Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 12:07 am GMT

PDB ID	:	2CZJ
Title	:	Crystal structure of the tRNA domain of tmRNA from Thermus thermophilus HB8
Authors	:	Bessho, Y.; Shibata, R.; Sekine, S.; Murayama, K.; Shirouzu, M.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on	:	2005-07-13
Resolution	:	3.01 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

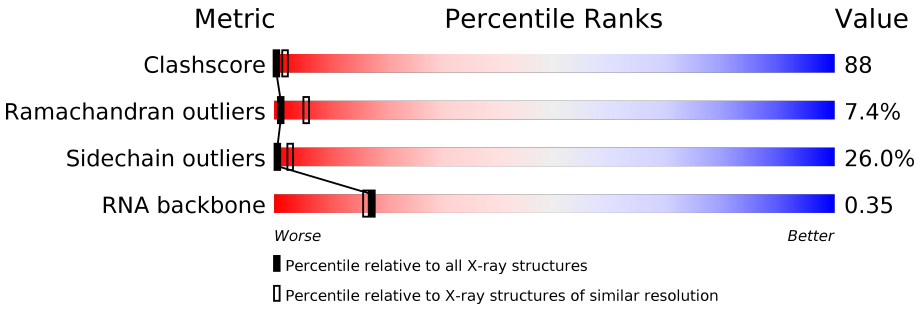
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.01 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	2279 (3.04-3.00)
Ramachandran outliers	110173	2207 (3.04-3.00)
Sidechain outliers	110143	2210 (3.04-3.00)
RNA backbone	2435	1023 (3.38-2.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	123	19% 59% 19%
1	C	123	15% 56% 24%
1	E	123	12% 63% 17% 7%
1	G	123	9% 57% 28%
2	B	63	17% 41% 27% 13%
2	D	63	5% 46% 40% 8%

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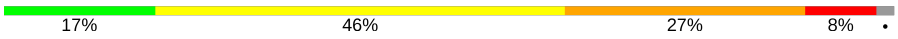
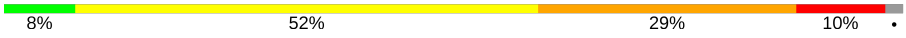
Mol	Chain	Length	Quality of chain
2	F	63	
2	H	63	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 9224 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 protein called SsrA-binding protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	122	Total	C	N	O	0	0	0
			993	637	181	175			
1	C	118	Total	C	N	O	0	0	0
			965	621	176	168			
1	E	122	Total	C	N	O	0	0	0
			993	637	181	175			
1	G	120	Total	C	N	O	0	0	0
			981	629	179	173			

- Molecule 2 is a RNA chain called tmRNA (63-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	62	Total	C	N	O	P	0	0	0
			1323	589	233	439	62			
2	D	62	Total	C	N	O	P	0	0	0
			1323	589	233	439	62			
2	F	62	Total	C	N	O	P	0	0	0
			1323	589	233	439	62			
2	H	62	Total	C	N	O	P	0	0	0
			1323	589	233	439	62			

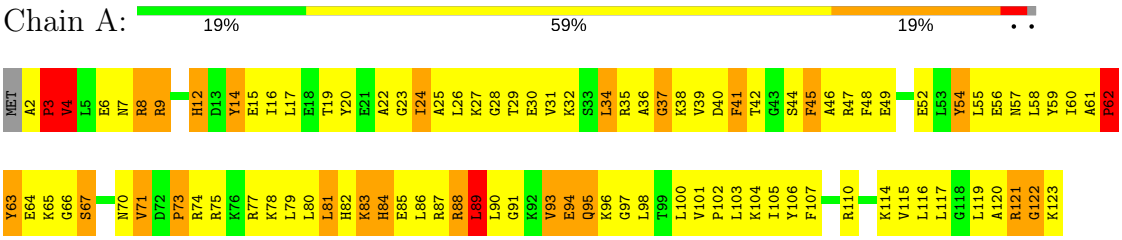
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

Note EDS was not executed.

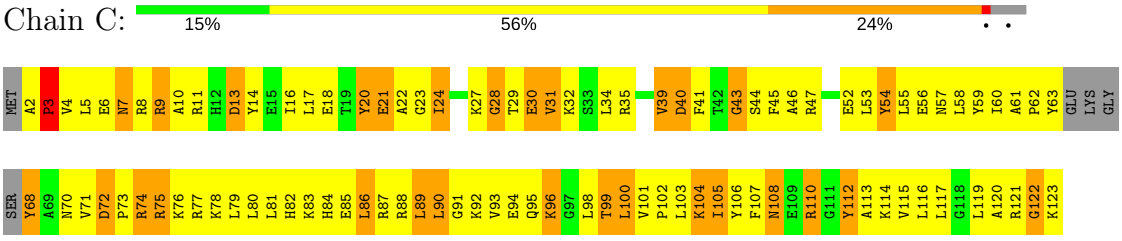
• Molecule 1: SsrA-binding protein

Chain A:



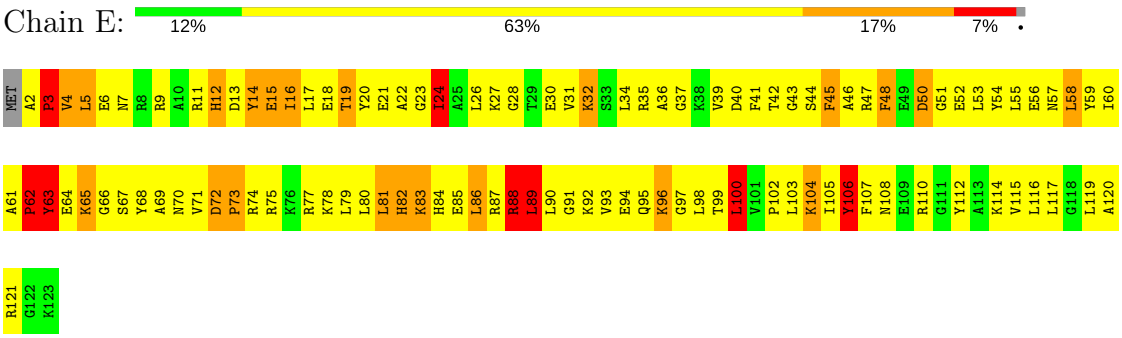
• Molecule 1: SsrA-binding protein

Chain C:



• Molecule 1: SsrA-binding protein

Chain E:

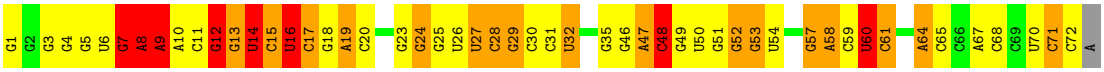


• Molecule 1: SsrA-binding protein

Chain G:

• Molecule 2: tmRNA (63-MER)

Chain B:

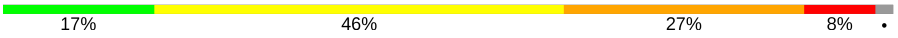


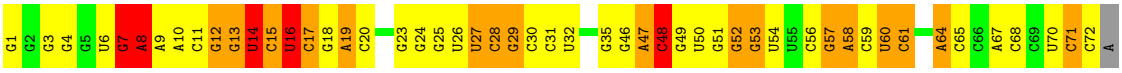
• Molecule 2: tmRNA (63-MER)

Chain D:

• Molecule 2: tmRNA (63-MER)

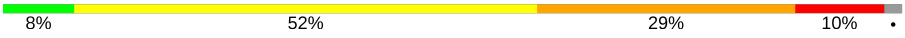
Chain F:





• Molecule 2: tmRNA (63-MER)

Chain H:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	84.78Å 67.96Å 178.66Å 90.00° 90.07° 90.00°	Depositor
Resolution (Å)	48.76 – 3.01	Depositor
% Data completeness (in resolution range)	96.7 (48.76-3.01)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.255 , 0.320	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9224	wwPDB-VP
Average B, all atoms (Å^2)	101.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.69	0/1011	1.01	5/1354 (0.4%)
1	C	1.04	1/982 (0.1%)	1.06	4/1315 (0.3%)
1	E	0.84	2/1011 (0.2%)	0.99	2/1354 (0.1%)
1	G	0.83	1/998 (0.1%)	1.15	6/1335 (0.4%)
2	B	0.94	2/1431 (0.1%)	1.14	13/2228 (0.6%)
2	D	1.09	11/1431 (0.8%)	1.35	30/2228 (1.3%)
2	F	0.94	2/1431 (0.1%)	1.05	8/2228 (0.4%)
2	H	0.98	6/1431 (0.4%)	1.12	17/2228 (0.8%)
All	All	0.94	25/9726 (0.3%)	1.13	85/14270 (0.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	2
1	E	0	1
1	G	0	1
2	B	0	2
2	F	0	3
2	H	0	1
All	All	0	11

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	43	GLY	C-O	-25.35	0.83	1.23
2	D	60	U	C3'-O3'	-10.09	1.28	1.42
2	D	57	G	O3'-P	-9.74	1.49	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	14	U	O3'-P	9.28	1.72	1.61
2	D	60	U	O3'-P	-8.00	1.51	1.61
2	D	59	C	C3'-O3'	-7.83	1.31	1.42
2	F	1	G	OP3-P	-7.71	1.51	1.61
2	D	57	G	C5'-C4'	-7.43	1.42	1.51
2	H	57	G	C5'-C4'	-7.38	1.42	1.51
2	D	19	A	O3'-P	-7.30	1.52	1.61
1	G	43	GLY	C-O	-7.24	1.12	1.23
2	D	57	G	P-O5'	-7.24	1.52	1.59
2	D	1	G	OP3-P	-7.22	1.52	1.61
2	B	1	G	OP3-P	-6.96	1.52	1.61
2	D	7	G	O3'-P	6.62	1.69	1.61
2	H	1	G	OP3-P	-6.61	1.53	1.61
2	D	61	C	P-OP1	-6.19	1.38	1.49
2	H	19	A	O3'-P	6.12	1.68	1.61
1	E	15	GLU	CB-CG	6.00	1.63	1.52
2	B	60	U	O3'-P	5.55	1.67	1.61
2	H	57	G	O3'-P	-5.53	1.54	1.61
2	H	57	G	P-O5'	-5.50	1.54	1.59
2	D	53	G	C3'-O3'	-5.23	1.34	1.42
2	H	57	G	O5'-C5'	-5.09	1.34	1.42
1	E	24	ILE	CA-CB	5.03	1.66	1.54

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	60	U	C4'-C3'-O3'	-13.33	81.41	109.40
1	G	66	GLY	N-CA-C	-12.89	80.88	113.10
1	C	43	GLY	CA-C-N	12.67	145.06	117.20
2	D	60	U	P-O3'-C3'	12.56	134.77	119.70
2	D	60	U	OP1-P-O3'	-12.41	77.89	105.20
2	D	48	C	O5'-P-OP2	-11.96	94.94	105.70
2	D	59	C	P-O3'-C3'	9.46	131.05	119.70
2	B	8	A	C2'-C3'-O3'	9.13	129.59	109.50
2	D	60	U	OP2-P-O3'	8.74	124.43	105.20
1	C	43	GLY	CA-C-O	-8.68	104.97	120.60
2	D	64	A	OP2-P-O3'	-8.42	86.67	105.20
2	D	57	G	O5'-P-OP2	-8.36	98.17	105.70
2	H	7	G	C4'-C3'-O3'	8.36	129.71	113.00
2	D	48	C	O5'-P-OP1	-8.21	98.31	105.70
2	D	59	C	C2'-C3'-O3'	-8.13	91.62	109.50
2	F	8	A	C2'-C3'-O3'	7.97	127.04	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	43	GLY	O-C-N	-7.97	109.94	122.70
2	H	60	U	C4'-C3'-O3'	-7.92	92.77	109.40
2	D	64	A	C4'-C3'-O3'	-7.51	93.63	109.40
1	E	3	PRO	N-CA-C	7.48	131.54	112.10
2	D	59	C	O4'-C4'-C3'	-7.48	96.52	104.00
2	B	58	A	O5'-P-OP2	-7.47	98.98	105.70
2	B	32	U	O5'-P-OP1	7.34	119.51	110.70
1	G	86	LEU	CA-CB-CG	7.27	132.03	115.30
2	H	7	G	OP2-P-O3'	7.07	120.74	105.20
1	G	58	LEU	CA-CB-CG	-7.01	99.18	115.30
2	D	56	C	OP2-P-O3'	6.84	120.24	105.20
1	E	100	LEU	CA-CB-CG	6.83	131.00	115.30
2	D	59	C	C4'-C3'-O3'	6.82	126.64	113.00
2	D	7	G	OP1-P-O3'	6.68	119.90	105.20
2	B	57	G	OP2-P-O3'	6.58	119.69	105.20
2	H	48	C	O5'-P-OP2	-6.57	99.79	105.70
2	D	58	A	O5'-P-OP2	6.34	118.31	110.70
2	D	48	C	N1-C1'-C2'	6.33	122.22	114.00
2	H	48	C	N1-C1'-C2'	6.14	121.98	114.00
1	A	4	VAL	N-CA-C	6.04	127.31	111.00
2	H	56	C	OP2-P-O3'	6.00	118.39	105.20
2	D	7	G	C2'-C3'-O3'	5.99	123.28	113.70
2	D	14	U	OP1-P-O3'	5.99	118.37	105.20
2	D	7	G	C4'-C3'-O3'	5.98	124.96	113.00
2	H	59	C	N1-C1'-C2'	-5.93	105.48	112.00
2	B	9	A	C4'-C3'-O3'	-5.71	97.42	109.40
2	H	7	G	C4'-C3'-C2'	5.71	108.31	102.60
2	D	57	G	O5'-P-OP1	-5.68	100.59	105.70
1	G	90	LEU	CA-CB-CG	5.67	128.35	115.30
2	D	60	U	C5'-C4'-O4'	5.67	115.90	109.10
2	D	14	U	OP2-P-O3'	-5.65	92.76	105.20
2	D	58	A	C5'-C4'-O4'	-5.64	102.33	109.10
2	B	24	G	N9-C1'-C2'	-5.63	105.81	112.00
2	H	47	A	OP1-P-O3'	5.63	117.59	105.20
2	B	14	U	OP2-P-O3'	-5.62	92.83	105.20
2	F	57	G	OP2-P-O3'	5.58	117.48	105.20
1	A	3	PRO	N-CA-C	5.58	126.60	112.10
1	G	7	ASN	N-CA-C	-5.56	95.98	111.00
2	D	47	A	OP2-P-O3'	5.52	117.35	105.20
2	B	7	G	C4'-C3'-C2'	5.50	108.10	102.60
1	G	43	GLY	CA-C-N	5.49	129.29	117.20
1	A	67	SER	N-CA-C	-5.45	96.28	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	71	C	N1-C1'-C2'	-5.45	106.00	112.00
2	H	59	C	C2'-C3'-O3'	-5.43	97.55	109.50
2	H	60	U	C5'-C4'-O4'	5.43	115.61	109.10
2	H	57	G	C4'-C3'-O3'	-5.41	98.05	109.40
2	D	47	A	OP1-P-O3'	5.40	117.07	105.20
2	B	48	C	N1-C1'-C2'	5.35	120.95	114.00
2	D	64	A	O3'-P-O5'	5.34	114.14	104.00
2	H	57	G	O5'-P-OP2	-5.33	100.90	105.70
1	C	39	VAL	CB-CA-C	-5.33	101.28	111.40
2	B	7	G	C2'-C3'-O3'	5.33	122.22	113.70
2	H	14	U	OP2-P-O3'	5.32	116.91	105.20
2	B	71	C	N1-C1'-C2'	-5.32	106.15	112.00
2	D	57	G	OP1-P-O3'	-5.31	93.51	105.20
2	F	52	G	N9-C1'-C2'	-5.28	106.20	112.00
1	A	93	VAL	N-CA-C	5.22	125.08	111.00
2	F	58	A	O5'-P-OP2	-5.21	101.02	105.70
2	H	59	C	O4'-C4'-C3'	-5.19	98.81	104.00
2	B	12	G	C5'-C4'-O4'	5.18	115.32	109.10
2	F	14	U	OP2-P-O3'	5.14	116.50	105.20
2	H	18	G	C2'-C3'-O3'	5.12	121.89	113.70
2	H	58	A	C5'-C4'-O4'	-5.07	103.01	109.10
2	B	52	G	N9-C1'-C2'	-5.05	106.44	112.00
2	D	7	G	OP2-P-O3'	-5.05	94.09	105.20
2	D	57	G	C4'-C3'-O3'	-5.05	98.80	109.40
2	F	48	C	N1-C1'-C2'	5.02	120.52	114.00
1	A	122	GLY	N-CA-C	5.01	125.64	113.10
2	F	7	G	C4'-C3'-C2'	5.01	107.61	102.60

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	54	TYR	Sidechain
2	B	16	U	Sidechain
2	B	27	U	Sidechain
1	C	112	TYR	Sidechain
1	C	20	TYR	Sidechain
1	E	106	TYR	Sidechain
2	F	16	U	Sidechain
2	F	27	U	Sidechain
2	F	48	C	Sidechain
1	G	68	TYR	Sidechain

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Mol	Chain	Res	Type	Group
2	H	8	A	Sidechain

5.2 Too-close contacts (i)

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	993	0	1030	190	0
1	C	965	0	1002	192	0
1	E	993	0	1030	296	0
1	G	981	0	1018	316	0
2	B	1323	0	672	120	0
2	D	1323	0	672	168	0
2	F	1323	0	672	150	0
2	H	1323	0	672	150	0
All	All	9224	0	6768	1400	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 88.

All (1400) 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:C:43:GLY:O	1:C:44:SER:N	1.73	1.21
1:E:21:GLU:O	2:F:18:G:N2	1.73	1.21
1:C:43:GLY:O	1:C:43:GLY:CA	1.89	1.20
2:H:22:G:H2'	2:H:23:G:H5"	1.23	1.18
1:E:55:LEU:HD11	1:E:102:PRO:HG3	1.20	1.17
1:A:60:ILE:O	1:A:62:PRO:HD3	1.40	1.16
2:D:22:G:H2'	2:D:23:G:H5"	1.21	1.14
1:G:17:LEU:HD12	1:G:119:LEU:HB3	1.24	1.13
1:A:55:LEU:HD11	1:A:102:PRO:HG3	1.32	1.12
1:G:95:GLN:HE22	1:G:98:LEU:HD13	1.04	1.11
1:G:114:LYS:HE3	2:H:16:U:H2'	1.33	1.11
1:C:93:VAL:HG22	1:C:100:LEU:HD23	1.31	1.09
1:C:85:GLU:O	1:C:89:LEU:HD23	1.53	1.08
1:G:45:PHE:CZ	1:G:57:ASN:HB2	1.89	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:106:TYR:CE1	1:G:114:LYS:HB2	1.88	1.08
1:G:39:VAL:HG12	1:G:60:ILE:HA	1.34	1.07
2:D:22:G:C2'	2:D:23:G:H5"	1.85	1.06
1:A:87:ARG:HA	1:A:90:LEU:HD21	1.36	1.06
2:B:50:U:H2'	2:B:51:G:C8	1.90	1.06
1:A:88:ARG:HA	1:A:88:ARG:HH11	1.20	1.05
2:F:50:U:H2'	2:F:51:G:C8	1.90	1.05
1:E:85:GLU:O	1:E:89:LEU:HD21	1.57	1.04
1:A:24:ILE:N	1:A:24:ILE:HD12	1.73	1.03
2:D:11:C:OP1	2:D:60:U:O2	1.76	1.03
1:C:43:GLY:C	1:C:43:GLY:O	0.83	1.02
2:H:22:G:C2'	2:H:23:G:H5"	1.89	1.02
1:A:2:ALA:HB1	1:A:3:PRO:HD2	1.39	1.01
1:E:89:LEU:H	1:E:89:LEU:HD23	1.24	1.01
1:E:45:PHE:HA	1:E:102:PRO:HD3	1.43	0.99
1:E:5:LEU:HG	1:E:105:ILE:HD11	1.41	0.99
2:B:64:A:H2'	2:B:65:C:C6	1.99	0.98
2:B:70:U:H2'	2:B:71:C:C6	1.98	0.98
1:E:114:LYS:HE2	2:F:17:C:OP1	1.63	0.98
1:G:7:ASN:CG	1:G:10:ALA:HB2	1.83	0.98
2:B:14:U:O2'	2:B:15:C:O5'	1.82	0.98
1:G:56:GLU:OE2	1:G:76:LYS:HB3	1.63	0.98
1:G:23:GLY:HA2	1:G:114:LYS:HZ2	1.23	0.98
1:E:98:LEU:HD21	1:E:119:LEU:HD22	1.45	0.97
1:A:24:ILE:HD12	1:A:24:ILE:H	1.30	0.96
2:B:26:U:O2	2:B:29:G:O6	1.84	0.96
2:F:6:U:H2'	2:F:7:G:H5"	1.46	0.96
2:F:13:G:H1	2:F:56:C:H42	1.10	0.96
2:F:26:U:O2	2:F:29:G:O6	1.84	0.96
1:E:21:GLU:HB3	2:F:17:C:H42	1.32	0.95
1:A:2:ALA:HB1	1:A:3:PRO:CD	1.96	0.94
1:E:82:HIS:HA	2:F:19:A:OP1	1.64	0.94
1:C:112:TYR:CD1	2:D:16:U:H1'	2.02	0.94
1:E:65:LYS:HG3	1:E:66:GLY:H	1.29	0.94
1:G:23:GLY:HA2	1:G:114:LYS:HD3	1.48	0.94
1:G:39:VAL:HB	1:G:59:TYR:O	1.67	0.94
1:G:89:LEU:HA	1:G:92:LYS:HE3	1.50	0.94
1:G:58:LEU:HG	1:G:59:TYR:N	1.83	0.94
1:G:95:GLN:NE2	1:G:98:LEU:HD13	1.82	0.93
1:G:89:LEU:HB2	1:G:92:LYS:HD2	1.49	0.93
2:D:19:A:N6	2:D:46:G:H21	1.65	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:LEU:C	2:B:18:G:O2'	2.07	0.93
2:F:64:A:H2'	2:F:65:C:C6	2.04	0.92
1:G:23:GLY:CA	1:G:114:LYS:HZ2	1.82	0.92
1:A:38:LYS:HE3	2:D:69:C:H1'	1.51	0.92
1:G:98:LEU:HD23	1:G:99:THR:N	1.82	0.92
1:A:86:LEU:HA	1:A:89:LEU:HD21	1.51	0.92
1:E:30:GLU:O	1:E:34:LEU:HG	1.69	0.92
1:E:5:LEU:O	1:E:5:LEU:HD12	1.69	0.92
1:G:114:LYS:NZ	2:H:16:U:O2	2.02	0.91
1:G:23:GLY:HA2	1:G:114:LYS:CD	2.00	0.91
1:E:22:ALA:O	1:E:115:VAL:HG12	1.70	0.91
1:C:9:ARG:HH22	2:B:5:G:H5'	1.36	0.91
1:E:5:LEU:HG	1:E:105:ILE:CD1	2.01	0.91
1:A:45:PHE:HA	1:A:102:PRO:HD3	1.53	0.90
2:B:6:U:H2'	2:B:7:G:H5"	1.52	0.90
1:C:9:ARG:HH12	2:B:5:G:H5"	1.37	0.90
1:E:89:LEU:O	1:E:93:VAL:HG23	1.70	0.90
1:E:4:VAL:HG23	1:E:106:TYR:CD2	2.06	0.90
2:D:28:C:H4'	2:D:29:G:C8	2.07	0.90
2:D:12:G:C2	2:D:57:G:N1	2.40	0.89
1:E:98:LEU:HD11	1:E:119:LEU:HB3	1.55	0.89
2:F:70:U:H2'	2:F:71:C:C6	2.07	0.89
1:G:46:ALA:HB3	1:G:100:LEU:HD12	1.52	0.88
1:A:38:LYS:CE	2:D:5:G:H21	1.86	0.88
1:E:93:VAL:HA	1:E:98:LEU:HB3	1.56	0.88
2:H:19:A:N6	2:H:46:G:H21	1.70	0.88
1:A:71:VAL:O	1:A:73:PRO:HD3	1.74	0.88
1:A:89:LEU:N	1:A:89:LEU:HD23	1.87	0.88
2:D:22:G:H2'	2:D:23:G:C5'	2.04	0.88
1:G:82:HIS:O	1:G:86:LEU:HD13	1.72	0.88
1:A:81:LEU:HD22	1:A:85:GLU:HB3	1.54	0.88
1:A:2:ALA:HA	1:A:35:ARG:O	1.73	0.88
2:H:28:C:H4'	2:H:29:G:C8	2.08	0.88
1:E:88:ARG:HD2	1:E:89:LEU:N	1.89	0.87
1:E:92:LYS:O	1:E:98:LEU:HD22	1.74	0.87
1:A:30:GLU:O	1:A:34:LEU:HD12	1.74	0.87
1:E:5:LEU:HD13	1:E:6:GLU:O	1.73	0.87
1:G:22:ALA:HB3	1:G:115:VAL:HG13	1.57	0.87
1:G:23:GLY:HA2	1:G:114:LYS:NZ	1.89	0.87
1:G:113:ALA:N	2:H:47:A:N1	2.22	0.87
1:E:44:SER:N	1:E:57:ASN:HD22	1.73	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:5:LEU:C	1:E:5:LEU:HD12	1.95	0.86
1:E:5:LEU:CG	1:E:105:ILE:HD11	2.05	0.86
1:A:60:ILE:O	1:A:62:PRO:CD	2.21	0.86
1:C:9:ARG:NH2	2:B:5:G:H5'	1.90	0.86
1:G:41:PHE:CE1	1:G:102:PRO:HB2	2.11	0.86
1:G:58:LEU:HD23	1:G:60:ILE:HD11	1.56	0.86
1:C:4:VAL:O	1:C:5:LEU:HD23	1.76	0.86
1:G:24:ILE:H	1:G:114:LYS:NZ	1.73	0.85
1:A:81:LEU:CD2	1:A:85:GLU:HB3	2.06	0.85
1:G:106:TYR:CZ	1:G:114:LYS:HB2	2.12	0.84
1:G:64:GLU:OE1	1:G:65:LYS:NZ	2.09	0.84
1:A:46:ALA:HB3	1:A:100:LEU:HB3	1.59	0.84
2:B:16:U:OP2	2:B:46:G:O6	1.95	0.84
1:E:98:LEU:CD2	1:E:119:LEU:HD22	2.08	0.84
1:G:26:LEU:CD2	1:G:34:LEU:HD11	2.08	0.84
1:E:81:LEU:HD21	1:E:85:GLU:HG2	1.57	0.83
1:A:81:LEU:O	2:B:18:G:O2'	1.96	0.83
1:A:37:GLY:O	2:D:6:U:O2'	1.96	0.83
2:F:6:U:C2'	2:F:7:G:H5"	2.07	0.83
1:G:26:LEU:HD22	1:G:34:LEU:HD11	1.60	0.83
1:A:59:TYR:CE1	1:A:73:PRO:HB3	2.13	0.83
1:E:81:LEU:C	2:F:18:G:O2'	2.16	0.83
1:G:9:ARG:HH21	1:G:13:ASP:HB2	1.42	0.82
2:B:14:U:C2'	2:B:15:C:O5'	2.28	0.82
1:E:20:TYR:CE2	1:E:89:LEU:HD22	2.13	0.82
1:C:22:ALA:HB1	1:C:79:LEU:HD22	1.61	0.82
1:E:26:LEU:HD13	1:E:34:LEU:HD11	1.60	0.82
1:G:91:GLY:HA2	1:G:94:GLU:CD	2.00	0.82
1:C:72:ASP:HB2	1:C:75:ARG:HG2	1.60	0.82
1:E:21:GLU:O	2:F:18:G:C2	2.32	0.82
1:E:21:GLU:HB3	2:F:17:C:N4	1.94	0.82
1:G:103:LEU:O	1:G:104:LYS:HG2	1.80	0.82
1:A:2:ALA:CB	1:A:3:PRO:HD2	2.10	0.81
1:G:27:LYS:HD2	1:G:27:LYS:N	1.96	0.81
1:G:38:LYS:HE2	1:G:64:GLU:HG3	1.61	0.81
2:H:22:G:H2'	2:H:23:G:C5'	2.07	0.81
2:B:6:U:C2'	2:B:7:G:H5"	2.09	0.81
1:G:114:LYS:HE3	2:H:16:U:C2'	2.11	0.81
1:E:98:LEU:HD21	1:E:119:LEU:HD13	1.63	0.81
1:G:24:ILE:CD1	1:G:114:LYS:HA	2.10	0.81
1:A:22:ALA:O	1:A:115:VAL:HG12	1.80	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:49:G:H22	2:D:66:C:H1'	1.47	0.80
1:E:27:LYS:HD3	1:E:30:GLU:OE1	1.80	0.80
1:E:86:LEU:HD23	1:E:87:ARG:N	1.96	0.80
1:G:63:TYR:CD2	1:G:66:GLY:O	2.35	0.79
1:A:89:LEU:H	1:A:89:LEU:HD23	1.46	0.79
1:E:22:ALA:HA	2:F:18:G:N1	1.97	0.79
1:A:82:HIS:CE1	2:B:18:G:O4'	2.36	0.79
1:C:23:GLY:HA2	1:C:114:LYS:HD3	1.63	0.79
1:E:78:LYS:HG2	1:E:79:LEU:N	1.96	0.79
1:C:18:GLU:HB3	1:C:119:LEU:HD12	1.64	0.79
1:G:45:PHE:HZ	1:G:57:ASN:HB2	1.42	0.79
1:G:87:ARG:O	1:G:90:LEU:HD22	1.83	0.79
1:A:48:PHE:CE1	1:A:90:LEU:HB3	2.18	0.78
2:B:50:U:H2'	2:B:51:G:H8	1.45	0.78
1:E:81:LEU:CD2	1:E:85:GLU:HG2	2.12	0.78
1:E:98:LEU:HD21	1:E:119:LEU:CD2	2.13	0.78
1:C:72:ASP:HB2	1:C:75:ARG:HE	1.49	0.78
1:E:88:ARG:HH12	1:E:119:LEU:HD21	1.48	0.78
2:B:64:A:H2'	2:B:65:C:H6	1.43	0.78
1:C:35:ARG:NH2	2:D:48:C:N3	2.29	0.78
1:E:102:PRO:HA	1:E:117:LEU:HD23	1.66	0.78
2:B:70:U:H2'	2:B:71:C:H6	1.45	0.78
1:G:59:TYR:CE1	1:G:74:ARG:HD3	2.18	0.78
1:G:23:GLY:HA2	1:G:114:LYS:CE	2.13	0.77
1:G:71:VAL:HB	1:G:75:ARG:HH21	1.49	0.77
1:G:115:VAL:HG22	1:G:116:LEU:N	1.99	0.77
1:G:58:LEU:HD23	1:G:60:ILE:CD1	2.13	0.77
1:C:72:ASP:CB	1:C:75:ARG:HE	1.98	0.77
2:F:50:U:H2'	2:F:51:G:H8	1.44	0.77
1:G:83:LYS:HG3	1:G:84:HIS:N	2.00	0.77
1:G:113:ALA:O	2:H:47:A:N6	2.17	0.77
1:G:17:LEU:CD1	1:G:119:LEU:HB3	2.12	0.77
1:G:120:ALA:O	1:G:121:ARG:HB2	1.83	0.77
1:A:30:GLU:OE1	1:A:75:ARG:NH1	2.18	0.77
2:F:64:A:H2'	2:F:65:C:H6	1.48	0.77
1:C:17:LEU:HB2	1:C:119:LEU:HB2	1.65	0.77
1:E:20:TYR:CZ	1:E:89:LEU:HD22	2.19	0.77
1:C:28:GLY:HA2	2:D:47:A:O2'	1.85	0.76
1:E:110:ARG:HG2	2:F:15:C:N4	2.00	0.76
1:E:78:LYS:CG	1:E:79:LEU:N	2.48	0.76
1:C:46:ALA:HB3	1:C:100:LEU:HB3	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3:PRO:HD2	1:C:35:ARG:O	1.84	0.76
1:E:81:LEU:HG	1:E:85:GLU:CD	2.05	0.76
1:G:24:ILE:HD11	1:G:115:VAL:H	1.50	0.76
1:A:9:ARG:NH1	1:A:42:THR:HG23	2.01	0.76
1:C:13:ASP:O	1:C:14:TYR:HD2	1.68	0.76
1:G:67:SER:O	1:G:68:TYR:CD2	2.40	0.75
1:A:59:TYR:HE1	1:A:73:PRO:HB3	1.51	0.75
1:C:24:ILE:HG23	1:C:79:LEU:CD2	2.16	0.75
1:G:46:ALA:CB	1:G:100:LEU:HD12	2.17	0.75
1:C:52:GLU:HG2	2:D:19:A:O2'	1.86	0.75
1:G:89:LEU:HB2	1:G:92:LYS:CD	2.17	0.75
2:H:10:A:H2'	2:H:11:C:H5"	1.69	0.75
1:G:106:TYR:HE1	1:G:114:LYS:HB2	1.50	0.75
1:G:39:VAL:CG1	1:G:60:ILE:HA	2.14	0.75
1:C:103:LEU:O	1:C:104:LYS:HB3	1.85	0.75
1:A:93:VAL:O	1:A:95:GLN:HG3	1.86	0.75
2:H:26:U:C2'	2:H:27:U:H5"	2.17	0.75
1:E:72:ASP:HB2	1:E:75:ARG:HH21	1.52	0.74
1:E:83:LYS:HG2	1:E:84:HIS:N	2.02	0.74
2:H:4:G:N2	2:H:70:U:H1'	2.01	0.74
1:E:62:PRO:HB3	1:E:70:ASN:HD22	1.52	0.74
1:G:112:TYR:HD2	2:H:47:A:C5	2.04	0.74
1:G:24:ILE:N	1:G:114:LYS:HZ2	1.85	0.74
1:A:46:ALA:HB2	1:A:55:LEU:HD12	1.70	0.74
2:B:12:G:N3	2:B:57:G:N2	2.35	0.74
1:E:47:ARG:C	1:E:53:LEU:HD12	2.06	0.74
1:A:47:ARG:HB3	1:A:56:GLU:OE2	1.89	0.73
1:E:43:GLY:C	1:E:57:ASN:HD22	1.91	0.73
1:A:60:ILE:C	1:A:62:PRO:HD3	2.08	0.73
1:A:90:LEU:HD12	1:A:91:GLY:N	2.02	0.73
1:C:27:LYS:H	1:C:30:GLU:HG3	1.52	0.73
1:G:24:ILE:HD11	1:G:114:LYS:HA	1.68	0.73
1:G:83:LYS:O	1:G:86:LEU:HD22	1.88	0.73
2:D:13:G:H1'	2:D:57:G:N2	2.03	0.73
1:G:24:ILE:HD11	1:G:115:VAL:N	2.02	0.73
1:G:7:ASN:ND2	1:G:10:ALA:HB2	2.02	0.73
2:D:54:5MU:C2	2:D:58:A:N6	2.56	0.73
1:E:63:TYR:HD2	1:E:64:GLU:N	1.86	0.73
1:G:72:ASP:HB3	1:G:75:ARG:CZ	2.18	0.73
1:G:21:GLU:O	2:H:18:G:N1	2.22	0.73
1:C:95:GLN:C	1:C:96:LYS:HD3	2.09	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:LYS:HD3	1:A:84:HIS:N	2.03	0.73
2:D:13:G:H1	2:D:56:C:H42	1.36	0.73
1:G:22:ALA:HB3	1:G:115:VAL:CG1	2.18	0.72
1:C:47:ARG:HB2	1:C:56:GLU:OE2	1.90	0.72
1:G:81:LEU:HD23	1:G:85:GLU:OE1	1.88	0.72
1:A:40:ASP:HB3	2:D:5:G:O2'	1.90	0.72
2:D:49:G:N2	2:D:66:C:H1'	2.04	0.72
2:H:16:U:O2	2:H:47:A:N6	2.22	0.72
1:G:81:LEU:C	2:H:18:G:O2'	2.28	0.72
1:A:87:ARG:O	1:A:90:LEU:HD11	1.90	0.72
1:G:71:VAL:HG23	1:G:72:ASP:N	2.05	0.72
1:G:59:TYR:HE1	1:G:74:ARG:HH11	1.36	0.72
2:D:30:C:H2'	2:D:31:C:C6	2.25	0.71
2:H:48:C:O2'	2:H:49:G:H5"	1.90	0.71
2:B:64:A:H2'	2:B:65:C:O4'	1.90	0.71
2:B:53:G:O2'	2:B:54:5MU:H5"	1.90	0.71
1:C:74:ARG:NH1	2:B:71:C:OP1	2.22	0.71
2:F:70:U:H2'	2:F:71:C:H6	1.55	0.71
1:G:19:THR:HG23	1:G:103:LEU:CD1	2.21	0.71
1:G:75:ARG:H	1:G:77:ARG:NH2	1.89	0.71
1:G:108:ASN:OD1	1:G:112:TYR:O	2.07	0.71
1:G:6:GLU:HA	1:G:104:LYS:HB3	1.72	0.71
1:E:112:TYR:HH	2:F:15:C:H6	1.38	0.71
1:E:83:LYS:HA	1:E:86:LEU:HD22	1.72	0.71
1:A:93:VAL:HG12	1:A:94:GLU:N	2.06	0.71
1:C:112:TYR:CG	2:D:16:U:H1'	2.25	0.71
1:G:103:LEU:HD11	1:G:117:LEU:O	1.89	0.71
1:G:89:LEU:O	1:G:92:LYS:HG3	1.91	0.71
1:A:16:ILE:HG21	1:A:19:THR:HG22	1.74	0.70
2:F:64:A:H2'	2:F:65:C:O4'	1.91	0.70
1:G:52:GLU:HG3	1:G:54:TYR:CE1	2.26	0.70
1:E:90:LEU:HD12	1:E:91:GLY:N	2.06	0.70
1:E:55:LEU:HD11	1:E:102:PRO:CG	2.12	0.70
2:D:55:PSU:C2	2:D:57:G:OP2	2.45	0.70
1:C:72:ASP:HB2	1:C:75:ARG:CG	2.22	0.70
1:C:24:ILE:HG23	1:C:79:LEU:HD21	1.71	0.70
1:G:31:VAL:O	1:G:34:LEU:HG	1.91	0.70
1:G:64:GLU:O	1:G:65:LYS:HD2	1.92	0.70
2:D:10:A:H2'	2:D:11:C:H5"	1.74	0.70
1:E:24:ILE:HG13	1:E:26:LEU:HD21	1.73	0.70
1:A:2:ALA:CB	1:A:3:PRO:CD	2.70	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:50:ASP:CG	1:E:51:GLY:N	2.46	0.69
2:F:12:G:H2'	2:F:13:G:C8	2.26	0.69
2:H:49:G:H22	2:H:66:C:H1'	1.56	0.69
2:D:66:C:N4	2:D:67:A:N6	2.40	0.69
1:A:48:PHE:CZ	1:A:90:LEU:HB3	2.27	0.69
1:C:31:VAL:HG11	2:D:48:C:C2	2.27	0.69
2:B:16:U:O2'	2:B:17:C:P	2.50	0.69
2:F:14:U:O2	2:F:15:C:H5	1.75	0.69
2:B:12:G:C2	2:B:57:G:C2	2.80	0.69
1:E:17:LEU:HB2	1:E:119:LEU:HB2	1.74	0.69
1:C:9:ARG:NH1	2:B:5:G:H5"	2.07	0.69
1:E:59:TYR:CE1	1:E:73:PRO:HB3	2.27	0.69
1:G:97:GLY:HA3	1:G:121:ARG:HE	1.58	0.69
1:G:15:GLU:HB3	1:G:121:ARG:O	1.93	0.69
1:A:82:HIS:HA	2:B:19:A:OP1	1.92	0.69
1:E:5:LEU:CD1	1:E:5:LEU:C	2.61	0.69
1:C:40:ASP:HB2	2:B:5:G:O2'	1.93	0.68
2:H:19:A:N6	2:H:46:G:N2	2.40	0.68
1:A:32:LYS:HD3	1:A:63:TYR:OH	1.93	0.68
2:D:26:U:C2'	2:D:27:U:H5"	2.23	0.68
1:G:82:HIS:HA	2:H:19:A:OP1	1.92	0.68
1:E:4:VAL:HG23	1:E:106:TYR:CE2	2.27	0.68
1:E:62:PRO:HB3	1:E:70:ASN:HB2	1.75	0.68
1:G:52:GLU:HG3	1:G:54:TYR:OH	1.91	0.68
2:H:23:G:H5'	2:H:23:G:H8	1.58	0.68
2:F:67:A:H2'	2:F:68:C:H6	1.58	0.68
1:A:9:ARG:HH12	1:A:42:THR:HG23	1.59	0.68
1:C:41:PHE:HZ	1:C:105:ILE:HG23	1.59	0.68
1:E:48:PHE:HZ	1:E:93:VAL:HG11	1.59	0.68
1:E:98:LEU:CD1	1:E:119:LEU:HB3	2.24	0.68
2:B:12:G:H4'	2:B:13:G:OP1	1.94	0.68
2:D:16:U:O2	2:D:47:A:N6	2.27	0.68
2:F:14:U:O2	2:F:15:C:C5	2.47	0.68
1:E:28:GLY:HA2	2:F:47:A:O2'	1.93	0.67
1:E:65:LYS:HG3	1:E:66:GLY:N	2.07	0.67
1:G:101:VAL:CG1	1:G:120:ALA:HB2	2.25	0.67
1:A:38:LYS:HE3	2:D:5:G:H21	1.57	0.67
1:A:93:VAL:O	1:A:95:GLN:N	2.28	0.67
1:E:81:LEU:HG	1:E:85:GLU:OE1	1.95	0.67
1:G:75:ARG:O	1:G:77:ARG:HD2	1.95	0.67
1:A:6:GLU:HG2	1:A:104:LYS:HG3	1.74	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:108:ASN:CG	1:G:112:TYR:O	2.32	0.67
1:A:49:GLU:HA	1:A:49:GLU:OE2	1.92	0.67
1:E:87:ARG:HA	1:E:90:LEU:HD21	1.76	0.67
1:G:21:GLU:CD	2:H:17:C:H42	1.98	0.67
1:C:10:ALA:O	1:C:14:TYR:HB2	1.94	0.67
1:E:112:TYR:HB2	1:E:114:LYS:HE3	1.76	0.67
2:F:29:G:C6	2:F:30:C:C2	2.83	0.67
2:F:67:A:H2'	2:F:68:C:C6	2.29	0.67
1:G:97:GLY:O	1:G:121:ARG:HG3	1.95	0.67
2:B:9:A:H62	2:D:9:A:H3'	1.59	0.66
1:E:72:ASP:CG	1:E:75:ARG:HE	1.97	0.66
1:E:27:LYS:HD3	1:E:30:GLU:CD	2.16	0.66
1:E:99:THR:OG1	1:E:120:ALA:HB3	1.95	0.66
2:H:30:C:H2'	2:H:31:C:C6	2.29	0.66
1:C:41:PHE:CZ	1:C:105:ILE:HG23	2.30	0.66
1:E:81:LEU:N	2:F:18:G:O2'	2.28	0.66
2:F:16:U:O2'	2:F:17:C:P	2.53	0.66
1:G:116:LEU:C	1:G:117:LEU:HD12	2.16	0.66
2:H:35:G:H3'	2:H:46:G:C8	2.29	0.66
2:D:19:A:H62	2:D:46:G:H21	1.42	0.66
1:E:11:ARG:HD3	1:E:12:HIS:CE1	2.31	0.66
1:G:89:LEU:CB	1:G:92:LYS:HD2	2.23	0.66
2:D:13:G:H1	2:D:56:C:N4	1.93	0.66
1:G:41:PHE:CE2	1:G:104:LYS:HA	2.30	0.66
1:E:11:ARG:HD3	1:E:12:HIS:ND1	2.11	0.66
1:E:52:GLU:HG3	1:E:54:TYR:HE1	1.60	0.66
2:F:35:G:O2'	2:F:46:G:H5'	1.95	0.66
1:E:14:TYR:HB3	1:E:120:ALA:HB1	1.78	0.66
1:E:62:PRO:O	1:E:63:TYR:HB2	1.96	0.66
1:E:114:LYS:HZ3	2:F:17:C:H5	1.43	0.66
2:H:54:5MU:C2	2:H:58:A:N6	2.64	0.66
1:C:29:THR:HG21	1:C:70:ASN:ND2	2.10	0.65
1:E:82:HIS:O	1:E:86:LEU:HB3	1.96	0.65
1:A:29:THR:HG22	2:B:49:G:H4'	1.78	0.65
2:B:67:A:H2'	2:B:68:C:C6	2.31	0.65
1:E:46:ALA:O	1:E:100:LEU:HD23	1.96	0.65
1:G:9:ARG:NH2	1:G:13:ASP:OD2	2.29	0.65
2:D:4:G:N2	2:D:70:U:H1'	2.10	0.65
1:E:64:GLU:O	1:E:65:LYS:C	2.32	0.65
1:E:48:PHE:HE2	1:E:93:VAL:HG21	1.62	0.65
1:G:41:PHE:CE1	1:G:102:PRO:CB	2.80	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:41:PHE:HE1	1:G:102:PRO:HB2	1.61	0.65
1:G:30:GLU:HB3	1:G:60:ILE:HG21	1.77	0.65
1:G:98:LEU:HD23	1:G:99:THR:H	1.59	0.65
1:C:16:ILE:O	1:C:17:LEU:HD23	1.95	0.65
1:E:80:LEU:HB3	2:F:18:G:H2'	1.78	0.65
1:A:89:LEU:H	1:A:89:LEU:CD2	2.10	0.65
1:G:112:TYR:CD2	2:H:47:A:C5	2.84	0.65
1:G:86:LEU:HD22	1:G:87:ARG:N	2.12	0.65
2:H:19:A:H62	2:H:46:G:N2	1.95	0.65
2:B:12:G:H2'	2:B:13:G:C8	2.31	0.65
1:E:79:LEU:CD2	1:E:115:VAL:HG11	2.27	0.65
1:A:6:GLU:HG2	1:A:104:LYS:CB	2.27	0.65
1:E:98:LEU:HD21	1:E:119:LEU:CD1	2.26	0.65
1:G:41:PHE:HE1	1:G:102:PRO:CB	2.09	0.65
1:A:81:LEU:HD22	1:A:85:GLU:CB	2.26	0.65
2:B:67:A:H2'	2:B:68:C:H6	1.60	0.65
1:C:5:LEU:O	1:C:105:ILE:N	2.28	0.65
1:C:90:LEU:HD12	1:C:91:GLY:N	2.12	0.65
1:C:112:TYR:CD1	2:D:16:U:C1'	2.78	0.65
2:B:25:G:H2'	2:B:26:U:O4'	1.97	0.65
1:E:21:GLU:O	2:F:18:G:N1	2.30	0.65
2:D:19:A:N6	2:D:46:G:N2	2.43	0.64
1:A:17:LEU:HB2	1:A:119:LEU:HB2	1.80	0.64
2:B:16:U:P	2:B:46:G:O6	2.56	0.64
2:B:59:C:H2'	2:B:60:U:O4'	1.98	0.64
1:G:86:LEU:HD22	1:G:87:ARG:H	1.60	0.64
2:H:55:PSU:C2	2:H:57:G:OP2	2.51	0.64
1:E:78:LYS:CG	1:E:79:LEU:H	2.11	0.64
1:E:2:ALA:HB1	2:H:9:A:OP1	1.97	0.64
1:A:9:ARG:CZ	1:A:42:THR:HG23	2.27	0.64
2:B:12:G:O2'	2:B:13:G:O5'	2.14	0.64
2:D:13:G:C1'	2:D:57:G:N2	2.60	0.64
1:G:25:ALA:HA	2:H:16:U:O4	1.96	0.64
1:E:61:ALA:HB1	1:E:64:GLU:OE2	1.96	0.64
1:G:115:VAL:CG2	1:G:116:LEU:N	2.60	0.64
1:G:81:LEU:HD23	1:G:85:GLU:CD	2.17	0.64
1:C:47:ARG:HB2	1:C:56:GLU:CD	2.18	0.64
1:C:72:ASP:HB2	1:C:75:ARG:NE	2.12	0.64
2:F:8:A:H2	2:F:10:A:OP2	1.81	0.64
1:A:32:LYS:HD2	2:B:49:G:OP2	1.97	0.64
1:A:55:LEU:HD11	1:A:102:PRO:CG	2.20	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:12:G:C2	2:D:57:G:C6	2.86	0.64
1:E:47:ARG:NH1	1:E:48:PHE:HE1	1.94	0.64
1:G:55:LEU:HD21	1:G:58:LEU:HB3	1.79	0.64
1:G:21:GLU:HG3	2:H:18:G:H22	1.63	0.64
1:A:8:ARG:O	1:A:8:ARG:HD3	1.96	0.64
1:G:91:GLY:HA2	1:G:94:GLU:OE2	1.98	0.64
1:A:86:LEU:CA	1:A:89:LEU:HD21	2.26	0.64
1:C:17:LEU:HD11	1:C:121:ARG:HG3	1.80	0.63
2:B:70:U:H2'	2:B:71:C:C5	2.33	0.63
1:A:89:LEU:N	1:A:89:LEU:CD2	2.59	0.63
1:C:7:ASN:HB3	1:C:10:ALA:HB2	1.80	0.63
1:A:24:ILE:CD1	1:A:24:ILE:N	2.47	0.63
1:E:108:ASN:ND2	1:E:114:LYS:NZ	2.47	0.63
2:F:13:G:H1	2:F:56:C:N4	1.92	0.63
2:F:59:C:H2'	2:F:60:U:O4'	1.99	0.63
1:E:62:PRO:CB	1:E:70:ASN:HD22	2.12	0.63
1:G:59:TYR:HE1	1:G:74:ARG:HD3	1.63	0.63
2:D:35:G:H2'	2:D:46:G:O4'	1.99	0.63
1:G:31:VAL:HG21	2:H:47:A:O2'	1.98	0.63
2:B:47:A:H5'	2:B:48:C:OP1	1.99	0.63
2:F:60:U:OP2	2:F:60:U:H6	1.82	0.63
1:E:13:ASP:C	1:E:14:TYR:HD2	2.02	0.63
1:E:81:LEU:O	2:F:19:A:H5'	1.99	0.63
1:A:52:GLU:CD	2:B:20:C:H5'	2.18	0.63
1:C:27:LYS:HD3	1:C:30:GLU:CD	2.19	0.63
2:D:16:U:H4'	2:D:17:C:OP2	1.97	0.63
1:A:9:ARG:NH2	1:A:42:THR:HG23	2.13	0.62
2:B:64:A:C2'	2:B:65:C:C6	2.79	0.62
1:E:50:ASP:CG	1:E:51:GLY:H	2.03	0.62
1:A:82:HIS:CE1	2:B:17:C:O2'	2.53	0.62
2:B:8:A:H2	2:B:10:A:OP2	1.81	0.62
1:E:71:VAL:HG12	1:E:72:ASP:N	2.14	0.62
1:G:82:HIS:CB	1:G:84:HIS:CE1	2.82	0.62
1:A:83:LYS:NZ	1:A:87:ARG:NH2	2.48	0.62
2:B:9:A:N6	2:D:9:A:H3'	2.14	0.62
1:G:105:ILE:C	1:G:105:ILE:HD12	2.20	0.62
1:C:123:LYS:HB2	1:C:123:LYS:NZ	2.14	0.62
2:D:13:G:N2	2:D:56:C:N3	2.45	0.62
1:E:48:PHE:CE2	1:E:93:VAL:HG21	2.35	0.62
2:H:32:U:H2'	2:H:33:U:C6	2.34	0.62
1:A:12:HIS:CD2	1:A:12:HIS:H	2.17	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:17:LEU:HB2	1:G:119:LEU:HB2	1.80	0.62
1:C:98:LEU:HD21	1:C:119:LEU:HD23	1.80	0.62
1:E:104:LYS:HD3	1:E:116:LEU:HD23	1.81	0.62
1:G:41:PHE:HE2	1:G:104:LYS:HA	1.64	0.62
2:H:10:A:H2'	2:H:11:C:O4'	2.00	0.62
1:A:89:LEU:O	1:A:93:VAL:HG23	1.99	0.62
1:C:6:GLU:HB3	1:C:104:LYS:CB	2.30	0.62
1:E:43:GLY:O	1:E:45:PHE:CE1	2.53	0.62
2:D:67:A:H2'	2:D:68:C:C6	2.34	0.62
1:A:6:GLU:CD	1:A:104:LYS:HB2	2.20	0.62
2:B:16:U:O2'	2:B:17:C:OP1	2.15	0.62
1:C:7:ASN:ND2	1:C:102:PRO:O	2.18	0.62
2:B:12:G:O2'	2:B:13:G:C5'	2.47	0.61
2:B:31:C:O2'	2:B:32:U:H5'	2.00	0.61
2:D:10:A:H2'	2:D:11:C:O4'	2.00	0.61
2:D:27:U:O2'	2:D:28:C:OP1	2.16	0.61
1:G:82:HIS:HB2	1:G:84:HIS:CE1	2.35	0.61
1:C:43:GLY:O	1:C:44:SER:CA	2.46	0.61
1:E:21:GLU:CD	2:F:17:C:H41	2.04	0.61
1:G:24:ILE:H	1:G:114:LYS:HZ2	1.38	0.61
2:H:16:U:H4'	2:H:17:C:OP2	1.99	0.61
2:D:28:C:H4'	2:D:29:G:N9	2.14	0.61
1:E:57:ASN:CG	1:E:57:ASN:O	2.39	0.61
1:E:62:PRO:CG	1:E:73:PRO:HG3	2.30	0.61
1:A:6:GLU:HG2	1:A:104:LYS:CG	2.30	0.61
1:A:24:ILE:HG23	1:A:79:LEU:HD23	1.81	0.61
2:H:66:C:N4	2:H:67:A:N6	2.47	0.61
1:A:74:ARG:HH11	1:A:74:ARG:HG3	1.65	0.61
1:C:44:SER:HA	1:C:57:ASN:O	2.01	0.61
1:G:22:ALA:HB1	1:G:79:LEU:HD22	1.82	0.61
1:E:32:LYS:HD2	2:F:49:G:H5'	1.83	0.61
2:H:49:G:N2	2:H:66:C:H1'	2.15	0.61
2:D:1:G:H2'	2:D:2:G:H8	1.64	0.61
2:D:33:U:H2'	2:D:34:U:C6	2.36	0.61
2:F:12:G:O2'	2:F:13:G:O5'	2.18	0.61
1:E:78:LYS:NZ	2:F:19:A:O2'	2.33	0.61
1:G:103:LEU:C	1:G:104:LYS:HG2	2.21	0.61
1:A:94:GLU:C	1:A:96:LYS:H	2.04	0.61
2:F:12:G:H4'	2:F:13:G:OP1	1.99	0.61
1:E:55:LEU:HB2	1:E:79:LEU:HD11	1.83	0.61
2:D:6:U:H2'	2:D:7:G:H5'	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:53:G:H3'	2:F:54:5MU:H71	1.81	0.60
2:B:60:U:H6	2:B:60:U:OP2	1.84	0.60
1:C:23:GLY:HA2	1:C:114:LYS:CD	2.31	0.60
1:E:20:TYR:OH	1:E:88:ARG:NE	2.34	0.60
1:E:114:LYS:HD2	2:F:18:G:O6	2.02	0.60
2:H:28:C:H4'	2:H:29:G:N9	2.15	0.60
1:C:7:ASN:HB3	1:C:10:ALA:CB	2.31	0.60
2:D:19:A:H61	2:D:46:G:H21	1.49	0.60
1:E:72:ASP:HB2	1:E:75:ARG:NH2	2.16	0.60
1:G:106:TYR:HE2	1:G:116:LEU:HD13	1.66	0.60
1:G:89:LEU:HA	1:G:92:LYS:CE	2.27	0.60
2:H:26:U:H2'	2:H:27:U:H5"	1.84	0.60
1:C:18:GLU:CB	1:C:119:LEU:HD12	2.29	0.60
1:E:108:ASN:ND2	1:E:114:LYS:HZ1	1.99	0.60
1:E:43:GLY:C	1:E:57:ASN:ND2	2.54	0.60
2:F:46:G:C8	2:F:46:G:O5'	2.54	0.60
2:B:46:G:O5'	2:B:46:G:C8	2.55	0.60
1:C:70:ASN:CG	1:C:71:VAL:H	2.05	0.60
1:C:81:LEU:C	2:D:18:G:O2'	2.40	0.60
1:G:106:TYR:CD1	1:G:106:TYR:C	2.74	0.60
1:E:63:TYR:OH	1:E:65:LYS:HE3	2.01	0.60
1:G:103:LEU:O	1:G:104:LYS:CG	2.50	0.60
1:E:81:LEU:HD12	2:F:18:G:N2	2.16	0.60
2:B:12:G:N3	2:B:57:G:C2	2.70	0.60
2:B:12:G:C2	2:B:57:G:N1	2.70	0.60
1:E:80:LEU:HG	2:F:19:A:N9	2.17	0.60
2:F:28:C:O2	2:F:28:C:H2'	2.02	0.60
1:G:93:VAL:O	1:G:93:VAL:HG12	2.02	0.60
1:C:62:PRO:CG	1:C:70:ASN:HD22	2.14	0.60
1:C:35:ARG:NH2	2:D:48:C:H42	2.00	0.60
1:E:63:TYR:HB3	1:E:67:SER:HB2	1.82	0.60
1:G:106:TYR:CE2	1:G:114:LYS:O	2.55	0.60
1:A:100:LEU:HD12	1:A:117:LEU:HD22	1.84	0.59
1:C:29:THR:HG21	1:C:70:ASN:CG	2.23	0.59
1:C:82:HIS:HB2	1:C:85:GLU:HG3	1.83	0.59
1:G:91:GLY:CA	1:G:94:GLU:CD	2.70	0.59
2:H:1:G:H2'	2:H:2:G:H8	1.66	0.59
2:D:23:G:H5'	2:D:23:G:H8	1.66	0.59
1:E:88:ARG:NH1	1:E:119:LEU:HD21	2.16	0.59
1:A:62:PRO:O	1:A:70:ASN:ND2	2.35	0.59
1:C:112:TYR:CE1	2:D:16:U:O4'	2.55	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:32:U:C2	2:D:33:U:C5	2.90	0.59
2:D:4:G:O2'	2:D:5:G:H5'	2.02	0.59
2:D:68:C:H2'	2:D:69:C:H6	1.67	0.59
1:G:98:LEU:HD21	1:G:119:LEU:HD22	1.83	0.59
2:D:32:U:H2'	2:D:33:U:C6	2.36	0.59
2:D:35:G:H3'	2:D:46:G:C8	2.36	0.59
1:E:72:ASP:CB	1:E:75:ARG:HE	2.15	0.59
1:G:26:LEU:C	1:G:27:LYS:HD2	2.22	0.59
1:G:38:LYS:HE2	1:G:64:GLU:CG	2.30	0.59
1:G:5:LEU:HD11	1:G:37:GLY:CA	2.32	0.59
1:A:55:LEU:HB2	1:A:79:LEU:HD11	1.84	0.59
1:C:52:GLU:OE2	2:D:20:C:H4'	2.02	0.59
2:F:48:C:H2'	2:F:48:C:O2	2.01	0.59
2:H:26:U:C2	2:H:28:C:O2	2.55	0.59
2:H:67:A:H2'	2:H:68:C:C6	2.37	0.59
1:G:52:GLU:CB	1:G:78:LYS:HE3	2.32	0.59
1:E:14:TYR:CB	1:E:120:ALA:HB1	2.32	0.59
2:F:25:G:H2'	2:F:26:U:O4'	2.03	0.59
2:F:31:C:O2'	2:F:32:U:H5'	2.02	0.59
2:H:14:U:H5	2:H:15:C:C2	2.21	0.59
1:G:52:GLU:HG3	1:G:54:TYR:CZ	2.38	0.59
1:A:123:LYS:HD2	1:A:123:LYS:N	2.18	0.59
2:B:48:C:O2	2:B:48:C:H2'	2.01	0.59
1:G:106:TYR:OH	1:G:114:LYS:CB	2.50	0.59
1:A:60:ILE:HD12	1:A:77:ARG:CZ	2.32	0.58
1:C:94:GLU:C	1:C:96:LYS:H	2.07	0.58
1:A:67:SER:OG	2:B:68:C:H5'	2.03	0.58
1:E:5:LEU:CD1	1:E:105:ILE:HD11	2.32	0.58
1:E:94:GLU:O	1:E:95:GLN:C	2.41	0.58
1:E:98:LEU:HD21	1:E:119:LEU:CG	2.32	0.58
2:F:35:G:C6	2:F:46:G:N2	2.71	0.58
1:A:14:TYR:CB	1:A:120:ALA:HB1	2.33	0.58
1:C:39:VAL:CG1	1:C:60:ILE:HG12	2.32	0.58
1:E:19:THR:HG22	1:E:103:LEU:HD11	1.84	0.58
1:G:114:LYS:CE	2:H:16:U:O2	2.51	0.58
1:G:24:ILE:O	2:H:16:U:N3	2.27	0.58
1:A:104:LYS:HE2	1:A:106:TYR:CD2	2.38	0.58
1:E:23:GLY:N	2:F:18:G:C6	2.71	0.58
1:A:7:ASN:OD1	1:A:9:ARG:HB3	2.03	0.58
2:B:28:C:H2'	2:B:28:C:O2	2.03	0.58
2:D:26:U:C2	2:D:28:C:O2	2.57	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:113:ALA:N	2:D:47:A:N1	2.42	0.58
2:H:22:G:C3'	2:H:23:G:H5"	2.33	0.58
2:B:29:G:C6	2:B:30:C:C2	2.91	0.58
1:G:27:LYS:O	1:G:31:VAL:HG23	2.04	0.58
1:G:72:ASP:OD1	1:G:75:ARG:NH1	2.36	0.58
1:C:45:PHE:CE1	1:C:56:GLU:HB2	2.38	0.58
2:D:8:A:N3	2:D:8:A:H2'	2.19	0.58
1:E:112:TYR:CE1	2:F:17:C:OP2	2.56	0.58
2:F:46:G:H8	2:F:46:G:O5'	1.85	0.58
1:G:71:VAL:HB	1:G:75:ARG:NH2	2.17	0.58
2:D:33:U:H2'	2:D:34:U:H6	1.69	0.58
1:E:78:LYS:CE	2:F:19:A:O2'	2.52	0.58
2:F:8:A:H2'	2:F:8:A:N3	2.18	0.58
1:G:100:LEU:HD12	1:G:117:LEU:HD23	1.86	0.58
1:C:20:TYR:O	1:C:116:LEU:HD12	2.03	0.58
1:E:22:ALA:HB2	1:E:81:LEU:CD1	2.34	0.58
1:C:9:ARG:HH12	2:B:5:G:C5'	2.15	0.57
2:D:22:G:C3'	2:D:23:G:H5"	2.33	0.57
1:E:112:TYR:CD2	2:F:16:U:H1'	2.39	0.57
1:A:24:ILE:CD1	1:A:24:ILE:H	2.10	0.57
2:B:46:G:O5'	2:B:46:G:H8	1.86	0.57
1:G:89:LEU:HB2	1:G:92:LYS:CE	2.34	0.57
1:G:86:LEU:O	1:G:90:LEU:HB3	2.03	0.57
2:H:68:C:H2'	2:H:69:C:H6	1.69	0.57
1:A:97:GLY:C	1:A:98:LEU:HD22	2.24	0.57
1:E:2:ALA:CB	2:H:9:A:OP1	2.52	0.57
2:F:16:U:O2'	2:F:17:C:OP1	2.19	0.57
1:G:106:TYR:OH	1:G:114:LYS:HB2	2.05	0.57
2:H:32:U:C2	2:H:33:U:C5	2.92	0.57
2:B:8:A:H2'	2:B:8:A:N3	2.19	0.57
1:C:93:VAL:CG2	1:C:100:LEU:HD23	2.21	0.57
2:F:12:G:O2'	2:F:13:G:C5'	2.53	0.57
2:H:6:U:H2'	2:H:7:G:H5'	1.85	0.57
1:E:19:THR:HG22	1:E:103:LEU:CD1	2.34	0.57
1:E:46:ALA:HA	1:E:55:LEU:HA	1.85	0.57
1:E:89:LEU:CD2	1:E:89:LEU:H	2.03	0.57
1:G:106:TYR:CZ	1:G:114:LYS:CB	2.86	0.57
2:B:12:G:HO2'	2:B:13:G:C5'	2.17	0.57
1:E:63:TYR:HD2	1:E:64:GLU:H	1.50	0.57
2:F:8:A:C2	2:F:10:A:OP2	2.57	0.57
1:G:7:ASN:OD1	1:G:10:ALA:HB2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:19:A:H62	2:D:46:G:N2	2.02	0.57
2:D:12:G:N1	2:D:57:G:C6	2.73	0.57
2:D:60:U:C2'	2:D:61:C:OP1	2.48	0.57
2:F:47:A:H2'	2:F:47:A:N3	2.20	0.57
2:F:64:A:C2'	2:F:65:C:C6	2.84	0.57
1:G:46:ALA:HB3	1:G:100:LEU:HB3	1.87	0.57
1:G:9:ARG:HH21	1:G:13:ASP:CB	2.16	0.57
2:B:8:A:C2	2:B:10:A:OP2	2.58	0.57
2:D:26:U:H2'	2:D:27:U:H5"	1.87	0.57
1:G:108:ASN:OD1	1:G:112:TYR:N	2.38	0.57
1:A:41:PHE:HD1	1:A:102:PRO:HB2	1.69	0.56
1:A:87:ARG:O	1:A:90:LEU:CD1	2.52	0.56
1:G:64:GLU:O	1:G:65:LYS:CD	2.52	0.56
2:H:10:A:C2'	2:H:11:C:H5"	2.33	0.56
2:F:47:A:H5'	2:F:48:C:OP1	2.05	0.56
1:G:112:TYR:CB	2:H:16:U:H1'	2.35	0.56
1:G:24:ILE:N	1:G:24:ILE:HD12	2.20	0.56
1:G:64:GLU:C	1:G:65:LYS:HD2	2.25	0.56
1:E:110:ARG:HG2	2:F:15:C:C4	2.40	0.56
1:E:40:ASP:HB3	2:H:5:G:O2'	2.06	0.56
1:G:19:THR:HG22	1:G:20:TYR:N	2.19	0.56
1:G:112:TYR:HD2	2:H:47:A:C6	2.24	0.56
1:A:23:GLY:HA2	1:A:114:LYS:HD3	1.87	0.56
2:D:16:U:O2'	2:D:17:C:P	2.62	0.56
2:D:13:G:H1'	2:D:57:G:C2	2.41	0.56
1:G:46:ALA:HB3	1:G:100:LEU:CD1	2.31	0.56
1:A:6:GLU:HG2	1:A:104:LYS:HB2	1.88	0.56
1:C:31:VAL:O	1:C:34:LEU:HB2	2.05	0.56
1:E:82:HIS:N	1:E:82:HIS:ND1	2.53	0.56
1:G:113:ALA:HB3	2:H:47:A:N1	2.20	0.56
1:A:104:LYS:HG2	1:A:106:TYR:HD2	1.71	0.56
1:C:3:PRO:CD	1:C:35:ARG:O	2.53	0.56
1:E:31:VAL:HA	1:E:34:LEU:HD12	1.88	0.56
1:A:17:LEU:HD11	1:A:121:ARG:HD3	1.88	0.56
2:D:52:G:O6	2:D:63:C:N4	2.39	0.56
1:A:86:LEU:O	1:A:90:LEU:CD2	2.53	0.56
2:D:12:G:N2	2:D:57:G:C2	2.74	0.56
1:G:104:LYS:O	1:G:116:LEU:HB2	2.05	0.56
1:G:55:LEU:CD2	1:G:77:ARG:HH11	2.19	0.56
1:C:27:LYS:N	1:C:27:LYS:HD2	2.20	0.56
1:C:6:GLU:HB3	1:C:104:LYS:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:16:U:O2	2:F:47:A:N6	2.39	0.56
1:G:20:TYR:O	1:G:116:LEU:HD12	2.06	0.56
1:G:80:LEU:O	1:G:81:LEU:HD12	2.05	0.56
1:C:54:TYR:N	1:C:54:TYR:CD1	2.73	0.56
2:D:12:G:C2	2:D:57:G:C2	2.93	0.56
2:D:66:C:N4	2:D:67:A:H62	2.04	0.56
1:G:9:ARG:HD2	1:G:12:HIS:HD2	1.71	0.56
1:E:47:ARG:HD2	1:E:48:PHE:CE1	2.41	0.55
1:G:98:LEU:CD2	1:G:99:THR:N	2.63	0.55
1:A:41:PHE:CD2	1:A:41:PHE:N	2.73	0.55
1:C:9:ARG:NH1	2:B:5:G:OP1	2.39	0.55
1:C:52:GLU:O	1:C:54:TYR:HE1	1.88	0.55
1:E:55:LEU:HD23	1:E:56:GLU:N	2.22	0.55
1:E:58:LEU:HG	1:E:58:LEU:O	2.03	0.55
1:E:98:LEU:CD2	1:E:119:LEU:HD13	2.35	0.55
1:E:32:LYS:HG3	2:F:49:G:H5'	1.88	0.55
1:C:3:PRO:HB3	1:C:5:LEU:HD21	1.87	0.55
2:D:68:C:H2'	2:D:69:C:C6	2.40	0.55
1:G:83:LYS:O	1:G:87:ARG:HB2	2.05	0.55
1:E:60:ILE:HG12	1:E:77:ARG:NH2	2.22	0.55
1:E:81:LEU:O	2:F:18:G:O2'	2.24	0.55
1:G:19:THR:HG23	1:G:103:LEU:HD11	1.88	0.55
1:G:31:VAL:HG21	2:H:47:A:H1'	1.87	0.55
1:C:4:VAL:C	1:C:5:LEU:HD23	2.27	0.55
1:E:102:PRO:HA	1:E:117:LEU:CD2	2.36	0.55
1:E:63:TYR:HE2	1:E:65:LYS:HG3	1.72	0.55
1:E:112:TYR:OH	2:F:15:C:H6	1.87	0.55
1:G:101:VAL:CG1	1:G:120:ALA:CB	2.84	0.55
2:H:46:G:H5"	2:H:47:A:OP2	2.07	0.55
2:B:64:A:C2'	2:B:65:C:H6	2.15	0.55
1:A:74:ARG:NH1	2:D:71:C:OP1	2.40	0.55
1:E:41:PHE:CD1	1:E:102:PRO:HB2	2.41	0.55
1:E:27:LYS:N	1:E:30:GLU:OE1	2.40	0.55
2:F:35:G:O6	2:F:46:G:N2	2.40	0.55
1:C:98:LEU:HD21	1:C:119:LEU:CD2	2.37	0.55
2:D:2:G:H2'	2:D:2:G:N3	2.22	0.55
1:E:63:TYR:CD2	1:E:64:GLU:N	2.71	0.55
1:E:68:TYR:CE1	2:F:49:G:O4'	2.60	0.55
2:F:31:C:C2'	2:F:32:U:H5'	2.37	0.55
2:H:8:A:N3	2:H:8:A:H2'	2.22	0.55
1:C:83:LYS:O	1:C:87:ARG:HB2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:13:G:N2	2:D:57:G:C8	2.75	0.55
1:G:17:LEU:HB2	1:G:119:LEU:CB	2.37	0.55
1:G:82:HIS:N	2:H:18:G:H1'	2.22	0.55
2:H:23:G:C6	2:H:24:G:N7	2.75	0.55
1:E:45:PHE:HB3	1:E:100:LEU:O	2.06	0.55
2:F:53:G:O2'	2:F:54:5MU:H5"	2.07	0.55
2:H:26:U:O2'	2:H:27:U:H5"	2.07	0.55
1:C:82:HIS:N	2:D:18:G:H1'	2.22	0.54
1:G:21:GLU:CG	2:H:18:G:H22	2.20	0.54
1:C:82:HIS:CE1	2:D:17:C:O2'	2.61	0.54
1:E:16:ILE:HA	1:E:119:LEU:O	2.07	0.54
1:E:89:LEU:N	1:E:89:LEU:HD23	2.07	0.54
2:F:70:U:H2'	2:F:71:C:C5	2.42	0.54
2:H:52:G:O6	2:H:63:C:N4	2.40	0.54
1:E:14:TYR:N	1:E:14:TYR:CD2	2.75	0.54
1:E:44:SER:N	1:E:57:ASN:ND2	2.51	0.54
1:E:62:PRO:HB3	1:E:70:ASN:ND2	2.19	0.54
1:E:68:TYR:HB3	2:F:67:A:H1'	1.89	0.54
1:G:23:GLY:C	1:G:114:LYS:HZ2	2.10	0.54
1:G:48:PHE:CE1	1:G:49:GLU:O	2.60	0.54
2:B:7:G:H5'	2:B:7:G:H8	1.73	0.54
1:E:78:LYS:HG3	1:E:79:LEU:H	1.72	0.54
1:E:81:LEU:CD1	2:F:18:G:N2	2.71	0.54
1:A:101:VAL:O	1:A:117:LEU:HD23	2.07	0.54
1:A:46:ALA:HA	1:A:55:LEU:HA	1.90	0.54
1:A:67:SER:OG	2:B:68:C:C5'	2.56	0.54
1:E:110:ARG:HB3	2:F:15:C:C4	2.42	0.54
1:G:23:GLY:CA	1:G:114:LYS:NZ	2.59	0.54
1:G:78:LYS:NZ	2:H:19:A:H2'	2.22	0.54
1:G:60:ILE:HD12	1:G:77:ARG:NH1	2.22	0.54
2:H:66:C:H3'	2:H:67:A:H8	1.73	0.54
1:A:44:SER:O	1:A:102:PRO:HD2	2.07	0.54
1:A:24:ILE:HG23	1:A:79:LEU:CD2	2.37	0.54
2:D:13:G:C2	2:D:57:G:C4	2.95	0.54
1:E:63:TYR:CG	1:E:67:SER:HA	2.42	0.54
1:E:83:LYS:CG	1:E:84:HIS:N	2.69	0.54
1:A:86:LEU:O	1:A:90:LEU:HD23	2.07	0.54
2:B:14:U:HO2'	2:B:15:C:C5'	2.14	0.54
2:F:64:A:C2'	2:F:65:C:H6	2.20	0.54
1:G:24:ILE:HD12	1:G:114:LYS:NZ	2.23	0.54
1:G:98:LEU:CD2	1:G:99:THR:H	2.20	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:LYS:HG2	1:A:106:TYR:CD2	2.42	0.54
1:A:82:HIS:N	2:B:18:G:H1'	2.23	0.54
1:C:70:ASN:ND2	1:C:71:VAL:H	2.04	0.54
2:D:10:A:C2'	2:D:11:C:H5"	2.38	0.54
2:D:23:G:C6	2:D:24:G:N7	2.76	0.54
1:G:48:PHE:CG	1:G:49:GLU:N	2.76	0.54
1:G:72:ASP:HB3	1:G:75:ARG:NH1	2.23	0.54
1:A:94:GLU:C	1:A:96:LYS:N	2.61	0.53
1:A:66:GLY:HA3	2:B:68:C:H4'	1.90	0.53
1:E:41:PHE:HA	1:E:44:SER:OG	2.09	0.53
1:E:93:VAL:O	1:E:98:LEU:HB2	2.09	0.53
1:C:39:VAL:HG12	1:C:60:ILE:HG12	1.90	0.53
1:C:6:GLU:OE1	1:C:6:GLU:N	2.41	0.53
2:F:13:G:N2	2:F:56:C:N3	2.49	0.53
2:H:68:C:H2'	2:H:69:C:C6	2.43	0.53
1:C:13:ASP:O	1:C:14:TYR:CD2	2.57	0.53
2:D:16:U:N3	2:D:47:A:N7	2.56	0.53
1:E:24:ILE:HB	1:E:26:LEU:HD21	1.89	0.53
1:A:82:HIS:CE1	2:B:18:G:C4'	2.91	0.53
1:E:13:ASP:C	1:E:14:TYR:CD2	2.81	0.53
1:E:63:TYR:HB3	1:E:67:SER:CB	2.38	0.53
1:E:93:VAL:O	1:E:98:LEU:CB	2.56	0.53
2:H:2:G:H2'	2:H:2:G:N3	2.22	0.53
1:A:104:LYS:HB3	1:A:116:LEU:HD23	1.91	0.53
1:C:52:GLU:O	1:C:54:TYR:CE1	2.61	0.53
1:E:85:GLU:O	1:E:89:LEU:CD2	2.46	0.53
1:G:13:ASP:C	1:G:14:TYR:CD1	2.81	0.53
2:H:26:U:H2'	2:H:27:U:C5'	2.39	0.53
2:H:27:U:O2'	2:H:28:C:OP1	2.22	0.53
1:A:98:LEU:HD13	1:A:120:ALA:O	2.09	0.53
1:A:2:ALA:CA	1:A:35:ARG:O	2.53	0.53
2:B:47:A:H2'	2:B:47:A:N3	2.23	0.53
1:E:98:LEU:CG	1:E:119:LEU:HB3	2.39	0.53
1:G:10:ALA:O	1:G:14:TYR:HB2	2.09	0.53
1:A:81:LEU:HA	2:B:18:G:N3	2.24	0.53
1:G:52:GLU:HG3	1:G:54:TYR:HE1	1.74	0.53
1:C:39:VAL:HG12	1:C:60:ILE:HA	1.91	0.53
1:C:81:LEU:HD23	2:D:18:G:H21	1.74	0.53
2:D:23:G:C6	2:D:24:G:C5	2.97	0.53
1:C:112:TYR:CE1	2:D:16:U:C1'	2.92	0.53
2:H:23:G:C6	2:H:24:G:C5	2.97	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:52:GLU:OE1	1:C:78:LYS:HD3	2.09	0.52
1:E:92:LYS:O	1:E:98:LEU:CD2	2.54	0.52
1:G:6:GLU:CA	1:G:104:LYS:HB3	2.38	0.52
1:G:47:ARG:HH12	1:G:99:THR:HG22	1.74	0.52
1:G:52:GLU:HB2	1:G:78:LYS:HE3	1.90	0.52
1:G:97:GLY:C	1:G:121:ARG:HG3	2.29	0.52
2:H:16:U:O2'	2:H:17:C:P	2.67	0.52
2:B:8:A:C2	2:B:10:A:P	3.03	0.52
1:C:22:ALA:CB	1:C:79:LEU:HD22	2.36	0.52
2:H:33:U:H2'	2:H:34:U:C6	2.44	0.52
1:C:16:ILE:CG2	1:C:17:LEU:N	2.72	0.52
1:G:5:LEU:CD1	1:G:37:GLY:HA2	2.39	0.52
1:A:16:ILE:HD12	1:A:103:LEU:HD21	1.91	0.52
1:C:9:ARG:NH1	2:B:5:G:C5'	2.71	0.52
2:D:57:G:H2'	2:D:57:G:N3	2.25	0.52
2:D:3:G:N2	2:D:71:C:H1'	2.24	0.52
1:E:63:TYR:C	1:E:67:SER:HB3	2.30	0.52
1:G:107:PHE:HA	1:G:113:ALA:HA	1.91	0.52
1:G:9:ARG:O	1:G:14:TYR:CE1	2.63	0.52
1:E:110:ARG:HB3	2:F:15:C:C5	2.45	0.52
2:H:31:C:H2'	2:H:32:U:O4'	2.10	0.52
2:H:57:G:N3	2:H:57:G:H2'	2.24	0.52
1:G:80:LEU:HG	2:H:19:A:C4	2.45	0.52
2:H:4:G:O2'	2:H:5:G:H5'	2.09	0.52
1:A:2:ALA:O	1:A:3:PRO:O	2.27	0.52
1:C:92:LYS:C	1:C:94:GLU:N	2.62	0.52
1:E:62:PRO:C	1:E:70:ASN:ND2	2.62	0.52
1:C:59:TYR:CE1	1:C:73:PRO:CB	2.93	0.52
1:E:39:VAL:HG12	1:E:60:ILE:HA	1.92	0.52
1:E:112:TYR:OH	2:F:15:C:C6	2.55	0.52
1:G:54:TYR:HB2	1:G:56:GLU:OE1	2.10	0.52
2:D:70:U:H2'	2:D:71:C:C6	2.45	0.52
2:F:7:G:C4	2:F:49:G:N7	2.78	0.52
1:G:113:ALA:CB	2:H:47:A:N1	2.73	0.52
1:G:21:GLU:HG3	2:H:18:G:N2	2.25	0.52
1:G:39:VAL:CB	1:G:59:TYR:O	2.50	0.52
1:G:60:ILE:O	1:G:60:ILE:HG22	2.10	0.52
1:A:45:PHE:HB2	1:A:100:LEU:O	2.08	0.52
1:A:14:TYR:HB2	1:A:120:ALA:HB1	1.92	0.52
1:C:55:LEU:HD21	1:C:58:LEU:CB	2.40	0.52
1:C:6:GLU:HA	1:C:104:LYS:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:55:PSU:N3	2:D:57:G:H5”	2.25	0.52
2:F:35:G:H2’	2:F:46:G:O4’	2.10	0.52
2:F:8:A:C2	2:F:10:A:P	3.03	0.52
1:G:71:VAL:CG2	1:G:72:ASP:N	2.72	0.52
1:E:87:ARG:HA	1:E:90:LEU:CD2	2.39	0.51
1:G:71:VAL:HG23	1:G:72:ASP:H	1.75	0.51
2:B:31:C:C2’	2:B:32:U:H5’	2.40	0.51
2:D:55:PSU:N3	2:D:57:G:OP2	2.43	0.51
1:E:62:PRO:O	1:E:70:ASN:ND2	2.43	0.51
2:H:21:A:H8	2:H:21:A:O5’	1.92	0.51
1:A:45:PHE:HA	1:A:102:PRO:CD	2.35	0.51
1:E:15:GLU:N	1:E:121:ARG:O	2.42	0.51
1:E:28:GLY:CA	1:E:31:VAL:HG23	2.39	0.51
1:E:81:LEU:C	2:F:18:G:HO2’	2.13	0.51
2:F:14:U:H2’	2:F:15:C:O5’	2.09	0.51
1:G:29:THR:OG1	1:G:62:PRO:HB3	2.09	0.51
1:A:9:ARG:HH22	1:A:42:THR:HG23	1.74	0.51
1:C:52:GLU:CG	2:D:19:A:O2’	2.57	0.51
1:E:57:ASN:OD1	1:E:74:ARG:NH2	2.38	0.51
1:E:58:LEU:HD12	1:E:59:TYR:N	2.26	0.51
2:H:14:U:C5	2:H:15:C:C2	2.98	0.51
1:C:68:TYR:OH	2:D:49:G:H1’	2.10	0.51
1:G:44:SER:HA	1:G:57:ASN:O	2.10	0.51
2:B:7:G:C8	2:B:7:G:H5’	2.46	0.51
1:C:62:PRO:HG3	1:C:70:ASN:HD22	1.74	0.51
1:G:6:GLU:CD	1:G:6:GLU:N	2.63	0.51
1:A:45:PHE:HD2	1:A:45:PHE:H	1.58	0.51
1:C:6:GLU:HA	1:C:104:LYS:CB	2.40	0.51
1:C:2:ALA:N	2:B:9:A:H8	2.09	0.51
2:D:63:C:H2’	2:D:64:A:O4’	2.10	0.51
2:F:7:G:H5’	2:F:7:G:H8	1.75	0.51
1:G:27:LYS:O	1:G:29:THR:N	2.43	0.51
2:H:3:G:N2	2:H:71:C:H1’	2.25	0.51
1:E:63:TYR:CD2	1:E:67:SER:HA	2.45	0.51
1:G:100:LEU:CD1	1:G:117:LEU:HB3	2.40	0.51
1:G:6:GLU:CD	1:G:6:GLU:H	2.14	0.51
2:B:35:G:O2’	2:B:46:G:H5’	2.10	0.51
2:B:3:G:N2	2:B:71:C:H1’	2.26	0.51
1:A:38:LYS:HE2	2:D:5:G:H21	1.69	0.51
1:G:5:LEU:HD11	1:G:37:GLY:HA2	1.93	0.51
1:C:53:LEU:C	1:C:54:TYR:CD1	2.85	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:83:LYS:O	1:C:87:ARG:CG	2.59	0.50
1:C:9:ARG:NH1	1:C:9:ARG:HB2	2.26	0.50
2:D:67:A:H2'	2:D:68:C:H6	1.77	0.50
1:E:83:LYS:O	1:E:86:LEU:CD2	2.59	0.50
1:G:82:HIS:HB3	1:G:84:HIS:CE1	2.45	0.50
2:B:16:U:OP1	2:B:46:G:N1	2.38	0.50
1:E:112:TYR:O	1:E:114:LYS:HG2	2.11	0.50
1:E:88:ARG:HD2	1:E:88:ARG:C	2.30	0.50
1:G:31:VAL:CA	1:G:34:LEU:HG	2.42	0.50
2:H:63:C:H5'	2:H:63:C:H6	1.75	0.50
1:A:6:GLU:CG	1:A:104:LYS:HB2	2.42	0.50
1:A:14:TYR:C	1:A:15:GLU:OE2	2.50	0.50
1:A:87:ARG:CA	1:A:90:LEU:HD21	2.26	0.50
2:D:66:C:H3'	2:D:67:A:H8	1.75	0.50
1:G:78:LYS:HD3	2:H:19:A:C2	2.47	0.50
2:H:63:C:H2'	2:H:64:A:O4'	2.10	0.50
1:A:100:LEU:CD1	1:A:117:LEU:HD22	2.41	0.50
2:D:23:G:C4	2:D:24:G:C8	3.00	0.50
1:C:83:LYS:O	1:C:87:ARG:HG3	2.12	0.50
2:D:31:C:H2'	2:D:32:U:O4'	2.11	0.50
2:H:33:U:H2'	2:H:34:U:H6	1.75	0.50
1:A:67:SER:O	2:B:67:A:O2'	2.29	0.50
1:C:92:LYS:C	1:C:94:GLU:H	2.14	0.50
1:E:104:LYS:CD	1:E:116:LEU:HD23	2.41	0.50
1:E:4:VAL:HG23	1:E:106:TYR:HD2	1.70	0.50
1:E:71:VAL:CG1	1:E:72:ASP:N	2.74	0.50
1:E:88:ARG:HD2	1:E:89:LEU:CA	2.42	0.50
1:A:41:PHE:CE1	1:A:105:ILE:HD11	2.46	0.50
2:B:58:A:C6	2:B:61:C:C4	2.99	0.50
1:G:63:TYR:HD2	1:G:66:GLY:O	1.92	0.50
1:G:112:TYR:HB3	2:H:16:U:H1'	1.94	0.50
2:D:6:U:H2'	2:D:7:G:C5'	2.42	0.50
1:E:47:ARG:NH1	1:E:48:PHE:CE1	2.78	0.50
2:D:62:C:O2	2:D:62:C:H2'	2.10	0.49
1:E:34:LEU:C	1:E:36:ALA:N	2.65	0.49
1:E:22:ALA:HA	2:F:18:G:C2	2.47	0.49
2:H:23:G:C4	2:H:24:G:C8	3.00	0.49
1:C:44:SER:HB2	1:C:102:PRO:HG2	1.93	0.49
1:C:105:ILE:HD12	1:C:106:TYR:N	2.28	0.49
2:D:68:C:O2'	2:D:69:C:H5'	2.12	0.49
1:E:105:ILE:O	1:E:105:ILE:HD12	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:106:TYR:CZ	1:G:114:LYS:O	2.65	0.49
1:G:26:LEU:HD21	1:G:34:LEU:HD11	1.91	0.49
1:G:59:TYR:OH	1:G:74:ARG:NH1	2.45	0.49
1:C:35:ARG:HH22	2:D:48:C:H42	1.60	0.49
1:E:60:ILE:HD11	1:E:77:ARG:HH21	1.76	0.49
1:G:20:TYR:HE2	1:G:89:LEU:HD13	1.77	0.49
1:G:48:PHE:CZ	1:G:49:GLU:O	2.65	0.49
1:G:67:SER:C	1:G:68:TYR:CD2	2.85	0.49
2:B:46:G:H5"	2:B:47:A:OP2	2.12	0.49
2:B:48:C:O2	2:B:48:C:C2'	2.60	0.49
1:G:21:GLU:O	2:H:18:G:C2	2.66	0.49
1:E:93:VAL:CA	1:E:98:LEU:HB3	2.35	0.49
1:G:103:LEU:HD11	1:G:117:LEU:C	2.32	0.49
1:G:75:ARG:N	1:G:77:ARG:NH2	2.58	0.49
1:G:103:LEU:HD12	1:G:116:LEU:HB3	1.94	0.49
2:H:62:C:O2	2:H:62:C:H2'	2.12	0.49
2:B:16:U:H3'	2:B:18:G:OP2	2.13	0.49
2:D:23:G:C2'	2:D:24:G:H5'	2.42	0.49
1:E:108:ASN:CG	1:E:114:LYS:HZ2	2.16	0.49
1:E:80:LEU:HG	2:F:19:A:C8	2.48	0.49
1:G:14:TYR:CD1	1:G:14:TYR:N	2.80	0.49
1:G:52:GLU:HB3	1:G:78:LYS:HE3	1.93	0.49
1:G:89:LEU:HG	1:G:89:LEU:O	2.10	0.49
1:A:39:VAL:HB	1:A:59:TYR:O	2.13	0.49
1:E:44:SER:O	1:E:102:PRO:HD2	2.13	0.49
1:G:31:VAL:HA	1:G:34:LEU:HG	1.94	0.49
1:A:44:SER:HA	1:A:57:ASN:HB3	1.95	0.49
1:C:6:GLU:HB3	1:C:104:LYS:HB3	1.94	0.49
1:C:55:LEU:HD21	1:C:58:LEU:HB3	1.95	0.49
1:E:46:ALA:HB3	1:E:100:LEU:HB3	1.94	0.49
1:E:78:LYS:NZ	2:F:20:C:O4'	2.45	0.49
2:H:58:A:H1'	2:H:60:U:H5	1.78	0.49
2:D:70:U:H2'	2:D:71:C:H6	1.77	0.49
1:E:59:TYR:HE1	1:E:73:PRO:HB3	1.74	0.49
2:H:19:A:H61	2:H:46:G:H21	1.57	0.49
1:A:28:GLY:HA2	2:B:47:A:O2'	2.13	0.48
2:D:13:G:N3	2:D:57:G:C4	2.81	0.48
2:F:19:A:H62	2:F:46:G:H21	1.59	0.48
1:C:16:ILE:HG22	1:C:17:LEU:N	2.28	0.48
1:C:27:LYS:O	1:C:29:THR:N	2.46	0.48
1:E:32:LYS:CD	2:F:49:G:H5'	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:52:G:N2	2:H:53:G:H1'	2.29	0.48
2:H:55:PSU:N3	2:H:57:G:H5"	2.28	0.48
2:H:70:U:H2'	2:H:71:C:C6	2.48	0.48
1:C:93:VAL:HA	1:C:98:LEU:O	2.14	0.48
2:D:19:A:H2'	2:D:20:C:O4'	2.13	0.48
2:D:27:U:C2'	2:D:28:C:OP1	2.61	0.48
1:E:52:GLU:CG	1:E:54:TYR:HE1	2.25	0.48
1:E:72:ASP:CB	1:E:75:ARG:HH21	2.24	0.48
2:F:48:C:C2'	2:F:48:C:O2	2.60	0.48
1:A:55:LEU:CD1	1:A:102:PRO:HG3	2.23	0.48
1:A:20:TYR:O	1:A:116:LEU:HD12	2.14	0.48
1:A:75:ARG:O	1:A:77:ARG:HG3	2.13	0.48
1:C:31:VAL:HG21	2:D:47:A:O2'	2.14	0.48
1:E:78:LYS:HD3	2:F:19:A:H1'	1.95	0.48
1:G:5:LEU:HD11	1:G:37:GLY:HA3	1.95	0.48
1:G:58:LEU:HD23	1:G:60:ILE:CG1	2.43	0.48
1:A:59:TYR:CD1	1:A:73:PRO:HB3	2.47	0.48
1:C:62:PRO:HG3	1:C:70:ASN:ND2	2.28	0.48
1:C:82:HIS:HE1	2:D:17:C:O2'	1.97	0.48
1:A:26:LEU:HD12	1:A:31:VAL:HG22	1.96	0.48
1:C:98:LEU:HD11	1:C:119:LEU:HB3	1.94	0.48
1:E:28:GLY:HA2	1:E:31:VAL:HG23	1.96	0.48
1:G:30:GLU:O	1:G:34:LEU:HG	2.14	0.48
1:A:6:GLU:OE1	1:A:104:LYS:HB2	2.13	0.48
1:E:27:LYS:CD	1:E:30:GLU:OE1	2.56	0.48
1:E:78:LYS:HE2	2:F:19:A:O2'	2.14	0.48
1:A:98:LEU:HD11	1:A:121:ARG:HD2	1.96	0.48
1:A:27:LYS:HB2	1:A:30:GLU:HG3	1.95	0.48
1:C:94:GLU:C	1:C:96:LYS:N	2.67	0.48
2:H:66:C:H2'	2:H:67:A:C8	2.49	0.48
1:A:98:LEU:N	1:A:98:LEU:HD22	2.29	0.48
1:C:62:PRO:HB3	1:C:70:ASN:ND2	2.29	0.48
2:D:66:C:H2'	2:D:67:A:C8	2.49	0.48
2:F:12:G:C2	2:F:58:A:C2	3.02	0.48
1:G:105:ILE:HG22	1:G:115:VAL:HG23	1.96	0.48
1:G:82:HIS:O	1:G:86:LEU:CD1	2.56	0.48
1:G:113:ALA:C	2:H:47:A:H61	2.14	0.48
2:B:57:G:H2'	2:B:58:A:H5'	1.95	0.48
1:C:81:LEU:HA	2:D:18:G:N3	2.28	0.48
1:E:48:PHE:CE2	1:E:100:LEU:HD21	2.49	0.48
2:F:19:A:C5	2:F:20:C:C5	3.02	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:7:G:H5'	2:F:7:G:C8	2.49	0.48
1:E:35:ARG:HD2	2:F:8:A:H1'	1.95	0.48
2:H:23:G:C5	2:H:24:G:C8	3.02	0.48
1:A:25:ALA:O	1:A:75:ARG:NH2	2.46	0.47
1:A:38:LYS:CG	1:A:38:LYS:O	2.62	0.47
1:C:110:ARG:NH2	2:D:15:C:O2	2.47	0.47
1:C:6:GLU:CB	1:C:104:LYS:HB3	2.44	0.47
1:C:81:LEU:O	2:D:18:G:O2'	2.32	0.47
1:C:90:LEU:HD12	1:C:91:GLY:H	1.78	0.47
1:G:54:TYR:N	1:G:54:TYR:CD1	2.82	0.47
1:A:90:LEU:HD12	1:A:91:GLY:H	1.74	0.47
1:A:82:HIS:N	2:B:18:G:O2'	2.48	0.47
2:D:31:C:H6	2:D:31:C:O5'	1.97	0.47
2:D:49:G:O2'	2:D:50:U:H5'	2.14	0.47
2:D:52:G:N2	2:D:53:G:H1'	2.28	0.47
1:E:53:LEU:HD23	1:E:79:LEU:HD13	1.96	0.47
1:G:89:LEU:C	1:G:92:LYS:HG3	2.34	0.47
2:H:19:A:H62	2:H:46:G:H21	1.49	0.47
2:H:9:A:N3	2:H:9:A:H2'	2.29	0.47
1:A:120:ALA:C	1:A:121:ARG:HG2	2.33	0.47
2:D:23:G:H2'	2:D:24:G:H5'	1.96	0.47
1:E:45:PHE:CB	1:E:100:LEU:O	2.62	0.47
1:G:9:ARG:HD2	1:G:12:HIS:CD2	2.50	0.47
2:H:27:U:C2'	2:H:28:C:OP1	2.62	0.47
1:A:16:ILE:HD13	1:A:16:ILE:N	2.29	0.47
1:A:34:LEU:C	1:A:36:ALA:N	2.67	0.47
1:C:5:LEU:O	1:C:104:LYS:HB2	2.14	0.47
1:C:83:LYS:O	1:C:87:ARG:CB	2.62	0.47
2:D:23:G:C5	2:D:24:G:C8	3.02	0.47
1:G:63:TYR:HD2	1:G:65:LYS:O	1.98	0.47
1:G:98:LEU:HG	1:G:120:ALA:O	2.14	0.47
1:C:81:LEU:O	1:C:86:LEU:HD11	2.14	0.47
1:E:17:LEU:CD2	1:E:119:LEU:HD12	2.45	0.47
1:E:24:ILE:CG1	1:E:26:LEU:HD21	2.44	0.47
2:F:6:U:H2'	2:F:7:G:C5'	2.32	0.47
1:A:123:LYS:HD2	1:A:123:LYS:H	1.79	0.47
1:C:115:VAL:HG22	1:C:116:LEU:N	2.28	0.47
2:D:68:C:H2'	2:D:69:C:O4'	2.14	0.47
2:D:9:A:N3	2:D:9:A:H2'	2.29	0.47
1:E:45:PHE:N	1:E:45:PHE:CD1	2.82	0.47
1:E:81:LEU:HD23	1:E:85:GLU:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:110:ARG:CG	2:F:15:C:N4	2.76	0.47
1:G:27:LYS:CD	1:G:27:LYS:N	2.74	0.47
1:G:56:GLU:HG3	1:G:76:LYS:HD3	1.96	0.47
1:A:28:GLY:O	1:A:32:LYS:HG2	2.13	0.47
2:B:14:U:H2'	2:B:15:C:O5'	2.12	0.47
1:G:20:TYR:CE2	1:G:89:LEU:HD13	2.49	0.47
2:H:10:A:H2'	2:H:11:C:C5'	2.42	0.47
2:H:23:G:H5'	2:H:23:G:C8	2.45	0.47
1:A:105:ILE:O	1:A:106:TYR:HB3	2.14	0.47
1:A:63:TYR:HB2	1:A:70:ASN:ND2	2.29	0.47
2:B:12:G:C4	2:B:57:G:N2	2.83	0.47
2:D:21:A:O5'	2:D:21:A:H8	1.98	0.47
2:D:26:U:H2'	2:D:27:U:C5'	2.44	0.47
1:A:52:GLU:OE1	2:B:19:A:O2'	2.19	0.47
1:E:7:ASN:ND2	1:E:41:PHE:HB2	2.30	0.47
2:H:31:C:O5'	2:H:31:C:H6	1.98	0.47
1:A:29:THR:CG2	2:B:49:G:H4'	2.44	0.47
1:C:112:TYR:CE1	2:D:16:U:H1'	2.50	0.47
1:E:83:LYS:O	1:E:86:LEU:HD22	2.13	0.47
2:H:6:U:H2'	2:H:7:G:C5'	2.45	0.47
1:A:98:LEU:CD1	1:A:121:ARG:HD2	2.44	0.47
1:E:34:LEU:C	1:E:36:ALA:H	2.18	0.47
1:E:110:ARG:HB3	2:F:15:C:N4	2.29	0.47
2:H:68:C:H2'	2:H:69:C:O4'	2.15	0.47
1:A:82:HIS:HB3	1:A:84:HIS:CE1	2.49	0.46
1:C:84:HIS:O	1:C:88:ARG:N	2.48	0.46
1:E:2:ALA:N	1:E:3:PRO:HD3	2.30	0.46
1:E:52:GLU:H	1:E:52:GLU:HG2	1.48	0.46
2:F:29:G:H2'	2:F:30:C:O4'	2.15	0.46
1:G:106:TYR:CD1	1:G:106:TYR:O	2.69	0.46
1:G:84:HIS:O	1:G:88:ARG:N	2.48	0.46
1:C:107:PHE:HA	1:C:113:ALA:HA	1.97	0.46
2:D:13:G:H1'	2:D:57:G:H21	1.76	0.46
2:F:3:G:N2	2:F:71:C:H1'	2.30	0.46
1:G:106:TYR:OH	1:G:114:LYS:HB3	2.15	0.46
1:G:101:VAL:HG11	1:G:120:ALA:HB2	1.96	0.46
1:G:17:LEU:HG	1:G:119:LEU:O	2.16	0.46
1:G:55:LEU:HD23	1:G:77:ARG:HH11	1.80	0.46
2:H:13:G:H8	2:H:13:G:OP2	1.98	0.46
1:C:22:ALA:HB3	1:C:115:VAL:HG13	1.95	0.46
1:C:82:HIS:O	1:C:86:LEU:CD1	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:32:U:H2'	2:D:33:U:H6	1.81	0.46
1:E:46:ALA:HB1	1:E:53:LEU:HD21	1.96	0.46
1:A:101:VAL:C	1:A:117:LEU:HD23	2.35	0.46
2:B:30:C:H2'	2:B:31:C:C6	2.51	0.46
1:C:41:PHE:CZ	1:C:104:LYS:HA	2.51	0.46
1:G:115:VAL:CG1	1:G:117:LEU:HD11	2.45	0.46
2:H:70:U:H2'	2:H:71:C:H6	1.80	0.46
2:D:16:U:O2'	2:D:17:C:OP1	2.33	0.46
1:E:65:LYS:CG	1:E:66:GLY:H	2.11	0.46
2:F:16:U:H3'	2:F:18:G:OP2	2.15	0.46
2:F:52:G:H2'	2:F:52:G:N3	2.30	0.46
1:G:30:GLU:OE2	1:G:60:ILE:HB	2.16	0.46
2:H:14:U:H5"	2:H:15:C:C5	2.50	0.46
1:E:68:TYR:HE1	2:F:49:G:O4'	1.97	0.46
1:A:16:ILE:HA	1:A:119:LEU:O	2.15	0.46
1:C:72:ASP:HB2	1:C:75:ARG:CD	2.45	0.46
1:C:86:LEU:O	1:C:90:LEU:HB3	2.16	0.46
1:E:85:GLU:O	1:E:85:GLU:HG2	2.16	0.46
1:G:108:ASN:ND2	1:G:112:TYR:O	2.48	0.46
1:G:106:TYR:CE2	1:G:116:LEU:HD13	2.48	0.46
1:G:75:ARG:O	1:G:77:ARG:CD	2.62	0.46
1:G:75:ARG:O	1:G:77:ARG:CZ	2.64	0.46
1:A:83:LYS:HZ3	1:A:87:ARG:NH2	2.13	0.46
1:A:71:VAL:O	1:A:73:PRO:CD	2.55	0.46
2:B:53:G:C2'	2:B:54:5MU:H5"	2.46	0.46
1:C:23:GLY:O	1:C:79:LEU:HD23	2.15	0.46
2:D:13:G:C2	2:D:57:G:C5	3.04	0.46
1:G:96:LYS:N	1:G:96:LYS:HD2	2.31	0.46
1:A:81:LEU:CD2	1:A:85:GLU:CB	2.85	0.46
2:D:13:G:C4	2:D:57:G:C2	3.03	0.46
1:E:34:LEU:O	1:E:36:ALA:N	2.49	0.46
2:F:58:A:C6	2:F:61:C:C4	3.03	0.46
1:A:110:ARG:HG2	2:B:15:C:N4	2.32	0.45
1:E:82:HIS:ND1	2:F:18:G:H1'	2.31	0.45
1:E:81:LEU:CD2	1:E:85:GLU:O	2.64	0.45
1:G:100:LEU:HD11	1:G:117:LEU:HB3	1.98	0.45
1:G:101:VAL:HG12	1:G:120:ALA:CB	2.46	0.45
1:A:103:LEU:HB2	1:A:116:LEU:O	2.15	0.45
1:A:34:LEU:C	1:A:36:ALA:H	2.19	0.45
1:C:21:GLU:O	2:D:18:G:N2	2.49	0.45
2:D:26:U:O2'	2:D:27:U:H5"	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:46:G:H5”	2:F:47:A:OP2	2.16	0.45
1:C:112:TYR:HD1	2:D:16:U:HO2’	1.61	0.45
2:D:58:A:H1’	2:D:60:U:H5	1.80	0.45
1:E:108:ASN:CG	1:E:114:LYS:NZ	2.69	0.45
1:E:81:LEU:CA	2:F:18:G:O2’	2.63	0.45
1:G:101:VAL:HG11	1:G:120:ALA:CB	2.47	0.45
1:G:18:GLU:HG2	1:G:119:LEU:HD12	1.98	0.45
1:G:98:LEU:O	1:G:99:THR:HG23	2.16	0.45
2:B:47:A:H2’	2:B:48:C:C6	2.51	0.45
1:C:23:GLY:HA2	1:C:114:LYS:CE	2.47	0.45
1:C:39:VAL:HG11	1:C:60:ILE:HG12	1.99	0.45
2:D:13:G:OP2	2:D:13:G:H8	2.00	0.45
2:D:63:C:H6	2:D:63:C:H5’	1.81	0.45
1:E:63:TYR:HE2	1:E:65:LYS:CG	2.29	0.45
1:G:115:VAL:HG13	1:G:117:LEU:HD11	1.99	0.45
1:G:92:LYS:HD3	1:G:119:LEU:HD11	1.99	0.45
1:G:97:GLY:CA	1:G:121:ARG:HE	2.29	0.45
1:G:60:ILE:HD12	1:G:77:ARG:CZ	2.46	0.45
2:H:68:C:O2’	2:H:69:C:H5’	2.17	0.45
1:C:82:HIS:HD2	1:C:85:GLU:OE2	2.00	0.45
1:G:98:LEU:HD21	1:G:119:LEU:CD2	2.47	0.45
1:G:82:HIS:HB3	1:G:84:HIS:HE1	1.81	0.45
2:H:66:C:H3’	2:H:67:A:C8	2.52	0.45
1:A:39:VAL:HG11	1:A:60:ILE:HG23	1.99	0.45
1:C:101:VAL:HA	1:C:102:PRO:HD3	1.74	0.45
1:C:6:GLU:CB	1:C:104:LYS:CB	2.95	0.45
2:D:52:G:C6	2:D:63:C:N4	2.85	0.45
1:C:24:ILE:HG23	1:C:79:LEU:HD23	1.96	0.45
2:D:12:G:C2	2:D:58:A:C2	3.04	0.45
1:E:20:TYR:O	1:E:116:LEU:HD12	2.16	0.45
1:E:62:PRO:CB	1:E:70:ASN:ND2	2.77	0.45
1:G:19:THR:CG2	1:G:20:TYR:N	2.80	0.45
1:G:31:VAL:CG2	2:H:47:A:H1’	2.46	0.45
2:D:49:G:C2	2:D:66:C:O2	2.69	0.45
1:E:22:ALA:HB2	1:E:81:LEU:HD12	1.99	0.45
1:E:48:PHE:CZ	1:E:93:VAL:HG11	2.46	0.45
1:G:83:LYS:O	1:G:87:ARG:HG3	2.17	0.45
1:G:9:ARG:O	1:G:14:TYR:HE1	1.98	0.45
1:C:59:TYR:CE1	1:C:73:PRO:HB3	2.52	0.45
2:D:54:5MU:N3	2:D:58:A:N6	2.64	0.45
1:E:17:LEU:HD22	1:E:119:LEU:HD12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:23:GLY:CA	1:G:114:LYS:HD3	2.33	0.45
1:G:103:LEU:HD21	1:G:118:GLY:HA3	1.99	0.45
1:G:4:VAL:O	1:G:5:LEU:HD23	2.16	0.45
2:H:47:A:H5'	2:H:48:C:OP1	2.17	0.45
2:B:29:G:H2'	2:B:30:C:O4'	2.16	0.45
2:B:52:G:N3	2:B:52:G:H2'	2.31	0.45
1:C:22:ALA:HB3	1:C:115:VAL:CG1	2.47	0.45
1:C:76:LYS:O	1:C:76:LYS:HG3	2.16	0.45
2:F:47:A:H2'	2:F:48:C:C6	2.52	0.45
2:H:18:G:HO2'	2:H:19:A:P	2.40	0.45
1:A:62:PRO:HG2	1:A:73:PRO:HG3	1.99	0.44
1:A:46:ALA:N	1:A:100:LEU:O	2.42	0.44
1:E:88:ARG:HB3	1:E:89:LEU:HD23	1.99	0.44
1:G:71:VAL:HG21	1:G:75:ARG:HE	1.82	0.44
2:H:32:U:H2'	2:H:33:U:H6	1.79	0.44
2:H:66:C:N4	2:H:67:A:H62	2.12	0.44
1:A:34:LEU:O	1:A:36:ALA:N	2.50	0.44
1:A:81:LEU:C	2:B:18:G:HO2'	2.08	0.44
2:D:51:G:C6	2:D:64:A:N1	2.85	0.44
1:E:26:LEU:HD13	1:E:34:LEU:CD1	2.40	0.44
2:F:12:G:HO2'	2:F:13:G:C5'	2.27	0.44
1:G:100:LEU:CD1	1:G:117:LEU:HD23	2.47	0.44
1:G:21:GLU:CG	2:H:17:C:H42	2.29	0.44
1:G:31:VAL:C	1:G:34:LEU:HG	2.38	0.44
1:G:92:LYS:O	1:G:95:GLN:NE2	2.43	0.44
2:H:60:U:C6	2:H:60:U:OP2	2.70	0.44
2:B:28:C:O2	2:B:28:C:C2'	2.66	0.44
1:C:17:LEU:HD11	1:C:121:ARG:CG	2.48	0.44
2:D:46:G:H5"	2:D:47:A:OP2	2.17	0.44
1:E:22:ALA:HB2	1:E:81:LEU:HD13	1.99	0.44
1:G:68:TYR:CE2	2:H:67:A:H1'	2.52	0.44
2:H:23:G:H2'	2:H:24:G:H5'	1.99	0.44
1:E:88:ARG:HH12	1:E:119:LEU:CD2	2.23	0.44
2:F:58:A:O2'	2:F:60:U:C5	2.69	0.44
1:G:81:LEU:O	1:G:86:LEU:HD12	2.18	0.44
1:A:74:ARG:NH1	1:A:74:ARG:HG3	2.32	0.44
1:A:82:HIS:ND1	2:B:18:G:H4'	2.32	0.44
2:B:54:5MU:HN3	2:B:58:A:H62	1.65	0.44
1:C:101:VAL:HG12	1:C:120:ALA:HB2	2.00	0.44
1:E:81:LEU:HA	2:F:18:G:H1'	2.00	0.44
2:F:54:5MU:HN3	2:F:58:A:H62	1.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:30:GLU:O	1:G:34:LEU:CD2	2.65	0.44
1:G:86:LEU:CD2	1:G:87:ARG:N	2.80	0.44
2:D:23:G:H2'	2:D:24:G:C5'	2.47	0.44
1:E:104:LYS:HD3	1:E:116:LEU:CD2	2.45	0.44
1:E:54:TYR:CE2	1:E:78:LYS:HB2	2.53	0.44
1:E:78:LYS:HZ3	2:F:19:A:C2'	2.29	0.44
2:H:23:G:C2'	2:H:24:G:H5'	2.48	0.44
1:E:31:VAL:HG21	2:F:47:A:O2'	2.18	0.44
2:F:58:A:H2'	2:F:60:U:OP2	2.18	0.44
1:G:27:LYS:C	1:G:29:THR:N	2.71	0.44
1:A:85:GLU:O	1:A:89:LEU:HD22	2.18	0.44
1:C:70:ASN:CG	1:C:71:VAL:N	2.71	0.44
1:E:40:ASP:N	1:E:40:ASP:OD1	2.50	0.44
1:E:4:VAL:HA	1:E:106:TYR:HB3	2.00	0.44
2:F:13:G:HO2'	2:F:14:U:C5'	2.31	0.44
1:E:78:LYS:HZ3	2:F:20:C:H5'	1.82	0.44
2:H:23:G:H2'	2:H:24:G:C5'	2.48	0.44
1:C:81:LEU:HD22	1:C:85:GLU:CB	2.47	0.43
1:C:87:ARG:O	1:C:90:LEU:HG	2.18	0.43
1:E:39:VAL:CG1	1:E:60:ILE:HA	2.48	0.43
1:E:32:LYS:HD3	1:E:63:TYR:CE1	2.53	0.43
1:E:93:VAL:O	1:E:98:LEU:N	2.46	0.43
1:G:61:ALA:O	1:G:63:TYR:N	2.51	0.43
1:G:67:SER:C	1:G:68:TYR:CG	2.91	0.43
1:G:71:VAL:CG2	1:G:75:ARG:NE	2.81	0.43
1:G:82:HIS:ND1	2:H:18:G:O4'	2.51	0.43
2:B:19:A:H62	2:B:46:G:H21	1.66	0.43
2:B:3:G:O2'	2:B:4:G:H5'	2.17	0.43
1:C:121:ARG:O	1:C:122:GLY:O	2.36	0.43
1:C:61:ALA:HA	1:C:62:PRO:HD3	1.82	0.43
1:G:89:LEU:CA	1:G:92:LYS:HG3	2.48	0.43
1:A:45:PHE:CD2	1:A:45:PHE:N	2.85	0.43
1:C:98:LEU:HD23	1:C:99:THR:O	2.17	0.43
2:D:13:G:N2	2:D:57:G:N9	2.66	0.43
1:G:108:ASN:HD22	1:G:114:LYS:HG3	1.84	0.43
1:G:61:ALA:O	1:G:62:PRO:C	2.57	0.43
1:G:70:ASN:HD22	1:G:70:ASN:C	2.19	0.43
2:H:26:U:O2	2:H:28:C:H1'	2.18	0.43
2:H:65:C:C2'	2:H:66:C:O5'	2.67	0.43
1:A:16:ILE:CG2	1:A:19:THR:HG22	2.45	0.43
2:B:23:G:H5'	2:B:24:G:OP2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:64:GLU:O	1:E:66:GLY:N	2.51	0.43
2:F:57:G:H2'	2:F:58:A:H5'	2.00	0.43
2:H:16:U:O2'	2:H:17:C:OP1	2.36	0.43
1:A:20:TYR:HE1	1:A:85:GLU:CD	2.21	0.43
1:A:38:LYS:HG3	1:A:38:LYS:O	2.19	0.43
1:C:31:VAL:HG12	1:C:32:LYS:N	2.30	0.43
1:C:35:ARG:NH2	2:D:48:C:N4	2.65	0.43
1:C:59:TYR:CE1	1:C:73:PRO:HB2	2.54	0.43
1:C:83:LYS:HZ3	2:D:19:A:H5"	1.83	0.43
1:E:96:LYS:HB2	1:E:96:LYS:HE3	1.79	0.43
2:F:14:U:C2'	2:F:15:C:O5'	2.66	0.43
2:F:19:A:N6	2:F:46:G:H21	2.16	0.43
1:G:27:LYS:C	1:G:29:THR:H	2.21	0.43
2:H:35:G:C3'	2:H:46:G:C8	2.99	0.43
2:H:55:PSU:N3	2:H:57:G:OP2	2.51	0.43
2:H:54:5MU:N3	2:H:58:A:N6	2.67	0.43
1:C:17:LEU:HG	1:C:119:LEU:O	2.18	0.43
1:E:78:LYS:NZ	2:F:20:C:H5'	2.34	0.43
1:G:101:VAL:HA	1:G:102:PRO:HD3	1.74	0.43
2:H:10:A:C3'	2:H:11:C:H5"	2.47	0.43
1:G:68:TYR:HE2	2:H:67:A:H1'	1.83	0.43
2:B:14:U:O2'	2:B:15:C:P	2.75	0.43
1:E:61:ALA:O	1:E:63:TYR:N	2.52	0.43
1:E:81:LEU:CD2	1:E:85:GLU:CG	2.92	0.43
2:F:28:C:O2	2:F:28:C:C2'	2.64	0.43
2:F:31:C:H2'	2:F:32:U:H5'	2.00	0.43
1:G:78:LYS:HD3	2:H:19:A:N3	2.34	0.43
1:A:4:VAL:CG1	1:A:104:LYS:HE3	2.49	0.43
1:A:52:GLU:OE1	2:B:20:C:H5'	2.18	0.43
1:C:113:ALA:O	2:D:47:A:N6	2.52	0.43
2:D:23:G:O2'	2:D:24:G:H5'	2.19	0.43
2:F:49:G:O2'	2:F:50:U:H5'	2.18	0.43
2:F:3:G:O2'	2:F:4:G:H5'	2.17	0.43
1:G:31:VAL:O	1:G:34:LEU:N	2.46	0.43
2:B:24:G:N2	2:B:32:U:O2	2.52	0.43
1:C:54:TYR:HD1	1:C:54:TYR:N	2.17	0.43
1:G:48:PHE:HA	1:G:53:LEU:HA	2.01	0.43
1:G:72:ASP:HA	1:G:73:PRO:HD2	1.90	0.43
1:E:22:ALA:HB1	1:E:80:LEU:O	2.19	0.43
1:E:82:HIS:ND1	2:F:18:G:C1'	2.82	0.43
2:F:59:C:H2'	2:F:60:U:C1'	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:71:VAL:CG2	1:G:75:ARG:HE	2.32	0.43
1:G:81:LEU:O	1:G:86:LEU:CD1	2.67	0.43
1:G:89:LEU:HB2	1:G:92:LYS:NZ	2.34	0.43
1:E:31:VAL:HA	1:E:34:LEU:CD1	2.48	0.42
1:E:53:LEU:HD23	1:E:79:LEU:CD1	2.49	0.42
1:G:41:PHE:HE1	1:G:102:PRO:HB3	1.81	0.42
1:G:6:GLU:HB3	1:G:104:LYS:HD2	2.01	0.42
1:C:72:ASP:HA	1:C:73:PRO:HD3	1.89	0.42
1:C:87:ARG:HA	1:C:90:LEU:HD23	2.00	0.42
1:E:46:ALA:CB	1:E:53:LEU:HD21	2.49	0.42
1:E:73:PRO:O	1:E:77:ARG:NH2	2.52	0.42
2:F:58:A:C5	2:F:61:C:C4	3.07	0.42
1:G:59:TYR:CE1	1:G:74:ARG:NH1	2.84	0.42
1:A:60:ILE:HD12	1:A:77:ARG:NH2	2.34	0.42
1:A:82:HIS:ND1	2:B:18:G:C4'	2.82	0.42
2:B:29:G:C8	2:B:29:G:H3'	2.54	0.42
2:D:17:C:O5'	2:D:17:C:H6	2.03	0.42
2:D:49:G:C2'	2:D:50:U:H5'	2.49	0.42
1:E:32:LYS:CG	2:F:49:G:H5'	2.48	0.42
2:H:51:G:C6	2:H:64:A:N1	2.87	0.42
2:H:52:G:C6	2:H:63:C:N4	2.87	0.42
1:C:16:ILE:C	1:C:17:LEU:HD23	2.40	0.42
1:C:45:PHE:HD1	1:C:47:ARG:HG3	1.85	0.42
1:C:84:HIS:CG	1:C:85:GLU:N	2.87	0.42
2:D:66:C:C4	2:D:67:A:N6	2.88	0.42
1:G:91:GLY:HA2	1:G:94:GLU:CG	2.49	0.42
1:C:31:VAL:O	1:C:34:LEU:N	2.49	0.42
1:G:24:ILE:HD12	1:G:114:LYS:HZ2	1.85	0.42
2:H:17:C:H6	2:H:17:C:O5'	2.02	0.42
1:C:31:VAL:CG2	2:D:47:A:N3	2.83	0.42
1:E:5:LEU:HD11	1:E:105:ILE:HD11	2.02	0.42
1:E:47:ARG:O	1:E:53:LEU:HD12	2.17	0.42
1:G:55:LEU:O	1:G:55:LEU:HG	2.15	0.42
2:H:26:U:O2	2:H:28:C:O2	2.38	0.42
1:A:49:GLU:HB2	1:A:54:TYR:CE1	2.54	0.42
2:B:50:U:H3	2:B:64:A:H61	1.67	0.42
1:C:60:ILE:O	1:C:60:ILE:HG22	2.19	0.42
1:A:9:ARG:HH22	1:A:42:THR:CG2	2.32	0.42
2:D:52:G:C6	2:D:63:C:C4	3.08	0.42
1:E:44:SER:HA	1:E:57:ASN:HB3	2.01	0.42
1:E:18:GLU:HB2	1:E:88:ARG:HH22	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:103:LEU:H	1:G:103:LEU:HG	1.55	0.42
1:G:15:GLU:O	1:G:121:ARG:O	2.37	0.42
2:H:14:U:H5	2:H:15:C:O2	2.02	0.42
1:A:66:GLY:CA	2:B:68:C:H4'	2.49	0.42
1:A:80:LEU:N	1:A:80:LEU:HD12	2.35	0.42
1:C:120:ALA:O	1:C:121:ARG:HG2	2.20	0.42
1:C:121:ARG:O	1:C:122:GLY:C	2.58	0.42
2:D:23:G:H5'	2:D:23:G:C8	2.52	0.42
2:D:23:G:C5	2:D:24:G:N7	2.88	0.42
1:E:72:ASP:HB3	1:E:75:ARG:HE	1.84	0.42
1:E:82:HIS:ND1	2:F:18:G:O4'	2.53	0.42
1:E:83:LYS:CA	1:E:86:LEU:HD22	2.46	0.42
1:E:87:ARG:O	1:E:90:LEU:HG	2.19	0.42
2:F:18:G:O2'	2:F:19:A:H5'	2.19	0.42
2:F:29:G:H3'	2:F:29:G:C8	2.54	0.42
2:B:59:C:H2'	2:B:60:U:C1'	2.50	0.42
1:C:84:HIS:NE2	1:C:85:GLU:HG2	2.35	0.42
2:D:66:C:H3'	2:D:67:A:C8	2.53	0.42
1:G:106:TYR:CZ	1:G:114:LYS:C	2.93	0.42
2:H:46:G:P	2:H:46:G:H8	2.43	0.42
1:A:65:LYS:HB2	1:A:65:LYS:NZ	2.35	0.41
2:D:27:U:O2'	2:D:28:C:P	2.77	0.41
2:F:67:A:C4	2:F:68:C:C5	3.08	0.41
1:G:78:LYS:HZ1	2:H:19:A:H2'	1.84	0.41
2:H:51:G:N3	2:H:51:G:H2'	2.35	0.41
1:A:78:LYS:HG2	1:A:79:LEU:N	2.35	0.41
1:C:43:GLY:O	1:C:43:GLY:HA3	2.03	0.41
2:D:49:G:H2'	2:D:50:U:C5'	2.50	0.41
2:D:6:U:C6	2:D:6:U:H3'	2.55	0.41
1:E:21:GLU:C	2:F:18:G:H1	2.22	0.41
1:E:81:LEU:HD23	1:E:85:GLU:C	2.40	0.41
1:A:23:GLY:CA	1:A:114:LYS:HD3	2.48	0.41
1:A:41:PHE:H	1:A:41:PHE:HD2	1.68	0.41
1:C:72:ASP:O	1:C:75:ARG:HG2	2.21	0.41
1:G:116:LEU:HA	1:G:116:LEU:HD12	1.63	0.41
1:G:21:GLU:HG2	1:G:21:GLU:H	1.68	0.41
2:H:62:C:O2	2:H:62:C:C2'	2.69	0.41
2:D:62:C:O2	2:D:62:C:C2'	2.69	0.41
1:G:24:ILE:HD11	1:G:114:LYS:CA	2.43	0.41
1:G:64:GLU:CD	1:G:65:LYS:NZ	2.73	0.41
1:G:28:GLY:HA2	2:H:47:A:O2'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:HIS:NE2	2:B:17:C:O2'	2.53	0.41
1:C:27:LYS:C	1:C:29:THR:H	2.24	0.41
1:E:81:LEU:HA	2:F:18:G:N3	2.35	0.41
2:F:23:G:H5'	2:F:24:G:OP2	2.20	0.41
2:F:50:U:H3	2:F:64:A:H61	1.68	0.41
1:G:107:PHE:CD1	1:G:107:PHE:N	2.86	0.41
1:A:110:ARG:NE	2:B:15:C:N3	2.69	0.41
2:D:13:G:H21	2:D:57:G:H1'	1.85	0.41
1:E:62:PRO:CD	1:E:73:PRO:HG3	2.50	0.41
2:H:52:G:C6	2:H:63:C:C4	3.08	0.41
2:B:57:G:C2'	2:B:58:A:H5'	2.51	0.41
1:C:7:ASN:CB	1:C:10:ALA:HB2	2.50	0.41
1:E:48:PHE:HA	1:E:52:GLU:O	2.20	0.41
1:E:110:ARG:CG	2:F:15:C:C4	3.04	0.41
2:H:23:G:C5	2:H:24:G:N7	2.89	0.41
1:C:98:LEU:HD21	1:C:119:LEU:HA	2.01	0.41
1:C:55:LEU:O	1:C:76:LYS:HA	2.21	0.41
2:D:52:G:N1	2:D:63:C:C4	2.89	0.41
1:E:62:PRO:HD3	1:E:73:PRO:HG3	2.02	0.41
1:E:86:LEU:HD23	1:E:87:ARG:HG2	2.02	0.41
1:G:58:LEU:HD23	1:G:60:ILE:HG13	2.03	0.41
1:G:6:GLU:OE2	1:G:6:GLU:N	2.53	0.41
1:A:107:PHE:N	1:A:107:PHE:CD2	2.88	0.41
1:A:6:GLU:HA	1:A:104:LYS:HA	2.03	0.41
2:D:5:G:H8	2:D:5:G:O5'	2.03	0.41
1:E:72:ASP:CB	1:E:75:ARG:NE	2.83	0.41
1:E:18:GLU:HB2	1:E:88:ARG:NH2	2.36	0.41
1:G:6:GLU:CB	1:G:104:LYS:HD2	2.51	0.41
2:H:22:G:C2	2:H:34:U:C2	3.09	0.41
2:H:5:G:N2	2:H:69:C:H1'	2.36	0.41
2:B:31:C:H2'	2:B:32:U:H5'	2.03	0.41
1:C:81:LEU:C	2:D:18:G:H1'	2.41	0.41
2:F:29:G:H8	2:F:29:G:H5"	1.86	0.41
2:F:32:U:H6	2:F:32:U:O5'	2.04	0.41
1:G:115:VAL:HG13	1:G:117:LEU:CD1	2.51	0.41
2:H:6:U:C6	2:H:6:U:H3'	2.56	0.41
2:B:58:A:H2'	2:B:60:U:OP2	2.21	0.41
2:D:10:A:H2'	2:D:11:C:C5'	2.48	0.41
1:E:39:VAL:HB	1:E:59:TYR:O	2.20	0.41
1:G:117:LEU:N	1:G:117:LEU:HD12	2.35	0.41
1:E:6:GLU:HA	1:E:104:LYS:HG3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:110:ARG:CB	2:F:15:C:N4	2.84	0.40
1:E:63:TYR:C	1:E:64:GLU:HG2	2.42	0.40
1:E:60:ILE:CD1	1:E:77:ARG:NH2	2.84	0.40
2:F:47:A:N3	2:F:47:A:C2'	2.83	0.40
2:H:14:U:H2'	2:H:15:C:H5'	2.03	0.40
2:H:52:G:N1	2:H:63:C:C4	2.89	0.40
1:A:30:GLU:C	1:A:34:LEU:HD12	2.40	0.40
1:C:27:LYS:HD3	1:C:30:GLU:OE1	2.20	0.40
2:D:10:A:C3'	2:D:11:C:H5"	2.51	0.40
2:D:22:G:C2	2:D:34:U:C2	3.09	0.40
1:G:24:ILE:N	1:G:114:LYS:NZ	2.45	0.40
1:C:2:ALA:N	2:B:9:A:C8	2.88	0.40
2:D:60:U:C6	2:D:60:U:C3'	3.04	0.40
1:E:107:PHE:HA	1:E:112:TYR:O	2.21	0.40
2:F:35:G:C2'	2:F:46:G:H5'	2.51	0.40
1:G:122:GLY:O	1:G:123:LYS:HB3	2.22	0.40
1:G:83:LYS:O	1:G:87:ARG:CB	2.69	0.40
1:A:58:LEU:HD12	1:A:58:LEU:HA	1.78	0.40
1:A:93:VAL:C	1:A:95:GLN:H	2.23	0.40
1:C:13:ASP:C	1:C:14:TYR:HD2	2.25	0.40
1:E:24:ILE:CB	1:E:26:LEU:HD21	2.52	0.40
1:E:32:LYS:HD3	1:E:63:TYR:HE1	1.85	0.40
1:E:70:ASN:C	1:E:71:VAL:HG23	2.41	0.40
1:G:21:GLU:HG3	2:H:18:G:H1	1.86	0.40
1:G:82:HIS:CD2	1:G:85:GLU:OE1	2.75	0.40
1:A:63:TYR:HB2	1:A:70:ASN:HD21	1.85	0.40
2:B:58:A:O2'	2:B:60:U:C5	2.73	0.40
2:B:67:A:C4	2:B:68:C:C5	3.10	0.40
1:C:108:ASN:OD1	1:C:112:TYR:O	2.39	0.40
1:C:80:LEU:HD12	1:C:80:LEU:N	2.37	0.40
1:E:24:ILE:HG13	1:E:26:LEU:HD11	2.04	0.40
1:E:62:PRO:O	1:E:70:ASN:CG	2.60	0.40
2:F:29:G:C8	2:F:29:G:C3'	3.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	120/123 (98%)	89 (74%)	22 (18%)	9 (8%)	1 5
1	C	114/123 (93%)	91 (80%)	17 (15%)	6 (5%)	2 13
1	E	120/123 (98%)	84 (70%)	24 (20%)	12 (10%)	1 2
1	G	118/123 (96%)	94 (80%)	16 (14%)	8 (7%)	1 7
All	All	472/492 (96%)	358 (76%)	79 (17%)	35 (7%)	1 6

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	PRO
1	A	4	VAL
1	A	94	GLU
1	C	108	ASN
1	E	3	PRO
1	E	65	LYS
1	G	108	ASN
1	G	121	ARG
1	A	37	GLY
1	A	122	GLY
1	C	122	GLY
1	E	37	GLY
1	E	62	PRO
1	E	63	TYR
1	E	97	GLY
1	G	28	GLY
1	G	31	VAL
1	C	28	GLY
1	C	31	VAL
1	C	104	LYS
1	E	89	LEU
1	E	96	LYS

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Mol	Chain	Res	Type
1	G	104	LYS
1	A	89	LEU
1	G	70	ASN
1	A	62	PRO
1	A	121	ARG
1	E	69	ALA
1	G	82	HIS
1	C	3	PRO
1	E	72	ASP
1	E	88	ARG
1	A	61	ALA
1	G	62	PRO
1	E	4	VAL

5.3.2 Protein sidechains (i)

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
1	A	101/102 (99%)	81 (80%)	20 (20%)	1 7
1	C	98/102 (96%)	72 (74%)	26 (26%)	0 3
1	E	101/102 (99%)	76 (75%)	25 (25%)	1 3
1	G	100/102 (98%)	67 (67%)	33 (33%)	0 1
All	All	400/408 (98%)	296 (74%)	104 (26%)	0 3

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	PRO
1	A	8	ARG
1	A	9	ARG
1	A	12	HIS
1	A	14	TYR
1	A	24	ILE
1	A	34	LEU
1	A	41	PHE

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Mol	Chain	Res	Type
1	A	45	PHE
1	A	62	PRO
1	A	63	TYR
1	A	64	GLU
1	A	71	VAL
1	A	73	PRO
1	A	81	LEU
1	A	83	LYS
1	A	84	HIS
1	A	88	ARG
1	A	89	LEU
1	A	95	GLN
1	C	3	PRO
1	C	7	ASN
1	C	8	ARG
1	C	9	ARG
1	C	11	ARG
1	C	13	ASP
1	C	21	GLU
1	C	24	ILE
1	C	30	GLU
1	C	40	ASP
1	C	54	TYR
1	C	63	TYR
1	C	68	TYR
1	C	72	ASP
1	C	74	ARG
1	C	75	ARG
1	C	77	ARG
1	C	86	LEU
1	C	89	LEU
1	C	90	LEU
1	C	96	LYS
1	C	99	THR
1	C	100	LEU
1	C	105	ILE
1	C	110	ARG
1	C	117	LEU
1	E	5	LEU
1	E	9	ARG
1	E	12	HIS
1	E	14	TYR

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Mol	Chain	Res	Type
1	E	16	ILE
1	E	19	THR
1	E	24	ILE
1	E	32	LYS
1	E	42	THR
1	E	45	PHE
1	E	48	PHE
1	E	50	ASP
1	E	58	LEU
1	E	62	PRO
1	E	63	TYR
1	E	73	PRO
1	E	81	LEU
1	E	82	HIS
1	E	83	LYS
1	E	86	LEU
1	E	88	ARG
1	E	89	LEU
1	E	100	LEU
1	E	104	LYS
1	E	106	TYR
1	G	6	GLU
1	G	8	ARG
1	G	13	ASP
1	G	16	ILE
1	G	24	ILE
1	G	32	LYS
1	G	40	ASP
1	G	41	PHE
1	G	45	PHE
1	G	48	PHE
1	G	55	LEU
1	G	56	GLU
1	G	59	TYR
1	G	63	TYR
1	G	64	GLU
1	G	68	TYR
1	G	70	ASN
1	G	73	PRO
1	G	74	ARG
1	G	81	LEU
1	G	83	LYS

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Mol	Chain	Res	Type
1	G	86	LEU
1	G	87	ARG
1	G	88	ARG
1	G	89	LEU
1	G	95	GLN
1	G	99	THR
1	G	100	LEU
1	G	101	VAL
1	G	103	LEU
1	G	104	LYS
1	G	107	PHE
1	G	116	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	70	ASN
1	C	70	ASN
1	C	82	HIS
1	E	70	ASN
1	E	108	ASN
1	G	12	HIS
1	G	70	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	61/63 (96%)	21 (34%)	0
2	D	61/63 (96%)	23 (37%)	0
2	F	61/63 (96%)	21 (34%)	0
2	H	61/63 (96%)	20 (32%)	0
All	All	244/252 (96%)	85 (34%)	0

All (85) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	7	G
2	B	8	A
2	B	9	A

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Mol	Chain	Res	Type
2	B	11	C
2	B	12	G
2	B	13	G
2	B	14	U
2	B	15	C
2	B	16	U
2	B	17	C
2	B	19	A
2	B	27	U
2	B	28	C
2	B	29	G
2	B	47	A
2	B	48	C
2	B	53	G
2	B	60	U
2	B	61	C
2	B	64	A
2	B	72	C
2	D	8	A
2	D	9	A
2	D	11	C
2	D	12	G
2	D	14	U
2	D	15	C
2	D	16	U
2	D	17	C
2	D	19	A
2	D	23	G
2	D	27	U
2	D	28	C
2	D	29	G
2	D	30	C
2	D	46	G
2	D	47	A
2	D	48	C
2	D	49	G
2	D	52	G
2	D	59	C
2	D	60	U
2	D	61	C
2	D	63	C
2	F	7	G

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Mol	Chain	Res	Type
2	F	8	A
2	F	9	A
2	F	11	C
2	F	12	G
2	F	13	G
2	F	14	U
2	F	15	C
2	F	16	U
2	F	17	C
2	F	19	A
2	F	27	U
2	F	28	C
2	F	29	G
2	F	47	A
2	F	48	C
2	F	53	G
2	F	60	U
2	F	61	C
2	F	64	A
2	F	72	C
2	H	8	A
2	H	9	A
2	H	11	C
2	H	12	G
2	H	14	U
2	H	16	U
2	H	17	C
2	H	19	A
2	H	23	G
2	H	27	U
2	H	28	C
2	H	29	G
2	H	30	C
2	H	46	G
2	H	47	A
2	H	48	C
2	H	52	G
2	H	59	C
2	H	60	U
2	H	63	C

There are no RNA pucker outliers to report.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	5MU	B	54	2	14,22,23	1.73	3 (21%)	16,32,35	1.84	4 (25%)
2	PSU	B	55	2	16,21,22	1.93	3 (18%)	20,30,33	6.12	7 (35%)
2	5MU	D	54	2	14,22,23	1.46	2 (14%)	16,32,35	2.04	3 (18%)
2	PSU	D	55	2	16,21,22	1.91	3 (18%)	20,30,33	6.14	5 (25%)
2	5MU	F	54	2	14,22,23	1.41	1 (7%)	16,32,35	2.06	3 (18%)
2	PSU	F	55	2	16,21,22	1.85	3 (18%)	20,30,33	6.11	7 (35%)
2	5MU	H	54	2	14,22,23	1.06	1 (7%)	16,32,35	2.07	3 (18%)
2	PSU	H	55	2	16,21,22	1.90	3 (18%)	20,30,33	6.13	5 (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
2	5MU	B	54	2	-	0/3/25/26	0/2/2/2
2	PSU	B	55	2	-	0/7/25/26	0/2/2/2
2	5MU	D	54	2	-	0/3/25/26	0/2/2/2
2	PSU	D	55	2	-	0/7/25/26	0/2/2/2
2	5MU	F	54	2	-	0/3/25/26	0/2/2/2
2	PSU	F	55	2	-	0/7/25/26	0/2/2/2
2	5MU	H	54	2	-	0/3/25/26	0/2/2/2
2	PSU	H	55	2	-	0/7/25/26	0/2/2/2

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	55	PSU	C5-C1'	-6.00	1.47	1.52
2	H	55	PSU	C5-C1'	-5.98	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	55	PSU	C5-C1'	-5.92	1.47	1.52
2	D	55	PSU	C5-C1'	-5.88	1.47	1.52
2	D	55	PSU	C6-C5	-3.07	1.34	1.38
2	H	55	PSU	C6-C5	-2.98	1.34	1.38
2	B	55	PSU	C6-C5	-2.65	1.34	1.38
2	F	55	PSU	C6-C5	-2.43	1.35	1.38
2	B	54	5MU	O3'-C3'	-2.33	1.37	1.43
2	B	54	5MU	C2-N3	2.07	1.42	1.38
2	H	55	PSU	C4-N3	2.43	1.37	1.33
2	F	55	PSU	C4-N3	2.43	1.37	1.33
2	B	55	PSU	C4-N3	2.50	1.37	1.33
2	D	55	PSU	C4-N3	2.62	1.37	1.33
2	D	54	5MU	C2-N3	2.62	1.43	1.38
2	H	54	5MU	C4-N3	3.24	1.38	1.33
2	F	54	5MU	C4-N3	3.85	1.40	1.33
2	D	54	5MU	C4-N3	4.43	1.41	1.33
2	B	54	5MU	C4-N3	4.99	1.42	1.33

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	55	PSU	N1-C2-N3	-18.47	115.11	128.40
2	B	55	PSU	N1-C2-N3	-18.35	115.20	128.40
2	F	55	PSU	N1-C2-N3	-18.16	115.34	128.40
2	H	55	PSU	N1-C2-N3	-18.05	115.42	128.40
2	H	55	PSU	C5-C4-N3	-14.49	113.54	125.43
2	D	55	PSU	C5-C4-N3	-14.00	113.95	125.43
2	F	55	PSU	C5-C4-N3	-13.83	114.09	125.43
2	B	55	PSU	C5-C4-N3	-13.60	114.27	125.43
2	D	54	5MU	C5-C4-N3	-5.00	119.72	125.24
2	H	54	5MU	C5-C4-N3	-4.83	119.92	125.24
2	F	54	5MU	C5-C4-N3	-4.35	120.44	125.24
2	B	54	5MU	C5-C6-N1	-3.93	117.90	122.15
2	B	54	5MU	C5-C4-N3	-3.62	121.25	125.24
2	F	55	PSU	C5-C1'-C2'	-3.58	109.38	115.55
2	B	55	PSU	C5-C1'-C2'	-3.44	109.62	115.55
2	H	55	PSU	C5-C1'-C2'	-3.30	109.86	115.55
2	D	55	PSU	C5-C1'-C2'	-3.25	109.95	115.55
2	D	54	5MU	C5-C6-N1	-2.88	119.03	122.15
2	B	55	PSU	O4'-C4'-C3'	-2.69	99.82	105.17
2	B	55	PSU	C4-C5-C1'	-2.61	116.09	121.15
2	F	55	PSU	C4-C5-C1'	-2.54	116.23	121.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	54	5MU	O3'-C3'-C2'	-2.19	104.83	111.83
2	F	55	PSU	O4'-C4'-C3'	-2.18	100.83	105.17
2	F	54	5MU	C5-C6-N1	-2.03	119.95	122.15
2	H	54	5MU	C5-C6-N1	-2.03	119.95	122.15
2	B	54	5MU	C4-N3-C2	2.62	117.45	115.16
2	F	55	PSU	C6-N1-C2	2.79	119.83	115.36
2	B	55	PSU	C6-N1-C2	2.80	119.85	115.36
2	H	55	PSU	C6-N1-C2	2.82	119.88	115.36
2	D	55	PSU	C6-N1-C2	2.98	120.13	115.36
2	D	54	5MU	C4-N3-C2	4.81	119.36	115.16
2	F	54	5MU	C4-N3-C2	5.38	119.87	115.16
2	H	54	5MU	C4-N3-C2	5.57	120.03	115.16
2	B	55	PSU	C4-N3-C2	13.37	126.86	115.16
2	F	55	PSU	C4-N3-C2	13.51	126.97	115.16
2	D	55	PSU	C4-N3-C2	13.59	127.05	115.16
2	H	55	PSU	C4-N3-C2	13.66	127.10	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	54	5MU	3	0
2	D	54	5MU	2	0
2	D	55	PSU	3	0
2	F	54	5MU	3	0
2	H	54	5MU	2	0
2	H	55	PSU	3	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.