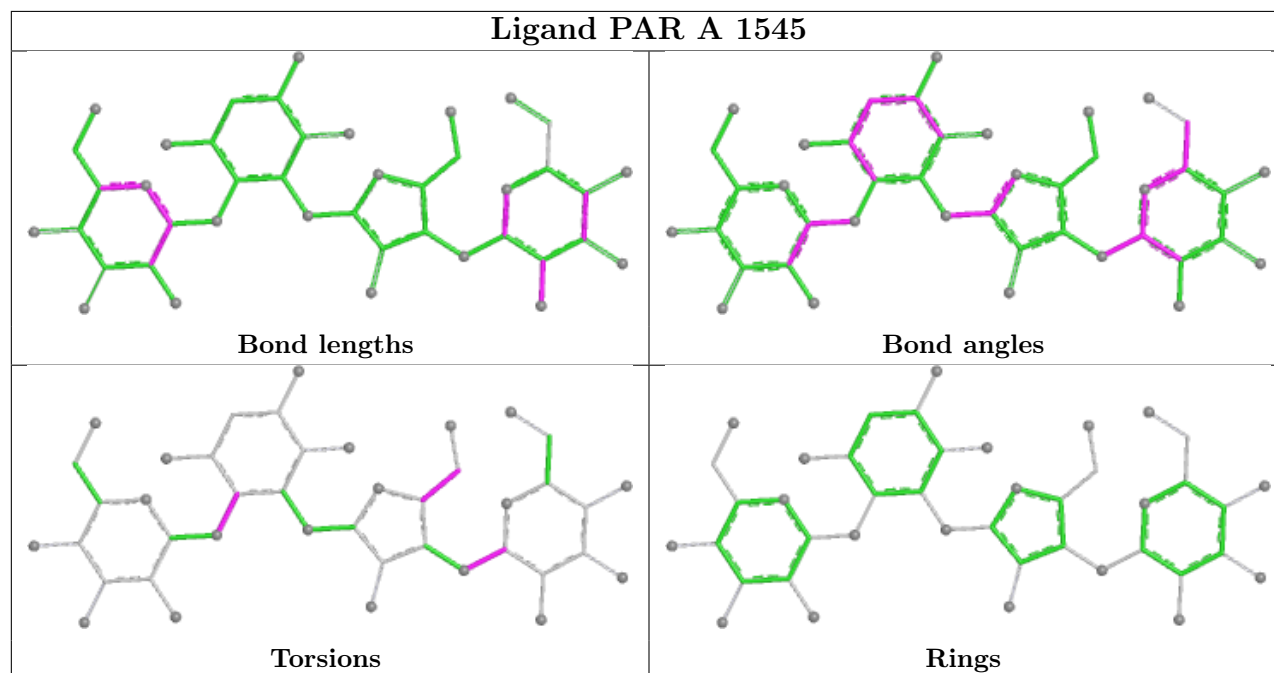
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	A	1545	PAR	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1506/1522 (98%)	0.52	151 (10%) 12 7	29, 61, 149, 201	0
2	W	4/4 (100%)	0.38	0 100 100	49, 53, 55, 126	0
3	X	10/11 (90%)	1.65	3 (30%) 1 1	63, 79, 146, 163	0
4	B	234/256 (91%)	0.94	28 (11%) 9 5	38, 106, 176, 201	0
5	C	206/239 (86%)	1.09	36 (17%) 4 3	41, 91, 159, 197	0
6	D	208/209 (99%)	0.63	20 (9%) 13 7	41, 72, 143, 200	0
7	E	150/162 (92%)	0.20	5 (3%) 49 28	33, 56, 107, 187	0
8	F	101/101 (100%)	0.81	7 (6%) 23 12	51, 99, 138, 167	0
9	G	155/156 (99%)	0.55	10 (6%) 25 13	34, 82, 151, 191	0
10	H	138/138 (100%)	0.14	1 (0%) 84 66	32, 53, 99, 163	0
11	I	127/128 (99%)	1.08	20 (15%) 5 3	43, 96, 148, 200	0
12	J	98/105 (93%)	1.70	35 (35%) 1 1	47, 127, 197, 201	0
13	K	119/129 (92%)	0.44	10 (8%) 17 9	37, 67, 120, 182	0
14	L	124/135 (91%)	0.40	11 (8%) 15 8	31, 56, 135, 175	0
15	M	125/126 (99%)	1.03	20 (16%) 5 3	47, 83, 165, 201	0
16	N	60/61 (98%)	1.47	16 (26%) 1 1	50, 81, 133, 200	0
17	O	88/89 (98%)	0.41	4 (4%) 38 20	39, 74, 135, 195	0
18	P	83/88 (94%)	0.22	1 (1%) 76 55	36, 52, 94, 174	0
19	Q	104/105 (99%)	0.46	11 (10%) 11 6	29, 57, 139, 201	0
20	R	73/88 (82%)	0.42	6 (8%) 17 9	50, 74, 161, 193	0
21	S	80/93 (86%)	1.22	16 (20%) 3 2	55, 105, 165, 201	0
22	T	99/106 (93%)	0.46	6 (6%) 27 14	28, 59, 118, 175	0
23	V	24/27 (88%)	1.09	5 (20%) 2 2	39, 67, 122, 166	0
All	All	3916/4078 (96%)	0.65	422 (10%) 11 6	28, 70, 158, 201	0

All (422) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	419	C	14.3
1	A	1361	G	9.5
1	A	425	G	9.0
1	A	412	A	8.8
1	A	418	C	8.6
15	M	123	ALA	8.4
1	A	190	C	7.7
1	A	1129	C	7.5
1	A	426	G	7.3
6	D	31	CYS	7.0
1	A	416	G	6.9
6	D	23	GLY	6.7
1	A	1027	C	6.6
1	A	413	G	6.5
1	A	411	A	6.5
15	M	118	ALA	6.3
21	S	2	PRO	6.1
1	A	424	G	6.0
1	A	417	C	5.9
6	D	9	CYS	5.9
1	A	1035	A	5.8
1	A	1540	U	5.6
12	J	17	ASP	5.6
1	A	423	G	5.5
1	A	631	G	5.4
15	M	126	LYS	5.3
15	M	7	VAL	5.2
15	M	106	ASN	5.2
6	D	24	GLU	5.2
1	A	1533	C	5.1
21	S	3	ARG	5.0
1	A	1362	C	5.0
1	A	1124	G	5.0
1	A	1125	U	5.0
16	N	22	THR	5.0
1	A	1126	U	4.9
6	D	33	MET	4.9
1	A	415	A	4.9
15	M	124	PRO	4.9
14	L	89	ARG	4.8
16	N	30	ALA	4.8
1	A	1539	C	4.7

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Mol	Chain	Res	Type	RSRZ
9	G	143	ARG	4.7
6	D	26	CYS	4.7
22	T	12	ALA	4.7
11	I	128	ARG	4.7
21	S	5	LEU	4.6
1	A	1021	G	4.6
1	A	1029	C	4.6
11	I	64	THR	4.6
4	B	16	HIS	4.6
1	A	1200	C	4.6
1	A	1256	A	4.6
1	A	190(A)	C	4.5
1	A	1541	U	4.5
1	A	481	G	4.5
1	A	1142	G	4.4
4	B	238	LEU	4.4
1	A	723	U	4.3
1	A	1033	G	4.3
3	X	30	G	4.3
1	A	1004	A	4.3
22	T	100	ILE	4.3
1	A	1017	G	4.3
1	A	420	U	4.3
1	A	1135	U	4.2
1	A	532	A	4.2
1	A	1003	G	4.2
16	N	57	ARG	4.1
12	J	36	GLY	4.1
1	A	1442	G	4.1
1	A	1022	G	4.1
6	D	19	LEU	4.0
1	A	204	U	4.0
15	M	8	GLU	4.0
18	P	83	GLU	4.0
1	A	1030	C	3.9
12	J	34	VAL	3.9
1	A	1005	A	3.9
1	A	1213	A	3.9
14	L	47	LYS	3.9
7	E	154	GLY	3.9
21	S	26	GLY	3.9
12	J	10	GLY	3.9

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Mol	Chain	Res	Type	RSRZ
4	B	220	ASP	3.9
5	C	154	SER	3.9
6	D	209	ARG	3.8
23	V	6	ARG	3.8
11	I	119	ALA	3.8
11	I	16	ARG	3.8
21	S	37	ARG	3.8
23	V	10	ARG	3.8
5	C	167	TRP	3.8
1	A	1196	U	3.8
1	A	1054	C	3.7
19	Q	105	ALA	3.7
1	A	1032	G	3.7
1	A	1127	G	3.7
1	A	1145	C	3.7
19	Q	101	ARG	3.7
1	A	1024	G	3.7
13	K	51	LYS	3.7
12	J	59	SER	3.6
1	A	1036	G	3.6
12	J	15	THR	3.6
1	A	1146	A	3.6
15	M	125	ARG	3.6
14	L	26	ALA	3.6
8	F	84	ASN	3.5
1	A	848	C	3.5
1	A	1028	C	3.5
1	A	1013	G	3.5
19	Q	102	GLY	3.5
1	A	1278	U	3.5
12	J	6	ILE	3.5
15	M	122	LYS	3.5
1	A	344	A	3.5
12	J	58	ASP	3.5
1	A	1002	G	3.5
1	A	1026	G	3.5
1	A	1281	U	3.5
1	A	1018	C	3.4
1	A	630	G	3.4
1	A	1370	G	3.4
12	J	5	ARG	3.4
1	A	1446	A	3.4

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Mol	Chain	Res	Type	RSRZ
13	K	52	GLY	3.4
21	S	53	ASN	3.4
5	C	205	GLY	3.4
23	V	25	LYS	3.4
12	J	70	ARG	3.4
1	A	1050	G	3.4
1	A	1143	G	3.4
1	A	1025	U	3.3
1	A	1260	C	3.3
3	X	40	C	3.3
7	E	83	GLU	3.3
5	C	75	VAL	3.3
21	S	6	LYS	3.3
16	N	2	ALA	3.3
6	D	21	LEU	3.3
11	I	30	GLY	3.3
1	A	1023	G	3.3
6	D	86	LYS	3.3
11	I	127	LYS	3.2
1	A	1031	G	3.2
1	A	1131	G	3.2
13	K	54	ARG	3.2
9	G	137	LYS	3.2
12	J	35	SER	3.2
16	N	13	THR	3.2
16	N	8	GLU	3.2
1	A	421	U	3.2
1	A	1128	C	3.2
12	J	75	ILE	3.2
1	A	414	A	3.1
14	L	28	LYS	3.1
21	S	77	THR	3.1
5	C	35	GLU	3.1
5	C	21	ARG	3.1
12	J	41	PRO	3.1
1	A	427	U	3.1
5	C	161	GLU	3.1
14	L	73	GLU	3.1
19	Q	13	ASP	3.1
16	N	21	TYR	3.1
17	O	23	GLY	3.0
22	T	101	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
5	C	62	ASP	3.0
1	A	88	A	3.0
9	G	2	ALA	3.0
4	B	140	HIS	3.0
5	C	96	GLY	3.0
1	A	422	C	3.0
12	J	77	PRO	3.0
9	G	16	LEU	3.0
4	B	206	ASP	3.0
1	A	1190	G	3.0
8	F	60	PHE	3.0
4	B	35	GLU	3.0
12	J	57	LYS	3.0
5	C	207	VAL	3.0
15	M	119	GLY	3.0
15	M	58	GLU	2.9
11	I	39	GLY	2.9
1	A	1134	G	2.9
1	A	1421	G	2.9
1	A	1130	A	2.9
1	A	1248	A	2.9
4	B	96	ARG	2.9
16	N	6	LEU	2.9
1	A	1006	C	2.9
5	C	13	GLY	2.9
4	B	127	ILE	2.9
15	M	11	ARG	2.9
13	K	36	ASP	2.9
22	T	106	ALA	2.9
11	I	22	GLY	2.9
5	C	82	GLU	2.9
4	B	122	PHE	2.9
14	L	115	LYS	2.9
1	A	991	U	2.8
12	J	64	GLU	2.8
14	L	128	ALA	2.8
1	A	1009	G	2.8
1	A	1094	G	2.8
1	A	1139	G	2.8
5	C	56	ASP	2.8
12	J	100	THR	2.8
16	N	18	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
10	H	98	LYS	2.8
15	M	120	LYS	2.8
12	J	8	LEU	2.8
6	D	32	ALA	2.8
1	A	1162	C	2.8
19	Q	96	GLN	2.8
23	V	24	ARG	2.8
5	C	87	LEU	2.8
19	Q	103	GLY	2.8
1	A	461	C	2.8
11	I	97	LYS	2.8
13	K	127	LYS	2.8
1	A	1034	G	2.8
1	A	1133	G	2.8
11	I	125	TYR	2.7
11	I	27	THR	2.7
16	N	61	TRP	2.7
1	A	993	G	2.7
9	G	154	TYR	2.7
12	J	78	ASN	2.7
21	S	49	ILE	2.7
21	S	62	ILE	2.7
11	I	12	GLU	2.7
21	S	81	ARG	2.7
4	B	19	HIS	2.7
12	J	72	VAL	2.7
4	B	44	LEU	2.7
4	B	86	GLU	2.7
7	E	50	GLU	2.7
1	A	202	U	2.7
1	A	1542	U	2.7
12	J	7	LYS	2.7
1	A	1020	U	2.7
13	K	117	ASN	2.7
7	E	20	GLN	2.6
17	O	9	GLN	2.6
16	N	28	GLY	2.6
17	O	7	GLU	2.6
1	A	266	G	2.6
1	A	460	A	2.6
1	A	1259	C	2.6
11	I	117	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
19	Q	104	LYS	2.6
1	A	1257	U	2.6
5	C	19	GLU	2.6
1	A	485	G	2.6
8	F	49	ALA	2.6
5	C	127	ARG	2.6
8	F	1	MET	2.6
1	A	1043	C	2.6
5	C	155	GLY	2.6
5	C	94	LEU	2.6
5	C	85	ARG	2.6
5	C	69	HIS	2.5
1	A	1300	G	2.5
4	B	209	ARG	2.5
12	J	73	ASP	2.5
6	D	34	GLU	2.5
4	B	148	TYR	2.5
6	D	3	ARG	2.5
13	K	128	ALA	2.5
1	A	251	G	2.5
1	A	1144	G	2.5
6	D	18	LYS	2.5
1	A	1012	U	2.5
1	A	1544	U	2.5
12	J	89	ASP	2.5
21	S	33	THR	2.5
4	B	10	LEU	2.5
6	D	36	ARG	2.5
9	G	151	TYR	2.5
1	A	1279	A	2.5
5	C	64	VAL	2.5
12	J	33	GLN	2.5
1	A	410	G	2.5
1	A	1038	C	2.5
16	N	35	ARG	2.5
19	Q	14	LYS	2.5
1	A	996	A	2.4
20	R	83	GLU	2.4
6	D	30	LYS	2.4
8	F	77	ARG	2.4
5	C	4	LYS	2.4
12	J	80	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
12	J	24	VAL	2.4
4	B	189	ASP	2.4
12	J	12	ASP	2.4
7	E	8	GLU	2.4
4	B	228	GLY	2.4
15	M	77	ASN	2.4
12	J	32	ALA	2.4
14	L	79	GLU	2.4
8	F	63	TYR	2.3
16	N	3	ARG	2.3
23	V	5	ASP	2.3
1	A	306	G	2.3
5	C	105	GLU	2.3
12	J	81	THR	2.3
5	C	60	ALA	2.3
15	M	9	ILE	2.3
1	A	980	C	2.3
5	C	91	LEU	2.3
4	B	131	PRO	2.3
4	B	192	SER	2.3
20	R	48	GLY	2.3
20	R	25	THR	2.3
1	A	1483	A	2.3
1	A	1019	C	2.3
4	B	136	VAL	2.3
11	I	65	VAL	2.3
20	R	29	PHE	2.3
1	A	1001	A	2.3
6	D	132	ARG	2.3
12	J	37	PRO	2.3
1	A	217	C	2.3
1	A	1277	C	2.3
12	J	3	LYS	2.3
5	C	88	ARG	2.3
1	A	1053	G	2.2
1	A	373	A	2.2
5	C	67	THR	2.2
11	I	78	LYS	2.2
13	K	53	SER	2.2
1	A	1484	C	2.2
9	G	5	ARG	2.2
12	J	45	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
4	B	7	VAL	2.2
5	C	110	ASN	2.2
19	Q	26	GLN	2.2
21	S	27	GLU	2.2
22	T	95	ALA	2.2
1	A	216	G	2.2
1	A	1258	G	2.2
16	N	9	LYS	2.2
1	A	992	U	2.2
1	A	975	A	2.2
1	A	1204	A	2.2
1	A	1268	A	2.2
1	A	999	C	2.2
1	A	1140	C	2.2
9	G	140	ASP	2.2
13	K	77	MET	2.2
14	L	92	ASP	2.2
5	C	30	ARG	2.2
5	C	76	VAL	2.2
1	A	1049	U	2.2
1	A	1212	U	2.2
1	A	190(K)	G	2.2
1	A	1176	A	2.2
1	A	1224	G	2.2
1	A	1475	G	2.2
11	I	102	LEU	2.2
12	J	93	GLY	2.2
19	Q	100	LYS	2.2
5	C	23	TYR	2.2
6	D	42	GLN	2.2
11	I	126	SER	2.2
21	S	4	SER	2.2
14	L	27	LEU	2.2
11	I	29	ASN	2.2
1	A	841	U	2.2
4	B	227	GLY	2.2
1	A	1182	G	2.2
15	M	73	GLU	2.1
13	K	111	ASP	2.1
4	B	229	VAL	2.1
17	O	48	LYS	2.1
15	M	75	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
5	C	63	ASN	2.1
15	M	16	ASP	2.1
5	C	97	LYS	2.1
12	J	87	THR	2.1
19	Q	17	LYS	2.1
6	D	35	ARG	2.1
9	G	110	GLN	2.1
1	A	1014	A	2.1
1	A	1041	A	2.1
1	A	1167	A	2.1
1	A	1373	G	2.1
12	J	71	LEU	2.1
3	X	33	U	2.1
4	B	128	GLU	2.1
20	R	46	GLU	2.1
16	N	60	SER	2.1
1	A	1502	A	2.1
20	R	88	LYS	2.1
4	B	23	ARG	2.1
11	I	66	ARG	2.1
1	A	1007	C	2.1
1	A	1198	G	2.1
1	A	1355	G	2.1
1	A	1443	G	2.1
5	C	2	GLY	2.1
9	G	56	GLN	2.1
6	D	37	PRO	2.1
8	F	31	GLU	2.1
4	B	97	TRP	2.0
4	B	48	MET	2.0
1	A	1275	A	2.0
14	L	61	THR	2.0
11	I	57	GLY	2.0
22	T	98	PRO	2.0
16	N	4	LYS	2.0
5	C	54	ARG	2.0
1	A	997	U	2.0
15	M	76	ALA	2.0
21	S	8	GLY	2.0
21	S	7	LYS	2.0
4	B	15	VAL	2.0
15	M	61	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
5	C	43	LEU	2.0
1	A	748	C	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	T6A	X	37	32/33	0.86	0.21	67,76,76,76	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
25	MG	A	441	1/1	0.45	0.39	29,29,29,29	1
25	MG	A	1562	1/1	0.60	0.74	29,29,29,29	1
25	MG	A	1595	1/1	0.67	0.63	29,29,29,29	1
25	MG	A	1585	1/1	0.68	0.61	29,29,29,29	1
25	MG	A	1613	1/1	0.70	0.74	29,29,29,29	1
25	MG	A	466	1/1	0.70	0.77	29,29,29,29	1
25	MG	A	1607	1/1	0.71	0.28	29,29,29,29	1
25	MG	A	1616	1/1	0.72	0.70	29,29,29,29	1
25	MG	A	1617	1/1	0.73	0.28	29,29,29,29	1
25	MG	N	423	1/1	0.73	0.57	29,29,29,29	1
25	MG	A	493	1/1	0.74	0.43	29,29,29,29	1
25	MG	A	214	1/1	0.75	0.64	29,29,29,29	1
25	MG	A	1632	1/1	0.76	0.32	29,29,29,29	1
25	MG	A	1608	1/1	0.78	0.58	29,29,29,29	1
25	MG	A	1610	1/1	0.80	0.44	29,29,29,29	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	MG	A	1565	1/1	0.80	0.36	29,29,29,29	1
25	MG	A	1631	1/1	0.80	0.20	29,29,29,29	1
25	MG	A	1583	1/1	0.82	0.29	29,29,29,29	0
25	MG	A	1612	1/1	0.82	0.24	29,29,29,29	1
25	MG	A	1586	1/1	0.82	0.29	29,29,29,29	0
25	MG	X	500	1/1	0.82	0.41	29,29,29,29	1
25	MG	A	1615	1/1	0.82	0.30	29,29,29,29	1
25	MG	A	1550	1/1	0.83	0.28	29,29,29,29	1
25	MG	A	1602	1/1	0.84	0.17	29,29,29,29	1
25	MG	A	1624	1/1	0.84	0.35	29,29,29,29	1
25	MG	A	1546	1/1	0.84	0.26	29,29,29,29	0
25	MG	A	1591	1/1	0.84	0.30	29,29,29,29	0
25	MG	A	1584	1/1	0.85	0.35	29,29,29,29	0
25	MG	A	1576	1/1	0.85	0.28	29,29,29,29	0
25	MG	A	1627	1/1	0.85	0.32	29,29,29,29	1
25	MG	A	1630	1/1	0.85	0.32	29,29,29,29	1
25	MG	A	1558	1/1	0.85	0.26	29,29,29,29	1
25	MG	A	1571	1/1	0.86	0.17	29,29,29,29	0
25	MG	A	1556	1/1	0.86	0.31	29,29,29,29	0
24	PAR	A	1545	42/42	0.86	0.14	28,28,28,28	0
25	MG	A	1609	1/1	0.86	0.41	29,29,29,29	1
25	MG	A	1597	1/1	0.86	0.12	29,29,29,29	0
25	MG	A	1600	1/1	0.87	0.33	29,29,29,29	1
25	MG	A	469	1/1	0.88	0.23	29,29,29,29	1
25	MG	A	210	1/1	0.88	0.22	29,29,29,29	1
25	MG	A	1548	1/1	0.88	0.36	29,29,29,29	1
25	MG	A	1547	1/1	0.88	0.29	29,29,29,29	0
25	MG	A	1579	1/1	0.88	0.27	29,29,29,29	1
25	MG	X	502	1/1	0.88	0.19	29,29,29,29	1
25	MG	A	1568	1/1	0.88	0.19	29,29,29,29	0
25	MG	A	1551	1/1	0.89	0.33	29,29,29,29	0
25	MG	A	1599	1/1	0.89	0.33	29,29,29,29	1
25	MG	A	1566	1/1	0.89	0.43	29,29,29,29	1
25	MG	A	473	1/1	0.89	0.28	29,29,29,29	1
25	MG	A	1596	1/1	0.89	0.30	29,29,29,29	0
25	MG	A	1626	1/1	0.90	0.25	29,29,29,29	1
25	MG	A	1578	1/1	0.90	0.23	29,29,29,29	0
25	MG	A	1629	1/1	0.90	0.23	29,29,29,29	1
25	MG	A	1633	1/1	0.90	0.38	29,29,29,29	1
25	MG	A	1620	1/1	0.90	0.44	29,29,29,29	1
25	MG	A	1623	1/1	0.90	0.13	29,29,29,29	1
25	MG	A	1552	1/1	0.90	0.26	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	MG	A	471	1/1	0.90	0.59	29,29,29,29	1
25	MG	A	1555	1/1	0.91	0.33	29,29,29,29	0
25	MG	A	1577	1/1	0.91	0.19	29,29,29,29	0
25	MG	A	1587	1/1	0.91	0.25	29,29,29,29	0
25	MG	A	1590	1/1	0.91	0.28	29,29,29,29	0
25	MG	A	1628	1/1	0.91	0.39	29,29,29,29	1
25	MG	A	1564	1/1	0.91	0.25	29,29,29,29	0
25	MG	A	1560	1/1	0.91	0.26	29,29,29,29	0
25	MG	A	1572	1/1	0.91	0.28	29,29,29,29	1
25	MG	A	1574	1/1	0.91	0.29	29,29,29,29	0
25	MG	A	1635	1/1	0.92	0.21	29,29,29,29	0
25	MG	A	1554	1/1	0.92	0.35	29,29,29,29	1
25	MG	A	71	1/1	0.92	0.36	29,29,29,29	1
25	MG	A	1569	1/1	0.92	0.39	29,29,29,29	1
25	MG	A	1570	1/1	0.93	0.19	29,29,29,29	0
25	MG	A	1621	1/1	0.93	0.43	29,29,29,29	1
25	MG	A	1567	1/1	0.93	0.48	29,29,29,29	1
25	MG	A	1557	1/1	0.93	0.27	29,29,29,29	0
25	MG	A	1625	1/1	0.93	0.26	29,29,29,29	0
25	MG	A	1614	1/1	0.93	0.15	29,29,29,29	0
25	MG	A	1634	1/1	0.93	0.53	29,29,29,29	1
25	MG	A	1603	1/1	0.93	0.52	29,29,29,29	1
25	MG	A	1563	1/1	0.93	0.26	29,29,29,29	1
25	MG	A	1588	1/1	0.93	0.31	29,29,29,29	0
25	MG	A	1618	1/1	0.93	0.20	29,29,29,29	0
25	MG	A	1575	1/1	0.93	0.44	29,29,29,29	1
25	MG	A	1581	1/1	0.94	0.43	29,29,29,29	1
25	MG	A	1601	1/1	0.94	0.07	29,29,29,29	0
25	MG	A	467	1/1	0.94	0.13	29,29,29,29	1
25	MG	A	1611	1/1	0.94	0.21	29,29,29,29	1
25	MG	A	1592	1/1	0.94	0.14	29,29,29,29	0
25	MG	A	1605	1/1	0.95	0.31	29,29,29,29	1
25	MG	A	1622	1/1	0.95	0.94	29,29,29,29	1
25	MG	A	86	1/1	0.95	0.23	29,29,29,29	1
25	MG	A	1561	1/1	0.95	0.16	29,29,29,29	1
25	MG	A	211	1/1	0.95	0.41	29,29,29,29	1
25	MG	A	1553	1/1	0.95	0.38	29,29,29,29	0
25	MG	A	1604	1/1	0.96	0.26	29,29,29,29	1
25	MG	A	87	1/1	0.96	0.45	29,29,29,29	1
25	MG	A	1606	1/1	0.96	0.14	29,29,29,29	0
25	MG	A	1582	1/1	0.96	0.27	29,29,29,29	0
25	MG	A	1593	1/1	0.96	0.29	29,29,29,29	0

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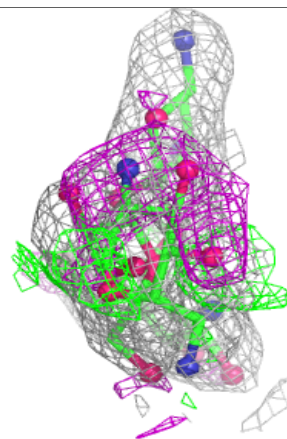
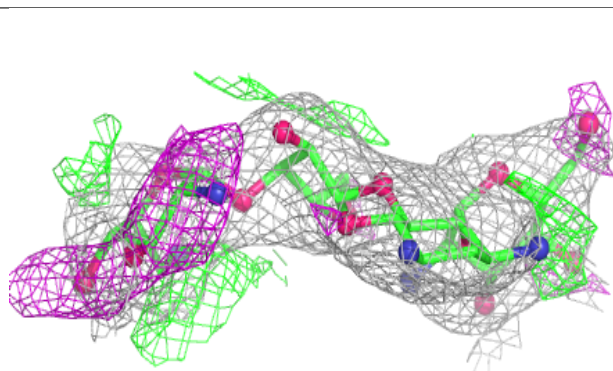
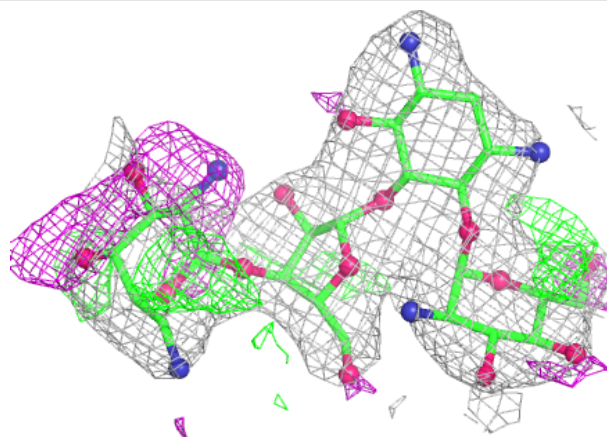
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	MG	A	1594	1/1	0.96	0.32	29,29,29,29	1
25	MG	A	470	1/1	0.96	0.25	29,29,29,29	1
25	MG	A	1559	1/1	0.96	0.25	29,29,29,29	1
25	MG	A	1573	1/1	0.96	0.27	29,29,29,29	0
25	MG	A	1549	1/1	0.97	0.34	29,29,29,29	1
25	MG	A	1598	1/1	0.97	0.19	29,29,29,29	0
25	MG	A	1619	1/1	0.97	0.20	29,29,29,29	0
25	MG	A	1580	1/1	0.98	0.55	29,29,29,29	1
26	ZN	D	306	1/1	0.98	0.18	29,29,29,29	1
25	MG	A	1589	1/1	0.99	0.36	29,29,29,29	0
26	ZN	N	307	1/1	1.00	0.05	29,29,29,29	1

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

Electron density around PAR A 1545:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.