Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:58 PM GMT

PDB ID	:	4JV5
Title	:	Crystal structures of pseudouridinilated stop codons with ASLs
Authors	:	Fernandez, I.S.; Ng, C.L.; Kelley, A.C.; Guowei, W.; Yu, Y.T.; Ramakrishnan, V.
Deposited on	:	2013-03-25
Resolution	:	3.16 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 (i) symbol.

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

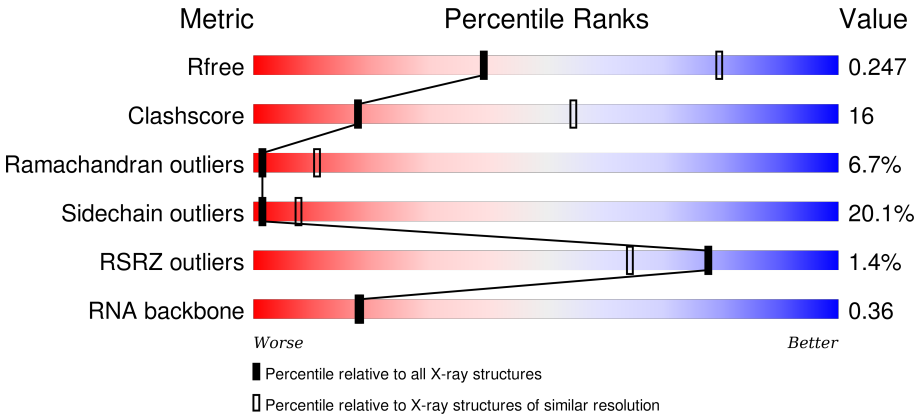
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.16 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1112 (3.20-3.12)
Clashscore	102246	1249 (3.20-3.12)
Ramachandran outliers	100387	1222 (3.20-3.12)
Sidechain outliers	100360	1221 (3.20-3.12)
RSRZ outliers	91569	1117 (3.20-3.12)
RNA backbone	2183	1046 (3.62-2.70)

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.

Mol	Chain	Length	Quality of chain
1	A	1517	43% 40% 15%
2	B	234	3% 45% 39% 14%
3	C	206	45% 43% 11%
4	D	208	2% 50% 34% 13%

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Mol	Chain	Length	Quality of chain
5	E	150	% 55% 35% 11%
6	F	101	% 56% 38% 6%
7	G	155	3% 57% 36% 6%
8	H	138	% 63% 25% 12%
9	I	127	43% 39% 18%
10	J	98	4% 36% 49% 14%
11	K	119	3% 59% 35% 6%
12	L	125	2% 49% 35% 15%
13	M	120	4% 39% 43% 17%
14	N	60	45% 32% 20%
15	O	88	68% 27% 5%
16	P	83	55% 31% 13%
17	Q	99	55% 37% 8%
18	R	70	73% 24%
19	S	78	3% 49% 37% 13%
20	T	99	56% 32% 8%
21	U	24	4% 54% 38% 8%
22	X	5	20% 60% 20%
23	Y	10	40% 40% 10% 10%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	MG	A	1607	-	-	-	X
24	MG	A	1608	-	-	-	X
24	MG	A	1610	-	-	-	X
24	MG	A	1614	-	-	-	X

2 Entry composition

There are 25 unique types of molecules in this entry. The entry contains 51923 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
			Total	C	N	O	P			
1	A	1511	32468	14453	6008	10497	1510	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	80	A	G	CONFLICT	GB 55771382

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	58	ARG	HIS	CONFLICT	UNP P80374

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	98	Total	C	N	O	S	0	0	0
			794	499	156	138	1			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	125	Total	C	N	O	S	0	0	0
			975	614	196	164	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	120	Total	C	N	O	S	0	0	0
			955	591	197	165	2			

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	R	70	Total	C	N	O	0	0	0
			574	367	112	95			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	S	78	Total	C	N	O	S	0	0	0
			629	403	114	110	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	T	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

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

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

- Molecule 22 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	X	5	Total	C	N	O	P	0	0	0
			104	48	19	33	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	Y	10	Total	C	N	O	P	0	0	0
			213	96	38	69	10			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	X	1	Total	Mg	0	0
			1	1		
24	A	15	Total	Mg	0	0
			15	15		
24	Y	1	Total	Mg	0	0
			1	1		

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

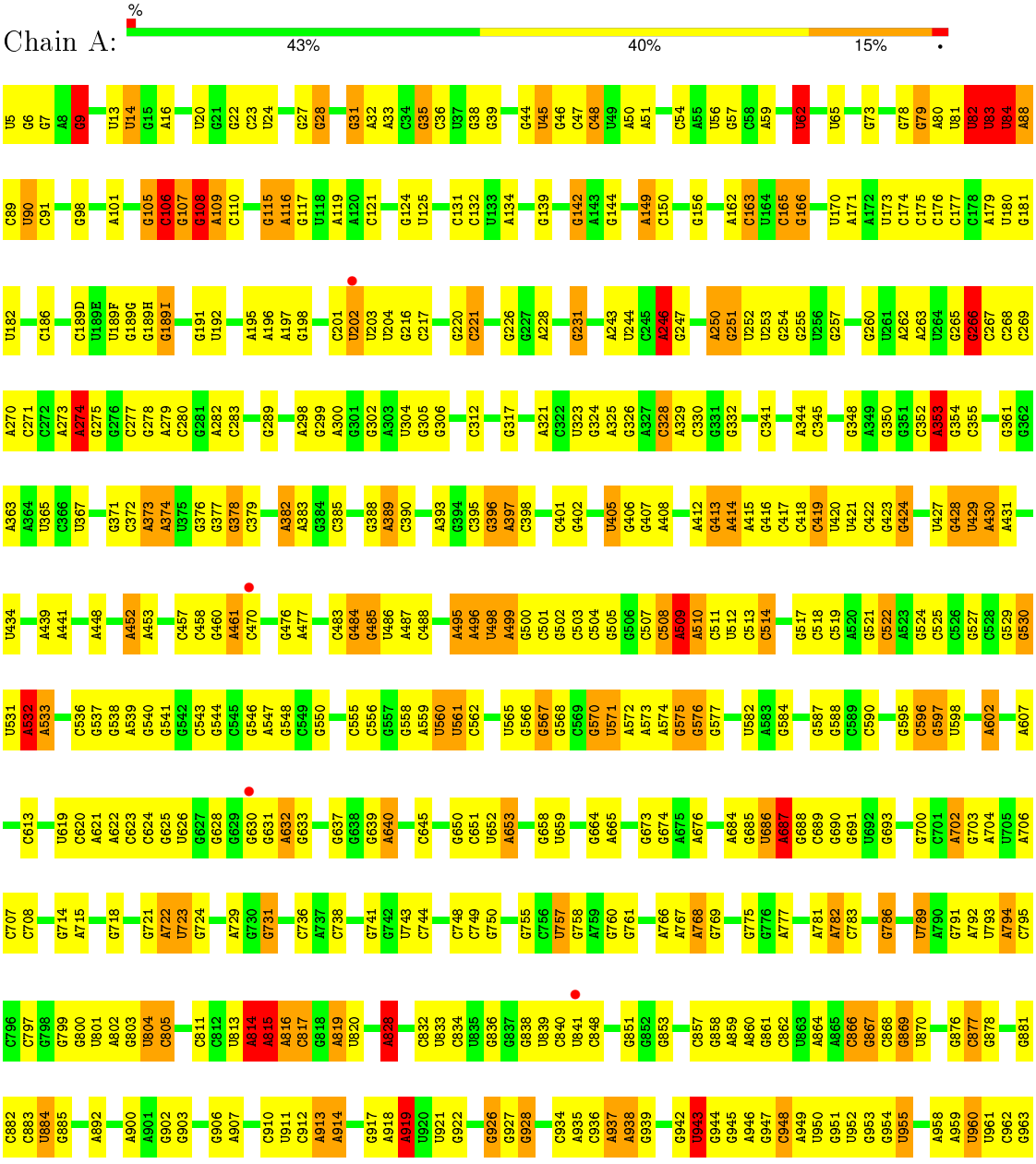
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	D	1	Total	Zn	0	0
			1	1		

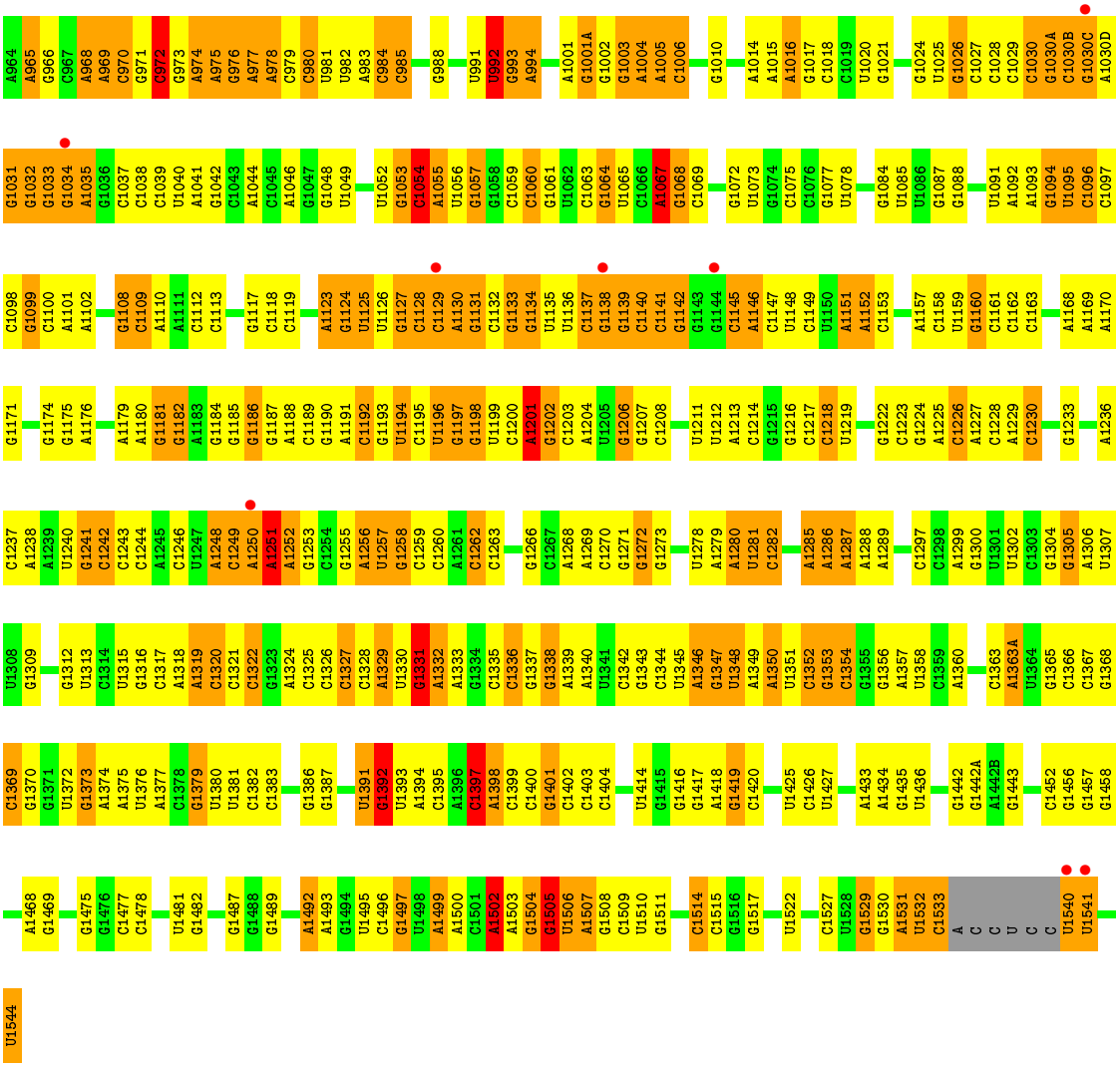
3 Residue-property plots (i)

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

- Molecule 1: 16S ribosomal RNA

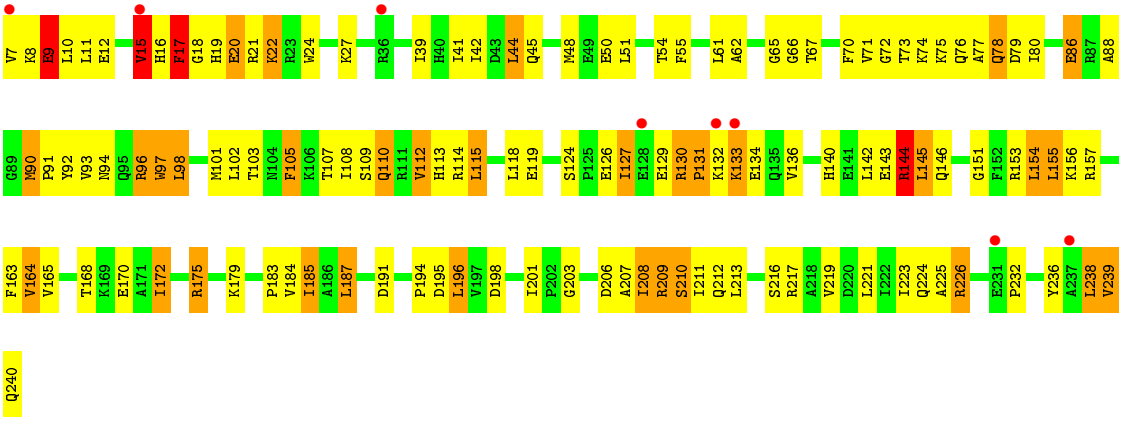
Chain A:





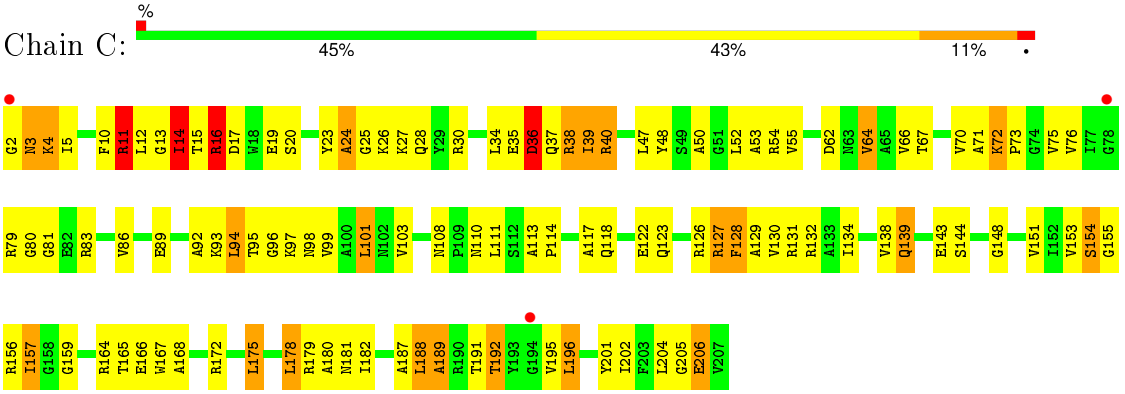
- Molecule 2: 30S ribosomal protein S2

Chain B:



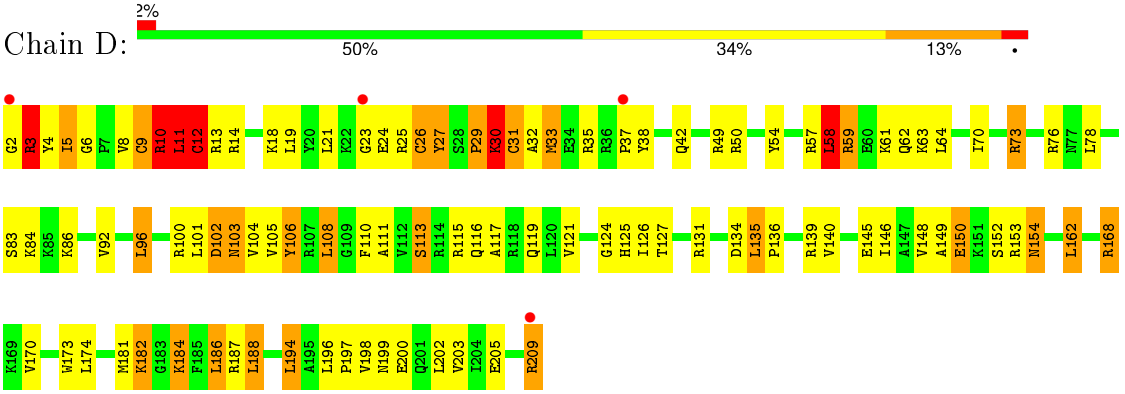
- Molecule 3: 30S ribosomal protein S3

Chain C:



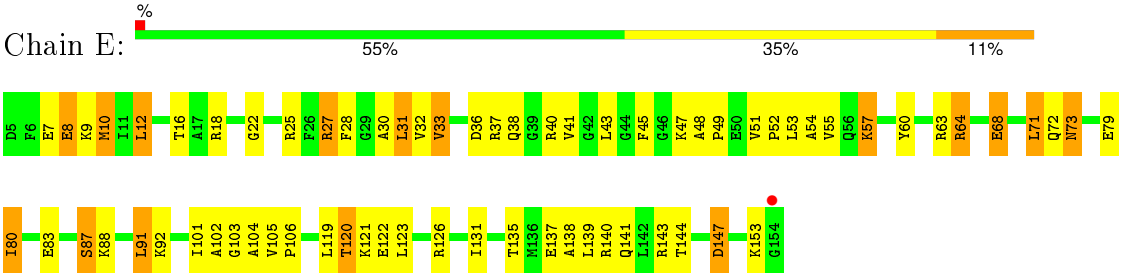
• Molecule 4: 30S ribosomal protein S4

Chain D:



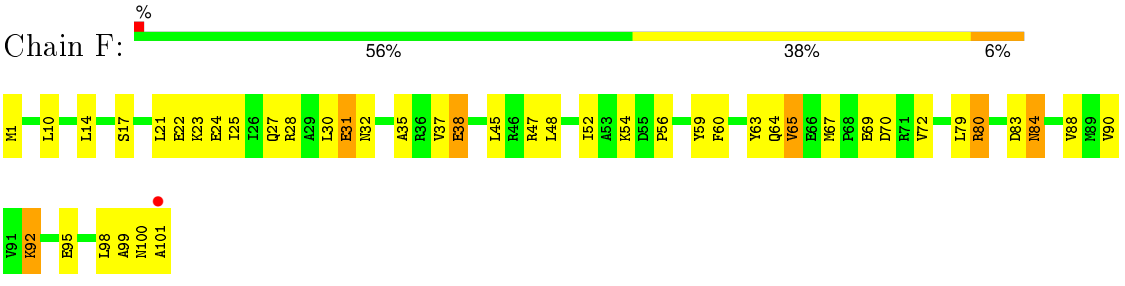
• Molecule 5: 30S ribosomal protein S5

Chain E:



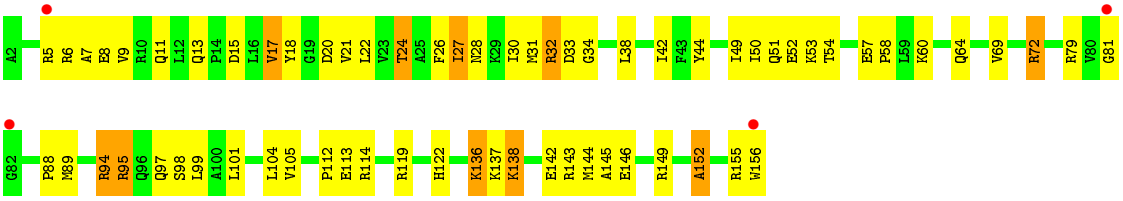
• Molecule 6: 30S ribosomal protein S6

Chain F:



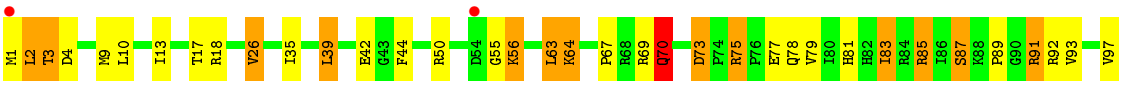
• Molecule 7: 30S ribosomal protein S7

Chain G:



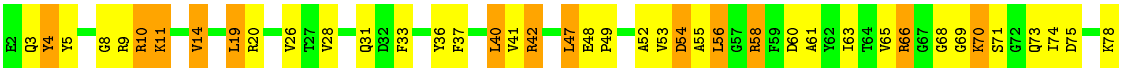
• Molecule 8: 30S ribosomal protein S8

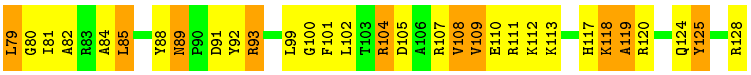
Chain H:



• Molecule 9: 30S ribosomal protein S9

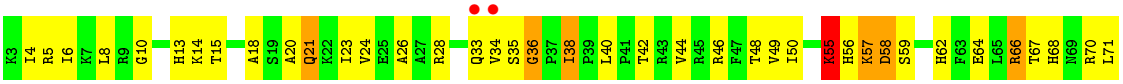
Chain I:

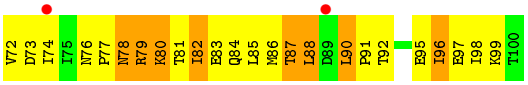




• Molecule 10: 30S ribosomal protein S10

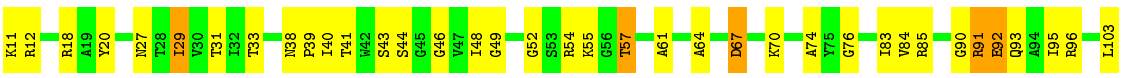
Chain J:

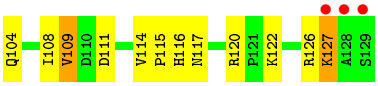




• Molecule 11: 30S ribosomal protein S11

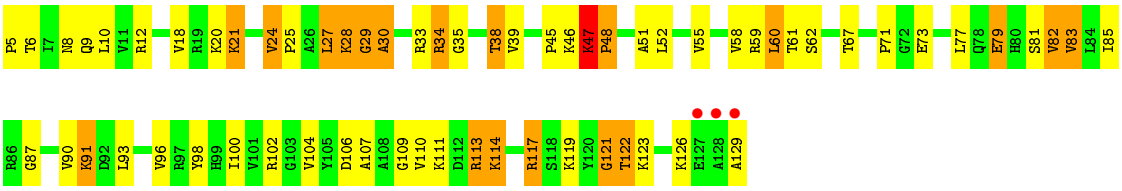
Chain K:



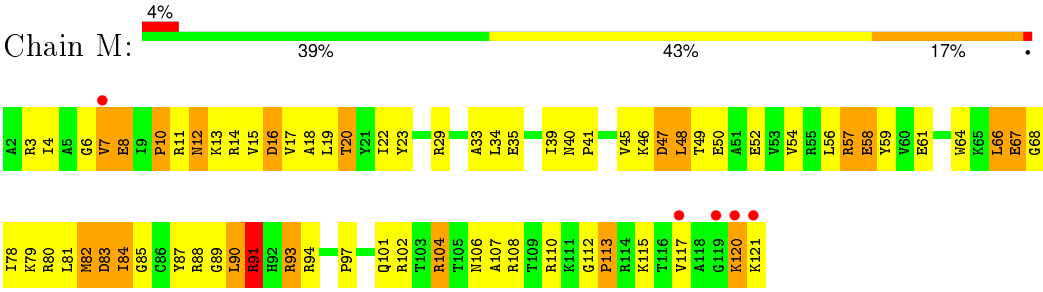


• Molecule 12: 30S ribosomal protein S12

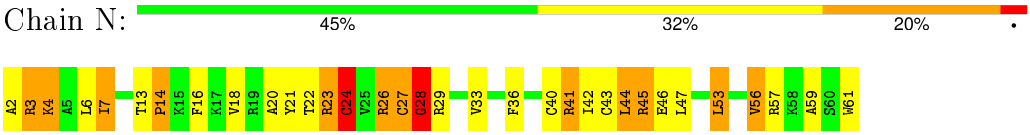
Chain L:



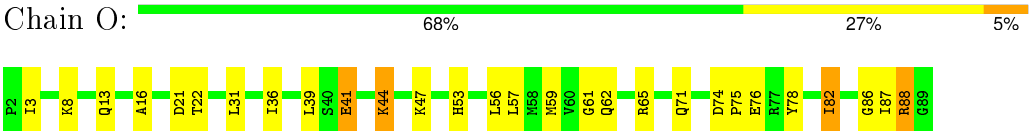
• Molecule 13: 30S ribosomal protein S13



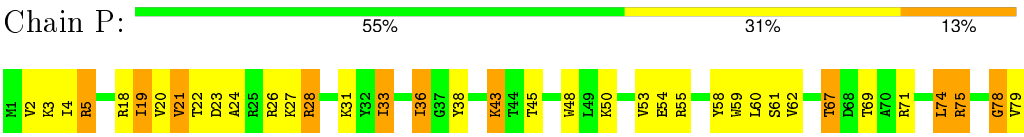
• Molecule 14: 30S ribosomal protein S14



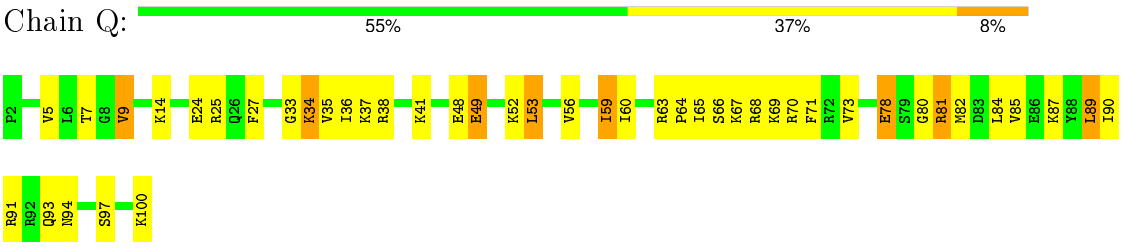
• Molecule 15: 30S ribosomal protein S15



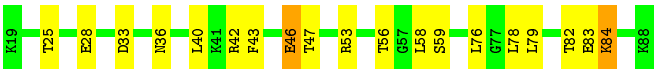
• Molecule 16: 30S ribosomal protein S16



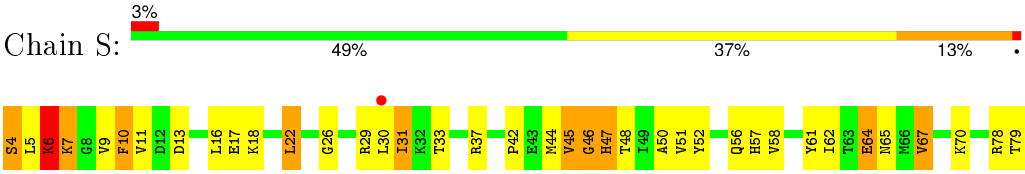
• Molecule 17: 30S ribosomal protein S17



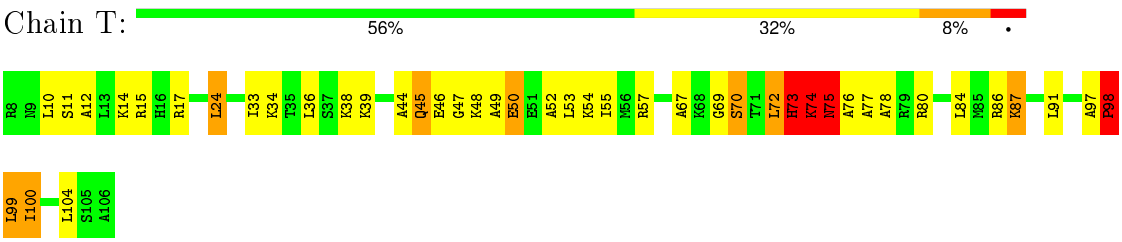
• Molecule 18: 30S ribosomal protein S18



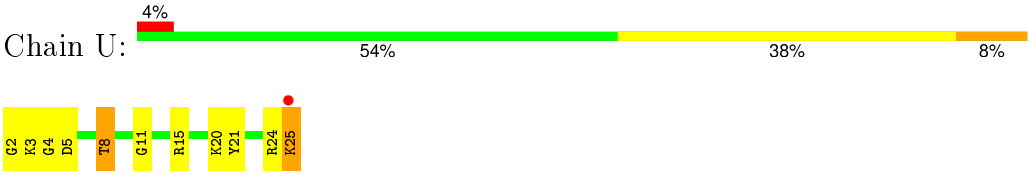
• Molecule 19: 30S ribosomal protein S19



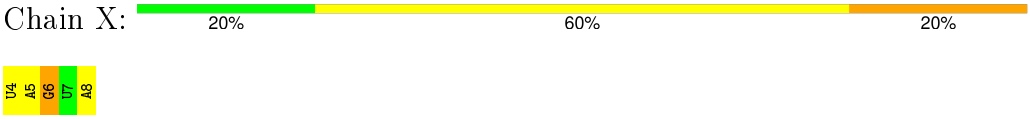
• Molecule 20: 30S ribosomal protein 20



• Molecule 21: 30S ribosomal protein THX



• Molecule 22: mRNA



• Molecule 23: ASL-tRNA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	401.00Å 401.00Å 176.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.88 – 3.16 29.88 – 3.16	Depositor EDS
% Data completeness (in resolution range)	95.4 (29.88-3.16) 95.6 (29.88-3.16)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.67 (at 3.18Å)	Xtriage
Refinement program	REFMAC 5.8.0016	Depositor
R, R_{free}	0.197 , 0.249 0.199 , 0.247	Depositor DCC
R_{free} test set	11558 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	81.3	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 68.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Outliers	0 of 231145 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	51923	wwPDB-VP
Average B, all atoms (Å^2)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.85% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, 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	0.50	7/36342 (0.0%)	0.92	105/56718 (0.2%)
2	B	0.55	0/1935	0.86	2/2609 (0.1%)
3	C	0.56	0/1636	0.86	4/2205 (0.2%)
4	D	0.60	1/1733 (0.1%)	0.96	9/2318 (0.4%)
5	E	0.67	0/1162	0.91	2/1564 (0.1%)
6	F	0.45	0/856	0.76	0/1154
7	G	0.47	0/1276	0.79	0/1709
8	H	0.65	0/1136	0.92	0/1527
9	I	0.52	0/1029	0.81	0/1378
10	J	0.55	0/807	0.79	0/1085
11	K	0.55	0/900	0.84	0/1213
12	L	0.61	0/991	0.92	0/1327
13	M	0.57	0/965	0.89	1/1292 (0.1%)
14	N	0.70	0/501	1.11	5/664 (0.8%)
15	O	0.54	0/745	0.83	0/992
16	P	0.60	0/716	0.95	2/963 (0.2%)
17	Q	0.66	0/836	0.95	1/1117 (0.1%)
18	R	0.52	0/579	0.80	0/768
19	S	0.58	0/642	0.84	0/865
20	T	0.57	0/765	0.87	0/1007
21	U	0.62	0/212	0.91	0/277
22	X	0.44	0/98	0.97	0/153
23	Y	1.01	2/237 (0.8%)	0.94	1/364 (0.3%)
All	All	0.53	10/56099 (0.0%)	0.90	132/83269 (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
2	B	0	1
3	C	0	2
4	D	0	2
9	I	0	2
11	K	0	1
14	N	0	1
20	T	0	5
All	All	0	14

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	Y	34	I	C4'-O4'	13.09	1.67	1.41
1	A	82	U	O3'-P	9.84	1.73	1.61
1	A	83	U	O3'-P	8.17	1.71	1.61
1	A	814	A	O3'-P	6.26	1.68	1.61
1	A	766	A	P-OP2	5.96	1.59	1.49
1	A	815	A	O3'-P	-5.54	1.54	1.61
1	A	1331	G	O3'-P	5.40	1.67	1.61
4	D	9	CYS	CB-SG	5.34	1.91	1.82
23	Y	34	I	C6-O6	5.23	1.33	1.23
1	A	6	G	O3'-P	-5.20	1.54	1.61

All (132) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	574	A	O5'-P-OP1	-15.93	91.36	105.70
1	A	1198	G	O5'-P-OP2	11.08	124.00	110.70
1	A	266	G	C2'-C3'-O3'	10.13	131.79	109.50
1	A	574	A	O5'-P-OP2	9.70	122.34	110.70
1	A	1078	U	O5'-P-OP1	-9.63	97.03	105.70
1	A	789	U	O5'-P-OP2	-9.30	97.33	105.70
3	C	11	ARG	NE-CZ-NH1	9.26	124.93	120.30
1	A	1078	U	O5'-P-OP2	9.09	121.61	110.70
1	A	970	C	O5'-P-OP2	8.62	121.05	110.70
1	A	1198	G	O5'-P-OP1	-8.50	98.05	105.70
1	A	783	C	O5'-P-OP2	-8.18	98.34	105.70
1	A	115	G	C2'-C3'-O3'	8.15	127.43	109.50
1	A	1505	G	O5'-P-OP2	8.03	120.34	110.70
1	A	913	A	C2'-C3'-O3'	8.03	127.17	109.50
1	A	1054	C	O5'-P-OP1	-7.95	98.54	105.70
1	A	1054	C	O5'-P-OP2	7.95	120.24	110.70
1	A	105	G	O5'-P-OP2	-7.80	98.68	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	106	C	C2'-C3'-O3'	7.79	126.64	109.50
1	A	576	G	O5'-P-OP2	-7.76	98.72	105.70
1	A	509	A	O5'-P-OP1	-7.67	98.79	105.70
1	A	508	C	P-O3'-C3'	7.65	128.88	119.70
1	A	6	G	C4'-C3'-O3'	-7.50	93.66	109.40
4	D	31	CYS	N-CA-C	-7.38	91.08	111.00
1	A	62	U	O5'-P-OP2	-7.35	99.08	105.70
1	A	231	G	O5'-P-OP2	-7.35	99.09	105.70
1	A	731	G	O5'-P-OP2	-7.30	99.13	105.70
4	D	9	CYS	CA-CB-SG	7.29	127.13	114.00
1	A	970	C	O5'-P-OP1	-7.19	99.23	105.70
1	A	509	A	C2'-C3'-O3'	7.18	125.31	109.50
1	A	1067	A	C2'-C3'-O3'	7.16	125.25	109.50
14	N	45	ARG	NE-CZ-NH1	7.14	123.87	120.30
1	A	1502	A	O5'-P-OP2	-7.08	99.33	105.70
1	A	702	A	C1'-O4'-C4'	-7.04	104.27	109.90
1	A	508	C	C4'-C3'-O3'	7.02	127.04	113.00
4	D	12	CYS	CA-CB-SG	6.95	126.50	114.00
1	A	405	U	C2'-C3'-O3'	6.91	124.76	113.70
1	A	567	G	O5'-P-OP1	-6.90	99.49	105.70
1	A	814	A	C2'-C3'-O3'	6.86	124.67	113.70
1	A	884	U	O5'-P-OP2	-6.82	99.56	105.70
17	Q	9	VAL	CB-CA-C	-6.76	98.55	111.40
1	A	389	A	O5'-P-OP1	-6.73	99.64	105.70
4	D	9	CYS	CB-CA-C	6.58	123.55	110.40
4	D	9	CYS	N-CA-C	-6.55	93.31	111.00
14	N	45	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	A	828	A	O5'-P-OP2	-6.53	99.83	105.70
1	A	862	C	O5'-P-OP1	-6.49	99.86	105.70
1	A	484	G	C2'-C3'-O3'	6.40	123.94	113.70
1	A	5	U	C5'-C4'-O4'	6.35	116.72	109.10
13	M	48	LEU	CA-CB-CG	6.28	129.75	115.30
1	A	757	U	O5'-P-OP2	-6.27	100.06	105.70
1	A	246	A	C2'-C3'-O3'	-6.22	95.81	109.50
1	A	943	U	O5'-P-OP2	6.20	118.14	110.70
4	D	26	CYS	CA-CB-SG	6.18	125.12	114.00
1	A	274	A	C4'-C3'-O3'	6.15	125.30	113.00
1	A	1077	G	O5'-P-OP2	-6.13	100.19	105.70
1	A	596	C	O5'-P-OP2	6.11	118.03	110.70
1	A	943	U	O5'-P-OP1	-6.08	100.23	105.70
4	D	31	CYS	CA-CB-SG	6.04	124.88	114.00
1	A	1489	G	O5'-P-OP1	5.99	117.88	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	105	G	O5'-P-OP1	5.94	117.82	110.70
1	A	1084	G	O5'-P-OP2	-5.93	100.36	105.70
1	A	84	U	N1-C1'-C2'	5.92	121.70	114.00
1	A	228	A	O5'-P-OP2	5.92	117.80	110.70
1	A	1251	A	O5'-P-OP2	5.92	117.80	110.70
1	A	82	U	N1-C1'-C2'	5.90	121.67	114.00
16	P	71	ARG	NE-CZ-NH1	5.87	123.24	120.30
1	A	757	U	O5'-P-OP1	5.84	117.70	110.70
1	A	266	G	P-O3'-C3'	5.83	126.70	119.70
14	N	24	CYS	CA-CB-SG	5.83	124.48	114.00
4	D	194	LEU	CA-CB-CG	5.82	128.68	115.30
1	A	928	G	O5'-P-OP1	-5.79	100.49	105.70
1	A	1260	C	O5'-P-OP1	-5.78	100.50	105.70
1	A	1506	U	O5'-P-OP1	5.77	117.62	110.70
1	A	9	G	O5'-P-OP2	-5.74	100.53	105.70
1	A	548	G	O5'-P-OP1	-5.73	100.55	105.70
1	A	108	G	C5'-C4'-O4'	5.71	115.95	109.10
2	B	144	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	A	1392	G	O5'-P-OP2	-5.69	100.58	105.70
1	A	16	A	O5'-P-OP2	5.68	117.51	110.70
1	A	175	C	O5'-P-OP1	-5.66	100.61	105.70
14	N	27	CYS	CA-CB-SG	-5.64	103.84	114.00
1	A	1505	G	C1'-C2'-O2'	-5.63	93.72	110.60
1	A	231	G	O5'-P-OP1	5.58	117.40	110.70
1	A	921	U	O5'-P-OP1	5.58	117.39	110.70
5	E	12	LEU	CA-CB-CG	5.57	128.12	115.30
1	A	919	A	O5'-P-OP2	-5.57	100.69	105.70
1	A	108	G	O4'-C4'-C3'	-5.54	98.46	104.00
1	A	532	A	C2'-C3'-O3'	5.54	122.56	113.70
1	A	228	A	O5'-P-OP1	-5.51	100.74	105.70
1	A	590	C	O5'-P-OP1	5.50	117.31	110.70
1	A	686	U	O5'-P-OP2	-5.45	100.80	105.70
5	E	27	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	A	522	C	O5'-P-OP2	-5.44	100.80	105.70
1	A	1077	G	O5'-P-OP1	5.41	117.19	110.70
1	A	452	A	O5'-P-OP1	-5.41	100.83	105.70
1	A	1504	G	O5'-P-OP1	-5.40	100.84	105.70
1	A	702	A	N9-C1'-C2'	5.40	121.02	114.00
3	C	11	ARG	NE-CZ-NH2	-5.39	117.61	120.30
1	A	992	U	C2'-C3'-O3'	5.38	122.31	113.70
1	A	1397	C	C4'-C3'-O3'	-5.36	98.15	109.40
14	N	28	GLY	N-CA-C	5.36	126.49	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	353	A	O5'-P-OP2	-5.34	100.89	105.70
1	A	115	G	O5'-P-OP2	-5.34	100.90	105.70
1	A	687	A	P-O3'-C3'	5.32	126.08	119.70
16	P	75	ARG	NE-CZ-NH1	5.30	122.95	120.30
23	Y	37	A	O5'-P-OP2	-5.30	100.93	105.70
1	A	1109	C	C2'-C3'-O3'	5.29	122.16	113.70
1	A	1251	A	O5'-P-OP1	-5.29	100.94	105.70
1	A	83	U	P-O3'-C3'	5.28	126.04	119.70
1	A	775	G	O5'-P-OP1	-5.27	100.95	105.70
1	A	948	C	O5'-P-OP1	5.27	117.03	110.70
2	B	175	ARG	NE-CZ-NH1	5.26	122.93	120.30
4	D	12	CYS	N-CA-CB	5.24	120.02	110.60
1	A	132	C	O5'-P-OP2	-5.23	100.99	105.70
1	A	1075	C	O5'-P-OP2	5.20	116.94	110.70
3	C	16	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	A	277	C	N1-C1'-C2'	-5.19	106.29	112.00
1	A	202	U	C2'-C3'-O3'	5.17	121.97	113.70
1	A	558	G	O5'-P-OP2	-5.15	101.06	105.70
3	C	94	LEU	CA-CB-CG	5.15	127.15	115.30
1	A	768	A	O5'-P-OP1	5.13	116.85	110.70
1	A	972	C	O5'-P-OP2	-5.11	101.10	105.70
1	A	1151	A	C2'-C3'-O3'	5.11	121.88	113.70
1	A	379	C	O5'-P-OP2	-5.10	101.11	105.70
1	A	1506	U	O5'-P-OP2	-5.10	101.11	105.70
1	A	786	G	O5'-P-OP2	5.06	116.77	110.70
1	A	257	G	O5'-P-OP1	5.05	116.77	110.70
1	A	972	C	O5'-P-OP1	5.05	116.76	110.70
1	A	134	A	O5'-P-OP2	-5.04	101.16	105.70
1	A	950	U	O5'-P-OP2	5.01	116.71	110.70
1	A	108	G	C4'-C3'-C2'	-5.01	97.59	102.60
1	A	1201	A	C2'-C3'-O3'	5.01	121.72	113.70

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	191	ASP	Peptide
3	C	14	ILE	Peptide
3	C	25	GLY	Peptide
4	D	11	LEU	Peptide
4	D	30	LYS	Peptide
9	I	117	HIS	Peptide

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Mol	Chain	Res	Type	Group
9	I	124	GLN	Peptide
11	K	127	LYS	Peptide
14	N	28	GLY	Peptide
20	T	12	ALA	Peptide
20	T	73	HIS	Peptide
20	T	74	LYS	Peptide
20	T	75	ASN	Peptide
20	T	98	PRO	Peptide

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	32468	0	16391	666	1
2	B	1900	0	1951	85	0
3	C	1612	0	1677	98	0
4	D	1703	0	1763	75	0
5	E	1146	0	1207	52	0
6	F	843	0	857	26	0
7	G	1257	0	1296	27	0
8	H	1116	0	1177	43	0
9	I	1011	0	1043	59	0
10	J	794	0	840	43	0
11	K	885	0	904	26	0
12	L	975	0	1062	42	0
13	M	955	0	1021	44	0
14	N	492	0	529	44	0
15	O	734	0	771	21	0
16	P	700	0	720	21	0
17	Q	823	0	891	35	0
18	R	574	0	644	11	0
19	S	629	0	652	25	0
20	T	763	0	861	30	0
21	U	208	0	221	7	0
22	X	104	0	54	8	0
23	Y	213	0	107	19	0
24	A	15	0	0	0	0
24	X	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	Y	1	0	0	0	0
25	D	1	0	0	0	0
All	All	51923	0	36639	1390	1

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 16.

All (1390) 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)
23:Y:34:I:O4'	23:Y:34:I:C4'	1.67	1.36
23:Y:34:I:C5'	23:Y:34:I:H8	1.53	1.20
4:D:31:CYS:O	4:D:33:MET:N	1.77	1.17
23:Y:34:I:C8	23:Y:34:I:H5'	1.82	1.15
3:C:154:SER:OG	3:C:155:GLY:N	1.74	1.12
12:L:47:LYS:HB3	12:L:48:PRO:HD3	1.33	1.11
1:A:1250:A:H1'	1:A:1251:A:N7	1.69	1.07
23:Y:34:I:C8	23:Y:34:I:C5'	2.39	1.02
1:A:1249:C:H42	1:A:1288:A:N6	1.56	1.01
1:A:1305:G:N2	1:A:1331:G:H2'	1.75	1.00
1:A:328:C:O2	1:A:328:C:H2'	1.59	0.99
12:L:90:VAL:O	12:L:91:LYS:HB3	1.59	0.99
12:L:28:LYS:O	12:L:30:ALA:N	1.97	0.98
1:A:1305:G:H22	1:A:1331:G:H2'	1.29	0.98
1:A:1248:A:H4'	1:A:1249:C:OP1	1.65	0.97
12:L:47:LYS:CB	12:L:48:PRO:HD3	1.95	0.96
12:L:47:LYS:HB3	12:L:48:PRO:CD	1.95	0.96
13:M:17:VAL:O	13:M:20:THR:HB	1.65	0.95
14:N:27:CYS:SG	14:N:27:CYS:O	2.24	0.95
1:A:1502:A:H2	1:A:1505:G:H1	1.15	0.95
1:A:1249:C:N4	1:A:1288:A:N6	2.14	0.94
14:N:24:CYS:HB2	14:N:40:CYS:H	1.30	0.94
1:A:1125:U:H5"	1:A:1125:U:C6	2.01	0.94
23:Y:34:I:H8	23:Y:34:I:H5'	1.17	0.93
1:A:1052:U:O2'	1:A:1055:A:OP2	1.85	0.93
17:Q:66:SER:O	17:Q:70:ARG:NH1	2.01	0.93
4:D:31:CYS:C	4:D:33:MET:H	1.68	0.93
1:A:1544:U:O3'	22:X:4:PSU:O5'	1.87	0.92
16:P:74:LEU:O	16:P:79:VAL:HG23	1.69	0.91
18:R:56:THR:HB	18:R:58:LEU:HD13	1.51	0.91
5:E:53:LEU:O	5:E:57:LYS:HB2	1.71	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1249:C:H42	1:A:1288:A:H62	1.21	0.89
1:A:1226:C:N4	13:M:104:ARG:HG3	1.87	0.88
13:M:90:LEU:O	13:M:91:ARG:HB2	1.72	0.88
1:A:84:U:H1'	1:A:88:A:OP2	1.75	0.87
14:N:36:PHE:O	14:N:36:PHE:CD1	2.27	0.87
1:A:1353:G:H2'	1:A:1354:C:H5'	1.57	0.86
3:C:30:ARG:NH1	3:C:30:ARG:HB2	1.90	0.85
17:Q:67:LYS:O	17:Q:68:ARG:HG2	1.77	0.84
9:I:70:LYS:O	9:I:74:ILE:HG13	1.78	0.83
1:A:1356:G:H2'	1:A:1357:A:C8	2.14	0.82
12:L:90:VAL:O	12:L:91:LYS:CB	2.28	0.82
1:A:867:G:O2'	1:A:868:C:H5'	1.77	0.82
13:M:3:ARG:HA	13:M:8:GLU:O	1.80	0.82
3:C:30:ARG:HH11	3:C:30:ARG:HB2	1.44	0.82
1:A:1240:U:H3'	1:A:1241:G:H5'	1.62	0.81
1:A:664:G:H22	1:A:741:G:H1	1.28	0.81
1:A:1540:U:H4'	1:A:1541:U:OP2	1.78	0.81
1:A:1366:C:H2'	1:A:1367:C:C6	2.15	0.81
4:D:2:GLY:O	4:D:3:ARG:O	1.97	0.81
1:A:1128:C:O2'	1:A:1130:A:N7	2.14	0.80
1:A:910:C:OP2	12:L:21:LYS:NZ	2.13	0.80
1:A:1499:A:O2'	1:A:1500:A:H5'	1.81	0.80
1:A:1038:C:H2'	1:A:1039:C:O2	1.82	0.80
1:A:1249:C:N4	1:A:1288:A:H61	1.77	0.80
1:A:1391:U:H2'	1:A:1392:G:C8	2.17	0.80
2:B:88:ALA:HB2	2:B:219:VAL:HG13	1.63	0.80
1:A:1353:G:C2'	1:A:1354:C:H5'	2.11	0.80
1:A:953:G:H5'	1:A:965:A:H61	1.46	0.79
14:N:27:CYS:HB3	14:N:43:CYS:HB3	1.62	0.79
1:A:78:G:H1	1:A:91:C:H5	1.31	0.79
4:D:30:LYS:HB3	4:D:35:ARG:HD2	1.64	0.79
11:K:40:ILE:HG22	11:K:41:THR:HG23	1.64	0.79
3:C:148:GLY:HA3	3:C:172:ARG:O	1.82	0.79
13:M:90:LEU:HA	13:M:93:ARG:HB2	1.65	0.78
3:C:134:ILE:HD11	3:C:153:VAL:HG23	1.65	0.78
1:A:1030(B):C:H2'	1:A:1030(C):G:H5'	1.66	0.78
7:G:32:ARG:O	7:G:34:GLY:N	2.15	0.78
17:Q:81:ARG:HB3	17:Q:84:LEU:HD12	1.66	0.78
1:A:1091:U:O2	1:A:1093:A:C8	2.37	0.77
23:Y:34:I:C8	23:Y:34:I:C4'	2.68	0.76
12:L:27:LEU:O	12:L:29:GLY:N	2.18	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:68:GLU:HG3	5:E:68:GLU:O	1.84	0.76
14:N:29:ARG:HD3	14:N:40:CYS:HB2	1.68	0.76
1:A:866:C:H2'	1:A:867:G:O5'	1.85	0.76
3:C:55:VAL:HG12	3:C:55:VAL:O	1.85	0.76
1:A:1249:C:C5	9:I:69:GLY:HA2	2.21	0.76
1:A:723:U:O2	1:A:723:U:H2'	1.85	0.76
1:A:685:G:OP1	11:K:11:LYS:NZ	2.17	0.76
3:C:70:VAL:HG12	3:C:72:LYS:H	1.52	0.75
1:A:1328:C:OP1	21:U:21:TYR:OH	2.03	0.75
6:F:48:LEU:HD13	6:F:52:ILE:HD12	1.68	0.75
13:M:87:TYR:O	13:M:90:LEU:O	2.05	0.75
2:B:187:LEU:HD23	2:B:201:ILE:O	1.86	0.75
1:A:804:U:H5"	1:A:805:C:OP2	1.87	0.74
1:A:1279:A:H5"	1:A:1280:A:OP1	1.88	0.74
18:R:46:GLU:CD	18:R:46:GLU:H	1.90	0.74
1:A:1125:U:H5"	1:A:1125:U:H6	1.50	0.74
3:C:23:TYR:CD1	3:C:24:ALA:N	2.56	0.74
19:S:64:GLU:O	19:S:67:VAL:HG23	1.86	0.73
23:Y:31:A:H2'	23:Y:31:A:N3	2.02	0.73
7:G:145:ALA:O	7:G:146:GLU:HB2	1.86	0.73
7:G:88:PRO:HG2	7:G:152:ALA:HB2	1.71	0.73
4:D:11:LEU:C	4:D:13:ARG:H	1.91	0.73
1:A:1270:C:OP2	21:U:24:ARG:NH2	2.22	0.72
1:A:707:C:H4'	11:K:20:TYR:CD2	2.25	0.72
19:S:18:LYS:O	19:S:22:LEU:HB2	1.89	0.72
1:A:62:U:H5"	1:A:385:C:O2	1.90	0.72
1:A:625:G:H2'	1:A:626:U:C6	2.25	0.71
12:L:24:VAL:CG1	12:L:24:VAL:O	2.38	0.71
9:I:3:GLN:HE22	9:I:20:ARG:HH21	1.38	0.71
1:A:1321:C:H3'	1:A:1322:C:H5"	1.73	0.71
1:A:1190:G:O2'	3:C:3:ASN:HB3	1.91	0.71
1:A:976:G:C8	1:A:1358:U:O2	2.44	0.71
1:A:1057:G:H5"	3:C:154:SER:OG	1.91	0.70
1:A:1366:C:H2'	1:A:1367:C:H6	1.54	0.70
2:B:51:LEU:HD22	2:B:55:PHE:CE2	2.26	0.70
1:A:420:U:O2	1:A:424:G:C2	2.44	0.70
10:J:49:VAL:HG13	14:N:41:ARG:HD2	1.73	0.70
9:I:58:ARG:NH1	9:I:58:ARG:HB2	2.07	0.70
1:A:1190:G:OP1	3:C:4:LYS:HA	1.92	0.70
1:A:1392:G:H21	1:A:1502:A:H8	1.40	0.70
2:B:136:VAL:O	2:B:140:HIS:N	2.22	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:96:ARG:O	2:B:98:LEU:HD23	1.91	0.69
1:A:974:A:OP2	14:N:29:ARG:NH2	2.25	0.69
12:L:38:THR:HG22	12:L:39:VAL:HG23	1.75	0.69
1:A:9:G:OP2	5:E:121:LYS:HD2	1.92	0.69
1:A:1054:C:N4	23:Y:34:I:C8	2.60	0.69
1:A:1226:C:N4	13:M:104:ARG:CG	2.56	0.69
1:A:189(G):G:H4'	1:A:189(H):G:OP2	1.93	0.69
3:C:73:PRO:O	3:C:76:VAL:HG22	1.92	0.69
23:Y:34:I:H8	23:Y:34:I:H5"	1.52	0.69
1:A:170:U:O2'	1:A:171:A:H5'	1.93	0.69
2:B:140:HIS:HA	2:B:143:GLU:HG2	1.75	0.68
2:B:15:VAL:H	2:B:16:HIS:CE1	2.10	0.68
2:B:19:HIS:CE1	2:B:206:ASP:HB2	2.29	0.68
4:D:11:LEU:C	4:D:13:ARG:N	2.47	0.68
3:C:14:ILE:HG22	3:C:15:THR:N	2.08	0.68
1:A:544:G:OP1	4:D:59:ARG:NH2	2.26	0.68
8:H:89:PRO:HA	8:H:92:ARG:NH1	2.09	0.68
8:H:10:LEU:HD22	8:H:83:ILE:HD11	1.75	0.68
1:A:299:G:H2'	1:A:300:A:C8	2.28	0.67
1:A:269:C:H2'	1:A:270:A:C8	2.29	0.67
20:T:45:GLN:HG2	20:T:91:LEU:HD22	1.75	0.67
1:A:1249:C:H2'	1:A:1250:A:OP1	1.93	0.67
2:B:16:HIS:CD2	2:B:209:ARG:HB2	2.30	0.67
5:E:45:PHE:CE2	5:E:47:LYS:HE2	2.29	0.67
4:D:25:ARG:C	4:D:27:TYR:H	1.97	0.67
1:A:979:C:H3'	1:A:980:C:H5"	1.77	0.67
1:A:1250:A:OP1	1:A:1250:A:O4'	2.12	0.67
1:A:866:C:C2'	1:A:867:G:O5'	2.40	0.67
12:L:47:LYS:CG	12:L:48:PRO:HD3	2.25	0.67
14:N:44:LEU:C	14:N:44:LEU:HD23	2.16	0.66
1:A:1262:C:H2'	1:A:1263:C:C6	2.30	0.66
1:A:1418:A:N6	1:A:1482:G:O2'	2.29	0.66
1:A:82:U:H6	1:A:82:U:OP2	1.78	0.66
15:O:16:ALA:HB1	15:O:21:ASP:HB3	1.78	0.66
7:G:51:GLN:OE1	7:G:51:GLN:HA	1.96	0.66
1:A:1532:U:O2	1:A:1532:U:H2'	1.96	0.66
9:I:5:TYR:O	9:I:84:ALA:HA	1.96	0.66
1:A:1502:A:H2	1:A:1505:G:N1	1.90	0.65
13:M:14:ARG:HB3	13:M:16:ASP:OD1	1.95	0.65
17:Q:68:ARG:H	17:Q:70:ARG:NH1	1.94	0.65
4:D:33:MET:HE2	4:D:37:PRO:HA	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:984:C:H2'	1:A:985:C:H6	1.61	0.65
12:L:47:LYS:CB	12:L:48:PRO:CD	2.67	0.65
1:A:1124:G:C2	1:A:1127:G:N2	2.65	0.65
11:K:46:GLY:O	11:K:48:ILE:O	2.15	0.65
1:A:1190:G:O2'	3:C:3:ASN:CB	2.44	0.65
2:B:110:GLN:HA	2:B:113:HIS:HB2	1.77	0.65
21:U:5:ASP:O	21:U:11:GLY:HA3	1.96	0.65
1:A:1031:G:N3	1:A:1032:G:N1	2.44	0.65
1:A:1544:U:O3'	22:X:4:PSU:C5'	2.44	0.65
6:F:37:VAL:HG12	6:F:38:GLU:O	1.97	0.65
6:F:10:LEU:HB2	6:F:59:TYR:HB3	1.79	0.65
20:T:73:HIS:C	20:T:74:LYS:HG3	2.16	0.65
1:A:994:A:N3	1:A:994:A:H2'	2.11	0.65
1:A:815:A:O2'	1:A:1527:C:H1'	1.95	0.65
1:A:559:A:P	5:E:126:ARG:HH22	2.20	0.64
2:B:61:LEU:HD23	2:B:66:GLY:HA3	1.79	0.64
1:A:1248:A:C2'	1:A:1249:C:H5'	2.27	0.64
1:A:1510:U:H2'	1:A:1511:G:C8	2.33	0.64
4:D:146:ILE:HD12	4:D:146:ILE:N	2.12	0.64
3:C:205:GLY:O	3:C:206:GLU:HB2	1.98	0.64
14:N:36:PHE:O	14:N:36:PHE:HD1	1.81	0.64
1:A:186:C:H5'	20:T:78:ALA:HB1	1.79	0.64
1:A:814:A:H2'	1:A:816:A:H5"	1.79	0.64
1:A:1368:G:O2'	1:A:1369:C:H5'	1.99	0.64
4:D:18:LYS:HD3	4:D:31:CYS:HB2	1.78	0.63
1:A:1368:G:C2'	1:A:1369:C:H5'	2.28	0.63
1:A:625:G:H2'	1:A:626:U:H6	1.62	0.63
1:A:1243:C:H5"	21:U:8:THR:HG22	1.81	0.63
5:E:102:ALA:HB1	5:E:106:PRO:HG2	1.79	0.63
5:E:10:MET:O	5:E:10:MET:HG3	1.96	0.63
1:A:192:U:O3'	20:T:57:ARG:HD2	1.99	0.63
8:H:112:LEU:HD12	8:H:112:LEU:C	2.18	0.63
1:A:1251:A:O2'	1:A:1252:A:C8	2.50	0.63
2:B:153:ARG:HG3	2:B:154:LEU:HD23	1.81	0.63
1:A:1343:G:H2'	1:A:1344:C:C6	2.34	0.63
12:L:24:VAL:HG12	12:L:24:VAL:O	1.97	0.62
3:C:11:ARG:HH11	3:C:11:ARG:CG	2.11	0.62
12:L:126:LYS:HA	12:L:129:ALA:O	2.00	0.62
1:A:266:G:H5"	1:A:268:C:H41	1.64	0.62
3:C:76:VAL:HG21	3:C:103:VAL:HG21	1.80	0.62
1:A:530:G:O6	22:X:6:G:H1'	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:8:VAL:O	4:D:10:ARG:N	2.33	0.62
6:F:21:LEU:O	6:F:24:GLU:HG2	2.00	0.62
1:A:706:A:C1'	11:K:29:ILE:HD11	2.29	0.62
1:A:1401:G:C2	1:A:1402:C:H1'	2.34	0.62
8:H:78:GLN:O	8:H:81:HIS:CE1	2.53	0.62
21:U:2:GLY:O	21:U:4:GLY:N	2.33	0.62
23:Y:33:U:H5'	23:Y:34:I:OP2	2.00	0.62
4:D:13:ARG:HA	4:D:33:MET:CE	2.29	0.62
1:A:1039:C:C6	1:A:1040:U:C5	2.87	0.62
1:A:791:G:C6	1:A:792:A:N7	2.68	0.62
5:E:101:ILE:HD11	5:E:119:LEU:CD2	2.30	0.62
1:A:83:U:O2'	1:A:84:U:O5'	2.15	0.62
1:A:376:G:OP2	16:P:67:THR:HG21	1.99	0.62
3:C:23:TYR:O	3:C:24:ALA:HB2	2.00	0.61
1:A:419:C:H5'	1:A:420:U:OP2	2.00	0.61
1:A:1251:A:N6	1:A:1287:A:C5	2.69	0.61
4:D:25:ARG:O	4:D:27:TYR:N	2.28	0.61
4:D:8:VAL:HG13	4:D:21:LEU:HD13	1.81	0.61
1:A:1346:A:OP1	9:I:120:ARG:NH1	2.27	0.61
1:A:1241:G:H2'	1:A:1242:C:C6	2.35	0.61
5:E:144:THR:OG1	5:E:147:ASP:OD1	2.11	0.61
1:A:1313:U:OP1	19:S:6:LYS:HG3	1.99	0.61
1:A:1348:U:O2'	1:A:1349:A:H5'	2.00	0.61
1:A:1499:A:C2'	1:A:1500:A:H5'	2.30	0.61
8:H:13:ILE:O	8:H:17:THR:HG23	2.01	0.61
1:A:401:C:O2'	1:A:402:G:H5'	2.01	0.61
4:D:30:LYS:CB	4:D:35:ARG:HD2	2.30	0.61
1:A:45:U:H2'	1:A:46:G:C8	2.35	0.61
14:N:29:ARG:HD3	14:N:40:CYS:CB	2.31	0.61
4:D:101:LEU:O	4:D:103:ASN:N	2.33	0.61
19:S:9:VAL:O	19:S:11:VAL:N	2.29	0.61
1:A:1147:C:O2'	9:I:5:TYR:OH	2.01	0.61
8:H:17:THR:HB	8:H:78:GLN:OE1	2.01	0.61
1:A:575:G:H4'	1:A:575:G:OP1	2.01	0.61
1:A:1331:G:OP1	1:A:1331:G:H4'	2.01	0.61
1:A:1069:C:O2'	1:A:1192:C:H1'	2.01	0.61
3:C:72:LYS:HG3	3:C:75:VAL:HG21	1.81	0.61
19:S:52:TYR:HA	19:S:56:GLN:O	2.00	0.61
1:A:1392:G:N2	1:A:1502:A:H8	1.98	0.61
1:A:269:C:H2'	1:A:270:A:H8	1.64	0.61
1:A:521:G:OP1	12:L:73:GLU:O	2.19	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:974:A:OP2	14:N:41:ARG:NH1	2.34	0.60
1:A:1030:C:H4'	1:A:1030(A):G:O5'	2.00	0.60
3:C:92:ALA:HB2	3:C:99:VAL:HG22	1.83	0.60
3:C:30:ARG:CB	3:C:30:ARG:NH1	2.64	0.60
1:A:1329:A:H2'	1:A:1330:U:H5'	1.83	0.60
1:A:537:G:OP1	12:L:113:ARG:NH2	2.34	0.60
20:T:69:GLY:O	20:T:73:HIS:CD2	2.54	0.60
1:A:376:G:H5"	16:P:5:ARG:HD3	1.83	0.60
3:C:14:ILE:HG22	3:C:15:THR:H	1.64	0.60
20:T:73:HIS:HB3	20:T:74:LYS:HG3	1.83	0.60
19:S:45:VAL:O	19:S:47:HIS:N	2.34	0.60
1:A:673:G:H2'	1:A:674:G:C8	2.35	0.60
1:A:189(I):G:H5"	1:A:189(I):G:H8	1.65	0.60
14:N:4:LYS:CE	14:N:7:ILE:HD11	2.31	0.60
5:E:80:ILE:HD12	5:E:91:LEU:HB2	1.84	0.60
1:A:1350:A:C2	1:A:1351:U:O2	2.54	0.60
1:A:1028:C:H2'	1:A:1029:C:O4'	2.02	0.60
11:K:85:ARG:NH1	11:K:111:ASP:OD2	2.34	0.60
15:O:87:ILE:HG22	15:O:88:ARG:N	2.16	0.60
5:E:83:GLU:HG3	5:E:88:LYS:HG3	1.83	0.60
3:C:11:ARG:HH11	3:C:11:ARG:HG3	1.67	0.60
1:A:1228:C:H2'	1:A:1229:A:H8	1.65	0.60
13:M:90:LEU:O	13:M:91:ARG:CB	2.48	0.59
1:A:631:G:H5"	1:A:632:A:OP1	2.03	0.59
1:A:62:U:C5'	1:A:385:C:O2	2.50	0.59
19:S:78:ARG:HH11	19:S:81:ARG:NH1	2.00	0.59
3:C:138:VAL:HG23	3:C:151:VAL:HG23	1.82	0.59
2:B:16:HIS:HD2	2:B:209:ARG:HB2	1.67	0.59
5:E:32:VAL:O	5:E:43:LEU:HD12	2.02	0.59
1:A:689:C:OP1	11:K:44:SER:OG	2.15	0.59
11:K:91:ARG:O	11:K:95:ILE:HG13	2.02	0.59
3:C:139:GLN:OE1	3:C:139:GLN:HA	2.01	0.59
10:J:48:THR:OG1	10:J:62:HIS:CD2	2.55	0.59
7:G:15:ASP:OD1	7:G:44:TYR:OH	2.20	0.59
1:A:1457:G:O2'	1:A:1458:G:H5'	2.03	0.59
6:F:64:GLN:C	6:F:65:VAL:HG12	2.22	0.59
4:D:12:CYS:O	4:D:33:MET:SD	2.61	0.59
1:A:1248:A:O2'	1:A:1249:C:H5'	2.03	0.59
1:A:1125:U:H6	1:A:1125:U:C5'	2.15	0.59
1:A:1363(A):A:H1'	1:A:1365:G:N7	2.18	0.59
1:A:82:U:C6	1:A:82:U:OP2	2.56	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:A:H2'	1:A:150:C:C6	2.38	0.59
5:E:36:ASP:OD2	5:E:40:ARG:HB2	2.03	0.59
1:A:1060:C:C5	3:C:2:GLY:HA3	2.38	0.59
1:A:1399:C:C2	1:A:1401:G:C5	2.90	0.59
9:I:118:LYS:O	9:I:119:ALA:HB3	2.03	0.59
12:L:71:PRO:O	12:L:102:ARG:HD2	2.02	0.59
1:A:1127:G:H5'	1:A:1128:C:OP2	2.02	0.59
3:C:134:ILE:HD11	3:C:153:VAL:CG2	2.33	0.59
8:H:17:THR:HG22	8:H:63:LEU:HG	1.83	0.59
1:A:1237:C:H3'	1:A:1336:C:H41	1.68	0.59
1:A:192:U:O2'	20:T:57:ARG:HG3	2.03	0.58
8:H:91:ARG:HH11	17:Q:33:GLY:HA3	1.67	0.58
3:C:181:ASN:HB3	3:C:205:GLY:HA3	1.84	0.58
17:Q:59:ILE:HD13	17:Q:73:VAL:HA	1.86	0.58
1:A:1201:A:O2'	1:A:1202:G:OP2	2.15	0.58
4:D:188:LEU:HD23	4:D:188:LEU:H	1.67	0.58
2:B:92:TYR:CD1	2:B:151:GLY:HA3	2.38	0.58
2:B:112:VAL:HG11	2:B:153:ARG:HA	1.84	0.58
1:A:524:G:H2'	1:A:525:C:C6	2.38	0.58
1:A:976:G:N7	1:A:1358:U:C2	2.70	0.58
6:F:21:LEU:O	6:F:25:ILE:HG13	2.03	0.58
1:A:706:A:H1'	11:K:29:ILE:HD11	1.84	0.58
2:B:91:PRO:HB3	2:B:151:GLY:O	2.03	0.58
1:A:948:C:O2'	1:A:949:A:H5'	2.02	0.58
1:A:969:A:OP1	10:J:55:LYS:HE3	2.03	0.58
1:A:328:C:O2	1:A:328:C:C2'	2.37	0.58
10:J:62:HIS:HB3	14:N:59:ALA:HB3	1.85	0.58
1:A:1286:A:H2'	1:A:1287:A:H4'	1.85	0.58
9:I:48:GLU:N	9:I:49:PRO:CD	2.66	0.58
1:A:983:A:H3'	1:A:984:C:H5'	1.86	0.58
15:O:36:ILE:HG13	15:O:59:MET:HE3	1.86	0.58
1:A:1195:C:O2	1:A:1195:C:H2'	2.04	0.58
1:A:1127:G:C5'	1:A:1128:C:OP2	2.52	0.58
1:A:1256:A:H5"	1:A:1258:G:H1'	1.86	0.58
1:A:1020:U:H2'	1:A:1021:G:C8	2.39	0.58
1:A:1248:A:C1'	1:A:1249:C:H5'	2.34	0.57
16:P:18:ARG:O	16:P:20:VAL:HG13	2.04	0.57
18:R:43:PHE:HD1	18:R:56:THR:HG22	1.69	0.57
1:A:1262:C:H2'	1:A:1263:C:H6	1.66	0.57
9:I:11:LYS:O	9:I:11:LYS:HG2	2.04	0.57
1:A:1226:C:C4	13:M:104:ARG:HG2	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:48:ALA:HB1	5:E:49:PRO:HD2	1.85	0.57
3:C:95:THR:O	3:C:97:LYS:N	2.35	0.57
10:J:96:ILE:H	10:J:96:ILE:HD13	1.70	0.57
1:A:1030(A):G:N1	1:A:1032:G:N7	2.53	0.57
1:A:1329:A:H5'	13:M:29:ARG:HD2	1.84	0.57
8:H:42:GLU:HG3	8:H:109:ILE:HD11	1.86	0.57
1:A:707:C:H2'	1:A:708:C:H6	1.70	0.57
2:B:225:ALA:O	2:B:226:ARG:HG3	2.04	0.57
1:A:1134:G:N7	1:A:1135:U:C5	2.73	0.57
3:C:154:SER:HG	3:C:155:GLY:H	1.44	0.57
14:N:24:CYS:HB2	14:N:40:CYS:N	2.10	0.57
1:A:363:A:OP2	12:L:34:ARG:NH1	2.37	0.57
1:A:1125:U:C6	1:A:1125:U:C5'	2.82	0.57
4:D:5:ILE:HG22	4:D:5:ILE:O	2.05	0.57
13:M:82:MET:O	13:M:85:GLY:HA2	2.05	0.57
1:A:945:G:C2	1:A:946:A:C8	2.92	0.57
2:B:78:GLN:NE2	2:B:94:ASN:O	2.38	0.57
5:E:103:GLY:O	5:E:106:PRO:HD2	2.04	0.57
12:L:34:ARG:NH1	12:L:61:THR:HG21	2.19	0.57
1:A:109:A:H2'	1:A:326:G:N2	2.20	0.57
1:A:165:C:H2'	1:A:166:G:O5'	2.05	0.57
12:L:87:GLY:HA2	12:L:98:TYR:HA	1.86	0.57
1:A:1056:U:O2'	1:A:1057:G:H5'	2.05	0.56
1:A:254:G:OP1	17:Q:67:LYS:O	2.21	0.56
1:A:1134:G:N7	1:A:1135:U:H5	2.03	0.56
2:B:96:ARG:O	2:B:98:LEU:CD2	2.53	0.56
8:H:44:PHE:HE2	8:H:109:ILE:HD12	1.68	0.56
10:J:38:ILE:HG13	10:J:71:LEU:HB3	1.87	0.56
3:C:55:VAL:O	3:C:55:VAL:CG1	2.53	0.56
1:A:976:G:C8	1:A:1358:U:C2	2.93	0.56
3:C:15:THR:O	3:C:16:ARG:HB2	2.05	0.56
5:E:101:ILE:HD11	5:E:119:LEU:HD23	1.86	0.56
1:A:38:G:H22	1:A:397:A:H5"	1.70	0.56
1:A:833:U:H2'	1:A:834:C:C6	2.40	0.56
1:A:1403:C:O2	1:A:1403:C:H2'	2.06	0.56
1:A:1249:C:H6	9:I:70:LYS:N	2.03	0.56
9:I:66:ARG:HH11	9:I:66:ARG:HB2	1.71	0.56
1:A:353:A:H5'	1:A:353:A:C8	2.41	0.56
1:A:1367:C:C2'	1:A:1368:G:O5'	2.54	0.56
7:G:26:PHE:CE2	7:G:30:ILE:HD11	2.41	0.56
2:B:97:TRP:CH2	2:B:101:MET:HB2	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:A:C2	1:A:383:A:C4	2.93	0.56
19:S:22:LEU:O	19:S:26:GLY:HA3	2.06	0.56
3:C:15:THR:HG22	3:C:15:THR:O	2.05	0.56
4:D:173:TRP:O	4:D:186:LEU:HB2	2.05	0.56
14:N:24:CYS:HB2	14:N:40:CYS:HB3	1.88	0.56
20:T:72:LEU:O	20:T:73:HIS:C	2.45	0.56
1:A:892:A:C2	1:A:907:A:C4	2.93	0.56
13:M:68:GLY:HA2	13:M:71:ARG:CB	2.36	0.56
15:O:41:GLU:OE2	15:O:41:GLU:HA	2.06	0.56
3:C:11:ARG:O	3:C:14:ILE:O	2.24	0.56
2:B:213:LEU:O	2:B:217:ARG:HG2	2.06	0.56
13:M:17:VAL:HG12	13:M:18:ALA:N	2.21	0.55
1:A:1028:C:C2'	1:A:1029:C:O4'	2.54	0.55
1:A:1279:A:C5'	1:A:1280:A:OP1	2.53	0.55
1:A:977:A:H2'	1:A:978:A:H5'	1.86	0.55
19:S:9:VAL:HG23	19:S:11:VAL:HG12	1.88	0.55
1:A:993:G:H4'	1:A:994:A:OP2	2.05	0.55
1:A:457:C:H2'	1:A:458:C:H6	1.71	0.55
9:I:104:ARG:O	9:I:104:ARG:HD2	2.05	0.55
22:X:6:G:OP2	22:X:6:G:N2	2.28	0.55
14:N:44:LEU:O	14:N:44:LEU:HD23	2.05	0.55
1:A:975:A:C5'	1:A:975:A:H8	2.19	0.55
12:L:5:PRO:HG2	12:L:10:LEU:HD21	1.89	0.55
4:D:108:LEU:HD13	4:D:174:LEU:HD13	1.87	0.55
1:A:1031:G:N3	1:A:1032:G:O6	2.39	0.55
7:G:15:ASP:HB3	7:G:20:ASP:H	1.72	0.55
1:A:265:G:H5'	17:Q:64:PRO:O	2.06	0.55
15:O:39:LEU:HD12	15:O:56:LEU:HD13	1.86	0.55
1:A:860:A:H2'	1:A:861:G:O4'	2.06	0.55
1:A:838:G:H8	1:A:838:G:O5'	1.88	0.55
9:I:54:ASP:C	9:I:56:LEU:H	2.10	0.55
11:K:20:TYR:CE1	11:K:83:ILE:HD13	2.41	0.55
1:A:928:G:O2'	1:A:1533:C:OP1	2.18	0.55
16:P:19:ILE:O	16:P:36:ILE:HG13	2.07	0.55
14:N:53:LEU:HB3	14:N:56:VAL:HG21	1.89	0.55
1:A:1226:C:C4	13:M:104:ARG:CG	2.90	0.55
8:H:91:ARG:NH1	17:Q:33:GLY:HA3	2.22	0.55
1:A:945:G:H2'	1:A:945:G:N3	2.22	0.55
1:A:946:A:H2'	1:A:947:G:C8	2.42	0.55
23:Y:34:I:H2'	23:Y:35:G:C8	2.42	0.55
1:A:1349:A:C2'	1:A:1350:A:O5'	2.55	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:53:VAL:O	9:I:54:ASP:HB2	2.06	0.55
1:A:1236:A:H4'	1:A:1304:G:H4'	1.89	0.55
1:A:1067:A:H5'	1:A:1067:A:C8	2.42	0.55
4:D:102:ASP:HB3	4:D:136:PRO:HB3	1.89	0.55
1:A:1315:U:O2'	1:A:1360:A:N3	2.35	0.55
1:A:1001(A):G:C6	1:A:1002:G:C6	2.95	0.55
1:A:1052:U:O2'	1:A:1055:A:P	2.65	0.54
2:B:223:ILE:C	2:B:225:ALA:H	2.10	0.54
1:A:1477:C:H2'	1:A:1478:C:C6	2.42	0.54
7:G:136:LYS:C	7:G:138:LYS:H	2.10	0.54
1:A:781:A:C3'	1:A:782:A:H5'	2.37	0.54
1:A:1003:G:N3	1:A:1004:A:H1'	2.23	0.54
13:M:112:GLY:O	13:M:113:PRO:C	2.45	0.54
1:A:1280:A:H5"	10:J:40:LEU:HD13	1.88	0.54
1:A:993:G:N3	1:A:993:G:H2'	2.22	0.54
1:A:255:G:OP1	17:Q:69:LYS:NZ	2.36	0.54
6:F:27:GLN:HA	6:F:30:LEU:HD12	1.89	0.54
4:D:149:ALA:HB3	4:D:152:SER:OG	2.07	0.54
17:Q:27:PHE:CZ	17:Q:36:ILE:HD11	2.42	0.54
15:O:62:GLN:HA	15:O:62:GLN:OE1	2.06	0.54
1:A:1063:C:OP2	1:A:1064:G:O2'	2.25	0.54
1:A:1252:A:OP1	1:A:1252:A:C8	2.60	0.54
1:A:1356:G:H2'	1:A:1357:A:H8	1.69	0.54
1:A:192:U:H4'	20:T:57:ARG:HD2	1.89	0.54
1:A:1148:U:H2'	1:A:1149:C:O4'	2.07	0.54
1:A:1425:U:H2'	1:A:1426:C:C6	2.43	0.54
1:A:1005:A:H2'	1:A:1006:C:O4'	2.07	0.54
8:H:122:ARG:CZ	8:H:122:ARG:HB2	2.38	0.54
1:A:1054:C:C4	23:Y:34:I:C8	2.96	0.54
1:A:1252:A:OP2	1:A:1252:A:O4'	2.25	0.54
1:A:1206:G:C6	1:A:1207:G:C5	2.96	0.54
10:J:48:THR:HG1	10:J:62:HIS:CD2	2.25	0.54
3:C:188:LEU:O	3:C:189:ALA:HB2	2.07	0.54
1:A:1169:A:C6	1:A:1170:A:C6	2.96	0.54
1:A:1031:G:N3	1:A:1032:G:C6	2.76	0.54
19:S:9:VAL:C	19:S:11:VAL:H	2.11	0.54
1:A:1059:C:O3'	14:N:45:ARG:NH2	2.41	0.54
3:C:129:ALA:HB3	3:C:132:ARG:HG2	1.90	0.54
1:A:1397:C:O4'	1:A:1397:C:O2	2.25	0.54
14:N:44:LEU:C	14:N:44:LEU:CD2	2.76	0.54
3:C:111:LEU:HD21	3:C:144:SER:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:50:ALA:HB1	19:S:57:HIS:HB3	1.89	0.54
3:C:19:GLU:HB3	3:C:40:ARG:NH2	2.23	0.54
3:C:70:VAL:HG12	3:C:71:ALA:H	1.72	0.53
16:P:75:ARG:O	16:P:78:GLY:N	2.40	0.53
8:H:1:MET:O	8:H:1:MET:HG2	2.08	0.53
1:A:1054:C:C5	23:Y:34:I:H5"	2.44	0.53
1:A:1399:C:H4'	1:A:1400:C:C5'	2.38	0.53
1:A:1192:C:C5	1:A:1193:G:C8	2.96	0.53
8:H:103:VAL:HG21	8:H:109:ILE:O	2.09	0.53
6:F:14:LEU:HD21	6:F:84:ASN:OD1	2.08	0.53
1:A:512:U:H1'	4:D:42:GLN:HE22	1.72	0.53
20:T:44:ALA:C	20:T:46:GLU:H	2.11	0.53
14:N:2:ALA:HB3	14:N:6:LEU:HD13	1.90	0.53
1:A:828:A:OP1	1:A:828:A:H4'	2.09	0.53
20:T:53:LEU:H	20:T:53:LEU:HD12	1.72	0.53
9:I:58:ARG:HB2	9:I:58:ARG:HH11	1.72	0.53
4:D:23:GLY:O	4:D:27:TYR:HD2	1.92	0.53
2:B:71:VAL:HG12	2:B:93:VAL:HB	1.90	0.53
12:L:6:THR:OG1	12:L:9:GLN:HG3	2.09	0.53
1:A:509:A:C6	1:A:510:A:N1	2.77	0.53
1:A:979:C:C3'	1:A:980:C:H5"	2.38	0.53
7:G:136:LYS:O	7:G:138:LYS:N	2.35	0.53
1:A:1347:G:N2	1:A:1373:G:H2'	2.24	0.53
1:A:1095:U:P	1:A:1108:G:H1	2.32	0.53
1:A:1179:A:C2'	1:A:1180:A:H5'	2.38	0.53
1:A:1492:A:H1'	22:X:5:A:O2'	2.09	0.53
1:A:353:A:H5'	1:A:353:A:H8	1.73	0.53
1:A:1001(A):G:H2'	1:A:1002:G:C8	2.44	0.53
1:A:323:U:H2'	1:A:324:G:O4'	2.09	0.53
1:A:302:G:N3	1:A:556:C:H4'	2.24	0.53
1:A:1250:A:H1'	1:A:1251:A:C8	2.42	0.53
14:N:24:CYS:CB	14:N:40:CYS:HB3	2.39	0.53
1:A:407:G:O2'	4:D:116:GLN:HG3	2.09	0.53
1:A:1352:C:H2'	1:A:1353:G:C8	2.44	0.53
1:A:501:C:H2'	1:A:502:G:C8	2.44	0.53
17:Q:67:LYS:O	17:Q:68:ARG:CG	2.54	0.53
14:N:4:LYS:HE2	14:N:7:ILE:HD11	1.91	0.53
2:B:78:GLN:O	2:B:94:ASN:OD1	2.27	0.53
12:L:8:ASN:O	12:L:12:ARG:HG3	2.09	0.53
1:A:937:A:C2	1:A:1379:G:C6	2.97	0.53
7:G:57:GLU:OE1	7:G:58:PRO:HD2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1271:G:H2'	1:A:1272:G:H5"	1.89	0.52
7:G:51:GLN:O	7:G:53:LYS:N	2.43	0.52
1:A:1002:G:H8	1:A:1002:G:O5'	1.92	0.52
1:A:1179:A:H2'	1:A:1180:A:H5'	1.91	0.52
1:A:1160:G:O6	1:A:1181:G:C6	2.62	0.52
2:B:22:LYS:HD2	2:B:22:LYS:N	2.24	0.52
1:A:878:G:H5'	8:H:89:PRO:HG2	1.91	0.52
1:A:979:C:H3'	1:A:980:C:C5'	2.39	0.52
1:A:1266:G:N2	1:A:1269:A:OP2	2.39	0.52
1:A:1313:U:O4	19:S:4:SER:N	2.42	0.52
1:A:969:A:H2'	1:A:970:C:H5'	1.89	0.52
4:D:121:VAL:O	4:D:134:ASP:HA	2.09	0.52
1:A:1257:U:OP2	1:A:1257:U:H4'	2.10	0.52
9:I:88:TYR:O	9:I:89:ASN:HB2	2.08	0.52
8:H:4:ASP:OD2	8:H:85:ARG:HD2	2.10	0.52
1:A:1347:G:C6	9:I:107:ARG:NH2	2.77	0.52
1:A:1160:G:H2'	1:A:1161:C:O5'	2.09	0.52
1:A:972:C:O3'	10:J:57:LYS:HG3	2.09	0.52
16:P:43:LYS:HB3	16:P:48:TRP:CD1	2.45	0.52
1:A:84:U:O2	1:A:84:U:H2'	2.08	0.52
11:K:48:ILE:HG22	11:K:49:GLY:H	1.73	0.52
20:T:67:ALA:O	20:T:73:HIS:ND1	2.43	0.52
14:N:24:CYS:SG	14:N:27:CYS:N	2.82	0.52
1:A:1544:U:O3'	22:X:4:PSU:H5"	2.09	0.52
1:A:1241:G:H2'	1:A:1242:C:H6	1.73	0.52
1:A:723:U:O2	1:A:723:U:C2'	2.56	0.52
2:B:70:PHE:O	2:B:92:TYR:HA	2.10	0.52
13:M:80:ARG:O	13:M:83:ASP:N	2.39	0.52
9:I:104:ARG:O	9:I:105:ASP:HB3	2.09	0.52
1:A:1118:C:H1'	1:A:1179:A:C4	2.44	0.52
3:C:52:LEU:H	3:C:52:LEU:HD23	1.75	0.52
13:M:3:ARG:NH1	13:M:7:VAL:HG12	2.24	0.52
1:A:1329:A:C2'	1:A:1330:U:H5'	2.39	0.52
1:A:975:A:H5'	1:A:975:A:H8	1.75	0.52
1:A:1399:C:H4'	1:A:1400:C:H5"	1.91	0.52
5:E:80:ILE:HG23	8:H:104:ARG:NH2	2.24	0.52
5:E:31:LEU:HD22	5:E:43:LEU:HD11	1.90	0.52
1:A:124:G:C5	1:A:125:U:C5	2.97	0.52
6:F:30:LEU:HD11	6:F:63:TYR:CE2	2.45	0.52
1:A:1331:G:OP1	1:A:1331:G:C4'	2.58	0.52
1:A:1031:G:O2'	1:A:1032:G:C5	2.63	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:103:GLY:O	5:E:104:ALA:C	2.48	0.52
8:H:122:ARG:NH1	8:H:122:ARG:HB2	2.25	0.52
1:A:718:G:C8	11:K:116:HIS:HB3	2.44	0.52
1:A:427:U:OP1	4:D:13:ARG:NH2	2.41	0.52
18:R:46:GLU:CD	18:R:46:GLU:N	2.62	0.52
4:D:64:LEU:HD13	4:D:198:VAL:HG11	1.92	0.52
1:A:498:U:O2'	1:A:499:A:OP2	2.28	0.52
12:L:81:SER:O	12:L:106:ASP:HB2	2.10	0.52
17:Q:68:ARG:H	17:Q:70:ARG:HH11	1.56	0.52
9:I:80:GLY:O	9:I:82:ALA:N	2.43	0.52
2:B:238:LEU:O	2:B:240:GLN:N	2.43	0.52
18:R:25:THR:HG21	18:R:42:ARG:HH11	1.75	0.52
1:A:1496:C:H2'	1:A:1497:G:O4'	2.10	0.52
4:D:33:MET:HE2	4:D:33:MET:HA	1.90	0.51
1:A:1351:U:O2'	1:A:1352:C:H5'	2.10	0.51
5:E:51:VAL:HB	5:E:52:PRO:HD3	1.91	0.51
23:Y:33:U:C5'	23:Y:34:I:OP2	2.58	0.51
1:A:1350:A:C6	1:A:1351:U:N3	2.76	0.51
1:A:270:A:H2'	1:A:271:C:C6	2.46	0.51
1:A:686:U:O2	1:A:687:A:C8	2.63	0.51
3:C:157:ILE:HG21	3:C:164:ARG:NH2	2.25	0.51
1:A:532:A:H2'	1:A:532:A:N3	2.24	0.51
7:G:143:ARG:O	7:G:145:ALA:O	2.27	0.51
5:E:45:PHE:HE2	5:E:47:LYS:HE2	1.75	0.51
1:A:407:G:H4'	4:D:116:GLN:HA	1.91	0.51
1:A:1100:C:O2'	1:A:1102:A:OP1	2.27	0.51
1:A:942:G:C2	1:A:943:U:C6	2.98	0.51
1:A:1252:A:P	1:A:1252:A:O4'	2.69	0.51
3:C:70:VAL:HG12	3:C:71:ALA:N	2.25	0.51
1:A:1001:A:H2'	1:A:1001(A):G:C8	2.45	0.51
1:A:881:G:P	12:L:12:ARG:HH22	2.34	0.51
11:K:108:ILE:O	11:K:109:VAL:HG23	2.11	0.51
7:G:9:VAL:HG11	7:G:94:ARG:HE	1.75	0.51
8:H:77:GLU:CG	8:H:78:GLN:H	2.23	0.51
19:S:45:VAL:HG23	19:S:46:GLY:N	2.26	0.51
1:A:1060:C:P	14:N:45:ARG:HH22	2.33	0.51
3:C:110:ASN:O	3:C:111:LEU:HD23	2.10	0.51
1:A:173:U:H4'	1:A:174:C:OP2	2.10	0.51
4:D:150:GLU:HA	4:D:153:ARG:HE	1.74	0.51
12:L:93:LEU:HB3	12:L:96:VAL:HG21	1.93	0.51
14:N:27:CYS:HB3	14:N:43:CYS:CB	2.36	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:954:G:O6	13:M:104:ARG:NH1	2.42	0.51
1:A:1493:A:C8	22:X:5:A:H1'	2.46	0.51
1:A:533:A:C2	1:A:536:C:C5	2.98	0.51
1:A:1251:A:N6	1:A:1287:A:N7	2.59	0.51
1:A:91:C:O2	1:A:91:C:O4'	2.29	0.51
1:A:1509:C:H2'	1:A:1510:U:O4'	2.11	0.51
2:B:142:LEU:O	2:B:146:GLN:HB2	2.11	0.51
3:C:50:ALA:HB1	3:C:70:VAL:HG11	1.92	0.51
1:A:623:C:C4	1:A:624:C:C4	2.99	0.51
4:D:31:CYS:C	4:D:33:MET:N	2.36	0.51
1:A:954:G:H2'	1:A:955:U:C6	2.46	0.51
3:C:30:ARG:CB	3:C:30:ARG:CZ	2.89	0.51
11:K:48:ILE:HD11	11:K:64:ALA:HA	1.92	0.51
1:A:1194:U:H2'	1:A:1195:C:H6	1.75	0.51
1:A:794:A:H2'	1:A:795:C:C6	2.46	0.51
1:A:959:A:C2	1:A:1222:G:O4'	2.63	0.51
1:A:1017:G:O5'	1:A:1017:G:H8	1.93	0.51
1:A:78:G:N1	1:A:91:C:H5	2.05	0.51
19:S:9:VAL:HG23	19:S:11:VAL:CG1	2.41	0.51
5:E:122:GLU:HG2	5:E:131:ILE:HD12	1.92	0.51
13:M:83:ASP:OD1	13:M:84:ILE:N	2.44	0.51
1:A:687:A:H2	1:A:700:G:N3	2.09	0.51
11:K:54:ARG:O	11:K:57:THR:OG1	2.28	0.51
13:M:33:ALA:HA	13:M:59:TYR:CE2	2.46	0.51
1:A:36:C:O2'	12:L:117:ARG:NH2	2.44	0.51
1:A:857:C:H2'	1:A:858:G:O4'	2.11	0.51
8:H:70:GLN:OE1	8:H:70:GLN:HA	2.11	0.51
1:A:1031:G:O2'	1:A:1032:G:C6	2.64	0.50
1:A:707:C:H2'	1:A:708:C:C6	2.46	0.50
2:B:88:ALA:HB2	2:B:219:VAL:CG1	2.39	0.50
1:A:7:G:H5'	1:A:298:A:O4'	2.11	0.50
20:T:100:ILE:O	20:T:100:ILE:HG22	2.11	0.50
1:A:417:C:H2'	1:A:418:C:C6	2.47	0.50
3:C:179:ARG:O	3:C:179:ARG:HG3	2.11	0.50
14:N:22:THR:O	14:N:23:ARG:HB2	2.09	0.50
1:A:1240:U:H3'	1:A:1241:G:C5'	2.39	0.50
7:G:145:ALA:O	7:G:146:GLU:CB	2.54	0.50
15:O:82:ILE:O	15:O:86:GLY:N	2.36	0.50
1:A:180:U:H2'	1:A:181:G:H5'	1.93	0.50
1:A:373:A:C2'	1:A:374:A:O5'	2.60	0.50
3:C:34:LEU:O	3:C:38:ARG:HG2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:11:LEU:CA	4:D:13:ARG:H	2.22	0.50
3:C:15:THR:O	3:C:15:THR:CG2	2.60	0.50
1:A:498:U:O2'	1:A:499:A:P	2.69	0.50
1:A:371:G:O2'	1:A:373:A:N7	2.42	0.50
1:A:1098:C:H2'	1:A:1099:G:O5'	2.11	0.50
1:A:1368:G:H2'	1:A:1369:C:H5'	1.92	0.50
1:A:1004:A:N6	1:A:1037:C:H42	2.09	0.50
17:Q:5:VAL:HA	17:Q:59:ILE:O	2.11	0.50
1:A:781:A:C5	1:A:802:A:C2	2.99	0.50
2:B:114:ARG:NH1	2:B:118:LEU:HD21	2.25	0.50
1:A:951:G:O2'	1:A:952:U:H5'	2.11	0.50
8:H:35:ILE:HG23	8:H:111:ILE:HD13	1.93	0.50
20:T:39:LYS:HD3	20:T:55:ILE:HD13	1.93	0.50
10:J:23:ILE:O	10:J:23:ILE:HG22	2.12	0.50
16:P:38:TYR:CE1	16:P:50:LYS:HD2	2.46	0.50
1:A:495:A:H4'	1:A:496:A:OP1	2.11	0.50
1:A:555:C:H2'	1:A:556:C:C6	2.47	0.50
20:T:99:LEU:O	20:T:100:ILE:C	2.50	0.50
1:A:1030(B):C:C2	1:A:1031:G:N1	2.79	0.50
2:B:97:TRP:CZ3	2:B:98:LEU:O	2.65	0.50
1:A:942:G:N3	1:A:943:U:C6	2.79	0.50
8:H:64:LYS:HG2	8:H:79:VAL:HG21	1.93	0.50
1:A:639:G:C2'	1:A:640:A:H5'	2.42	0.50
19:S:48:THR:HG22	19:S:61:TYR:HA	1.94	0.50
12:L:29:GLY:O	12:L:30:ALA:O	2.29	0.50
1:A:685:G:N2	1:A:704:A:OP2	2.38	0.49
3:C:180:ALA:O	3:C:181:ASN:HB3	2.12	0.49
13:M:68:GLY:HA2	13:M:71:ARG:HB3	1.94	0.49
6:F:30:LEU:O	6:F:35:ALA:HB3	2.11	0.49
1:A:1514:C:C2'	1:A:1515:C:H5'	2.42	0.49
1:A:304:U:H2'	1:A:305:G:C8	2.47	0.49
1:A:1110:A:H8	1:A:1110:A:O5'	1.95	0.49
10:J:26:ALA:HB3	10:J:85:LEU:HD21	1.94	0.49
4:D:58:LEU:HD22	4:D:62:GLN:HG2	1.95	0.49
1:A:35:G:H2'	1:A:36:C:C6	2.47	0.49
1:A:1039:C:H2'	1:A:1040:U:C6	2.47	0.49
1:A:1034:G:N3	1:A:1034:G:H2'	2.28	0.49
5:E:30:ALA:O	5:E:45:PHE:HA	2.12	0.49
1:A:401:C:O2'	1:A:621:A:N3	2.29	0.49
4:D:54:TYR:HE1	4:D:209:ARG:HH21	1.60	0.49
1:A:116:A:H2'	1:A:117:G:C8	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1251:A:C8	9:I:68:GLY:HA2	2.47	0.49
17:Q:60:ILE:O	17:Q:71:PHE:HA	2.12	0.49
4:D:196:LEU:HB3	4:D:198:VAL:HG12	1.94	0.49
4:D:61:LYS:HB2	4:D:203:VAL:HG22	1.93	0.49
2:B:163:PHE:HA	2:B:185:ILE:O	2.12	0.49
1:A:1188:A:H2'	1:A:1189:C:O4'	2.13	0.49
1:A:767:A:H2'	1:A:768:A:O4'	2.12	0.49
1:A:1091:U:O2	1:A:1093:A:N7	2.45	0.49
1:A:165:C:C2'	1:A:166:G:O5'	2.60	0.49
1:A:686:U:C2	1:A:687:A:N7	2.81	0.49
1:A:943:U:H2'	1:A:944:G:H5'	1.94	0.49
1:A:417:C:H6	1:A:417:C:O5'	1.96	0.49
10:J:42:THR:HG23	10:J:67:THR:O	2.12	0.49
1:A:250:A:H4'	1:A:251:G:O5'	2.13	0.49
10:J:4:ILE:O	10:J:73:ASP:HA	2.12	0.49
13:M:45:VAL:O	13:M:47:ASP:N	2.45	0.49
13:M:50:GLU:O	13:M:54:VAL:HG23	2.12	0.49
1:A:938:A:N6	1:A:939:G:C5	2.80	0.49
2:B:172:ILE:H	2:B:172:ILE:HD12	1.76	0.49
8:H:73:ASP:OD1	8:H:75:ARG:HD3	2.13	0.49
1:A:532:A:N6	1:A:1206:G:O2'	2.45	0.49
1:A:977:A:C2'	1:A:978:A:H5'	2.43	0.49
19:S:16:LEU:O	19:S:17:GLU:C	2.50	0.49
17:Q:56:VAL:HB	17:Q:78:GLU:HG3	1.94	0.49
1:A:1419:G:OP2	1:A:1419:G:H8	1.96	0.49
13:M:58:GLU:OE2	13:M:58:GLU:HA	2.13	0.49
1:A:1351:U:C2'	1:A:1352:C:H5'	2.42	0.49
5:E:80:ILE:HD13	5:E:138:ALA:HB1	1.94	0.49
9:I:49:PRO:O	9:I:52:ALA:HB3	2.13	0.49
5:E:72:GLN:O	5:E:73:ASN:HB3	2.12	0.49
1:A:981:U:O5'	1:A:981:U:H6	1.95	0.49
14:N:21:TYR:HD1	14:N:22:THR:O	1.96	0.49
1:A:1366:C:C2	1:A:1367:C:C5	3.01	0.49
10:J:56:HIS:O	10:J:58:ASP:O	2.30	0.49
1:A:1095:U:H2'	1:A:1096:C:C6	2.48	0.49
1:A:499:A:H4'	1:A:500:G:OP1	2.13	0.49
5:E:51:VAL:O	5:E:54:ALA:HB3	2.13	0.49
1:A:373:A:H2'	1:A:374:A:O5'	2.13	0.49
9:I:100:GLY:C	9:I:102:LEU:H	2.15	0.49
1:A:1399:C:H4'	1:A:1400:C:O5'	2.12	0.49
1:A:1133:G:N3	1:A:1142:G:N2	2.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:G:C6	1:A:125:U:C4	3.01	0.49
13:M:10:PRO:O	13:M:11:ARG:HB2	2.13	0.49
1:A:596:C:OP2	1:A:597:G:OP2	2.31	0.49
3:C:5:ILE:O	3:C:5:ILE:HD12	2.12	0.49
1:A:1366:C:O2'	1:A:1367:C:H5'	2.13	0.49
3:C:14:ILE:O	3:C:16:ARG:N	2.46	0.49
1:A:1379:G:OP2	7:G:6:ARG:HG3	2.12	0.49
1:A:1157:A:H4'	1:A:1158:C:O5'	2.12	0.49
10:J:77:PRO:O	10:J:79:ARG:NH2	2.44	0.49
16:P:22:THR:HA	16:P:33:ILE:HG13	1.95	0.49
1:A:1053:G:C3'	1:A:1054:C:H5'	2.43	0.48
23:Y:34:I:HO2'	23:Y:35:G:P	2.36	0.48
2:B:96:ARG:HA	2:B:96:ARG:CZ	2.42	0.48
9:I:118:LYS:O	9:I:119:ALA:CB	2.61	0.48
1:A:1134:G:N2	1:A:1141:C:C2	2.81	0.48
5:E:51:VAL:O	5:E:55:VAL:HG23	2.13	0.48
10:J:8:LEU:HD11	10:J:20:ALA:HB1	1.95	0.48
2:B:144:ARG:HG3	2:B:145:LEU:N	2.27	0.48
1:A:1014:A:H2'	1:A:1015:A:C8	2.48	0.48
8:H:67:PRO:O	8:H:69:ARG:HG3	2.13	0.48
1:A:377:G:O2'	1:A:378:G:H5'	2.13	0.48
5:E:147:ASP:OD1	5:E:147:ASP:N	2.46	0.48
5:E:83:GLU:HA	5:E:87:SER:O	2.13	0.48
5:E:7:GLU:OE1	5:E:37:ARG:NE	2.32	0.48
7:G:95:ARG:NH2	7:G:99:LEU:HD21	2.28	0.48
1:A:1133:G:C2	1:A:1142:G:N1	2.81	0.48
1:A:501:C:H2'	1:A:502:G:H8	1.78	0.48
1:A:1345:U:C4	1:A:1377:A:C2	3.02	0.48
4:D:18:LYS:CD	4:D:31:CYS:HB2	2.41	0.48
4:D:6:GLY:O	4:D:8:VAL:HG23	2.14	0.48
7:G:24:THR:HA	7:G:27:ILE:HG13	1.96	0.48
1:A:413:G:N2	1:A:428:G:H1'	2.27	0.48
3:C:83:ARG:O	3:C:86:VAL:N	2.47	0.48
1:A:273:A:C2'	1:A:274:A:O5'	2.61	0.48
1:A:80:A:H61	1:A:89:C:H42	1.61	0.48
1:A:1269:A:C2	1:A:1313:U:O4'	2.66	0.48
17:Q:33:GLY:O	17:Q:34:LYS:C	2.51	0.48
12:L:35:GLY:HA3	12:L:58:VAL:CG1	2.44	0.48
19:S:29:ARG:C	19:S:31:ILE:H	2.16	0.48
4:D:162:LEU:HG	4:D:181:MET:HG2	1.96	0.48
5:E:8:GLU:HA	5:E:33:VAL:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:546:G:OP1	4:D:73:ARG:HB2	2.14	0.48
1:A:757:U:H2'	1:A:758:G:O4'	2.13	0.48
2:B:18:GLY:HA3	2:B:41:ILE:HA	1.93	0.48
20:T:75:ASN:C	20:T:75:ASN:OD1	2.52	0.48
1:A:1033:G:HO2'	1:A:1034:G:P	2.36	0.48
1:A:300:A:H1'	1:A:565:U:O2	2.14	0.48
1:A:45:U:H2'	1:A:46:G:H8	1.77	0.48
10:J:4:ILE:HB	10:J:74:ILE:HG13	1.96	0.48
1:A:1252:A:N3	1:A:1252:A:H2'	2.28	0.48
14:N:24:CYS:HB2	14:N:40:CYS:CB	2.43	0.48
1:A:13:U:O2'	1:A:14:U:H5'	2.13	0.48
1:A:1468:A:H2'	1:A:1469:G:O4'	2.13	0.48
10:J:15:THR:HA	10:J:18:ALA:HB3	1.95	0.48
3:C:23:TYR:CG	3:C:24:ALA:N	2.82	0.48
8:H:10:LEU:HD12	8:H:85:ARG:HG2	1.96	0.48
2:B:107:THR:HA	2:B:110:GLN:NE2	2.29	0.48
20:T:72:LEU:O	20:T:73:HIS:O	2.32	0.48
1:A:502:G:C2	1:A:503:C:C2	3.01	0.48
4:D:105:VAL:HG12	4:D:117:ALA:HB1	1.95	0.48
4:D:106:TYR:CD1	4:D:106:TYR:C	2.86	0.48
1:A:1030(C):G:C8	1:A:1030(C):G:H5"	2.49	0.48
1:A:418:C:H1'	1:A:540:G:O2'	2.14	0.48
1:A:27:G:H2'	1:A:28:G:O4'	2.14	0.48
1:A:864:A:H2	1:A:917:G:N3	2.12	0.48
1:A:390:C:O3'	16:P:28:ARG:NH2	2.47	0.48
3:C:35:GLU:O	3:C:37:GLN:N	2.46	0.48
1:A:953:G:C5'	1:A:965:A:H61	2.22	0.47
1:A:937:A:C2	1:A:1379:G:O6	2.67	0.47
1:A:1191:A:OP1	3:C:3:ASN:OD1	2.31	0.47
5:E:105:VAL:HB	5:E:106:PRO:CD	2.44	0.47
7:G:27:ILE:HA	7:G:30:ILE:HD12	1.95	0.47
15:O:39:LEU:HD11	15:O:56:LEU:HB2	1.97	0.47
1:A:1179:A:OP2	9:I:93:ARG:NH2	2.37	0.47
1:A:858:G:O6	1:A:869:G:H3'	2.14	0.47
1:A:176:C:H2'	1:A:177:C:H6	1.79	0.47
1:A:31:G:O2'	1:A:48:C:N4	2.47	0.47
1:A:560:U:H4'	1:A:561:U:O5'	2.14	0.47
13:M:97:PRO:HA	13:M:110:ARG:HD3	1.95	0.47
15:O:53:HIS:NE2	15:O:57:LEU:HD21	2.29	0.47
19:S:10:PHE:CD1	19:S:10:PHE:N	2.82	0.47
2:B:97:TRP:CZ2	2:B:101:MET:HB2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:87:SER:HG	8:H:93:VAL:H	1.62	0.47
13:M:16:ASP:OD1	13:M:16:ASP:N	2.47	0.47
17:Q:27:PHE:CD1	17:Q:27:PHE:N	2.82	0.47
4:D:63:LYS:HD3	4:D:197:PRO:O	2.13	0.47
10:J:10:GLY:O	10:J:67:THR:HA	2.15	0.47
1:A:918:A:H2'	1:A:919:A:C8	2.50	0.47
2:B:127:ILE:HD13	2:B:127:ILE:O	2.14	0.47
4:D:8:VAL:HG12	4:D:9:CYS:N	2.29	0.47
1:A:1250:A:N3	1:A:1250:A:H2'	2.29	0.47
3:C:108:ASN:HD21	3:C:144:SER:HB3	1.78	0.47
11:K:33:THR:HG22	11:K:39:PRO:HA	1.96	0.47
11:K:92:GLU:HB3	11:K:96:ARG:NH1	2.29	0.47
1:A:1499:A:H5'	1:A:1499:A:H8	1.80	0.47
3:C:134:ILE:HG22	3:C:168:ALA:HB3	1.97	0.47
1:A:1031:G:C2	1:A:1032:G:O6	2.67	0.47
3:C:50:ALA:O	3:C:70:VAL:CG1	2.62	0.47
1:A:977:A:O2'	1:A:979:C:OP2	2.32	0.47
1:A:1135:U:O2	1:A:1137:C:O2	2.32	0.47
2:B:194:PRO:O	2:B:196:LEU:N	2.48	0.47
1:A:82:U:O2	1:A:83:U:O2	2.33	0.47
1:A:1069:C:H4'	1:A:1192:C:O2	2.13	0.47
10:J:96:ILE:HD13	10:J:96:ILE:N	2.29	0.47
20:T:75:ASN:OD1	20:T:76:ALA:N	2.47	0.47
18:R:33:ASP:O	18:R:40:LEU:HD11	2.14	0.47
1:A:1026:G:N3	1:A:1026:G:H2'	2.30	0.47
4:D:33:MET:CE	4:D:33:MET:HA	2.45	0.47
1:A:1251:A:H8	9:I:68:GLY:HA2	1.80	0.47
1:A:91:C:O2	1:A:91:C:O5'	2.32	0.47
3:C:72:LYS:HA	3:C:72:LYS:CE	2.44	0.47
4:D:25:ARG:C	4:D:27:TYR:N	2.66	0.47
6:F:64:GLN:C	6:F:65:VAL:CG1	2.83	0.47
5:E:36:ASP:OD1	5:E:38:GLN:N	2.48	0.47
17:Q:27:PHE:CE2	17:Q:36:ILE:HD11	2.49	0.47
1:A:1347:G:OP2	9:I:107:ARG:HG2	2.15	0.47
1:A:116:A:H2'	1:A:117:G:H8	1.79	0.47
2:B:50:GLU:O	2:B:54:THR:OG1	2.29	0.47
1:A:1134:G:C8	1:A:1135:U:H5	2.33	0.47
3:C:188:LEU:HD22	3:C:188:LEU:HA	1.82	0.47
1:A:533:A:C2	1:A:536:C:C6	3.03	0.47
17:Q:63:ARG:O	17:Q:65:ILE:HD12	2.15	0.47
1:A:1316:G:N2	1:A:1318:A:H3'	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1346:A:C8	1:A:1348:U:C2	3.03	0.47
16:P:4:ILE:N	16:P:4:ILE:HD12	2.30	0.47
1:A:1365:G:C5	1:A:1366:C:C5	3.03	0.47
5:E:71:LEU:O	5:E:72:GLN:HG2	2.15	0.47
10:J:44:VAL:HG13	10:J:66:ARG:HB3	1.97	0.47
14:N:26:ARG:HH11	14:N:47:LEU:HG	1.80	0.47
3:C:175:LEU:HD11	3:C:201:TYR:CD2	2.49	0.47
1:A:960:U:H2'	1:A:960:U:O2	2.15	0.47
1:A:1028:C:O2'	1:A:1029:C:O4'	2.32	0.46
1:A:1030(C):G:H8	1:A:1030(C):G:H3'	1.80	0.46
2:B:97:TRP:CE3	2:B:98:LEU:O	2.68	0.46
8:H:9:MET:HG3	8:H:26:VAL:HG21	1.96	0.46
9:I:26:VAL:HG13	9:I:61:ALA:HB3	1.97	0.46
1:A:799:G:C2'	1:A:800:G:H5'	2.44	0.46
10:J:78:ASN:HB2	10:J:80:LYS:HB2	1.97	0.46
1:A:749:C:OP2	1:A:750:G:OP2	2.33	0.46
4:D:29:PRO:O	4:D:30:LYS:HD3	2.14	0.46
2:B:16:HIS:HB3	2:B:210:SER:OG	2.14	0.46
4:D:117:ALA:O	4:D:121:VAL:HG23	2.15	0.46
1:A:1027:C:O2	1:A:1035:A:N1	2.48	0.46
1:A:221:C:O2	1:A:221:C:H2'	2.15	0.46
1:A:1367:C:H2'	1:A:1368:G:O5'	2.15	0.46
1:A:1541:U:C6	1:A:1541:U:H5'	2.50	0.46
9:I:4:TYR:CD2	9:I:19:LEU:HB2	2.50	0.46
1:A:1229:A:C2	1:A:1230:C:C4	3.03	0.46
1:A:418:C:O5'	1:A:418:C:H6	1.98	0.46
1:A:251:G:H4'	1:A:252:U:O5'	2.15	0.46
10:J:21:GLN:HA	10:J:24:VAL:HG23	1.97	0.46
2:B:183:PRO:HA	2:B:198:ASP:OD2	2.16	0.46
1:A:1249:C:C6	9:I:70:LYS:N	2.83	0.46
1:A:722:A:O2'	1:A:723:U:C2	2.68	0.46
1:A:624:C:H2'	1:A:625:G:H8	1.80	0.46
20:T:72:LEU:HD21	20:T:80:ARG:NE	2.30	0.46
1:A:949:A:C2	1:A:1233:G:N3	2.83	0.46
9:I:42:ARG:HE	9:I:71:SER:HG	1.62	0.46
1:A:1085:U:C2	1:A:1094:G:O6	2.68	0.46
5:E:139:LEU:C	5:E:141:GLN:H	2.19	0.46
1:A:570:G:H2'	1:A:571:U:C6	2.50	0.46
1:A:791:G:C5	1:A:792:A:N7	2.84	0.46
5:E:80:ILE:HD12	5:E:91:LEU:CB	2.43	0.46
1:A:1201:A:H4'	1:A:1202:G:O5'	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:A:N3	1:A:397:A:H3'	2.29	0.46
1:A:1095:U:OP1	1:A:1108:G:N2	2.43	0.46
1:A:1160:G:C2'	1:A:1161:C:O5'	2.63	0.46
9:I:28:VAL:HG22	9:I:63:ILE:HB	1.98	0.46
1:A:262:A:C6	1:A:263:A:C6	3.03	0.46
1:A:1268:A:N3	1:A:1326:C:O2'	2.44	0.46
17:Q:90:ILE:HA	17:Q:93:GLN:HG2	1.98	0.46
2:B:19:HIS:O	2:B:20:GLU:O	2.33	0.46
1:A:1152:A:O2'	1:A:1153:C:O4'	2.23	0.46
1:A:1457:G:C2'	1:A:1458:G:H5'	2.46	0.46
1:A:1194:U:H2'	1:A:1195:C:C6	2.50	0.46
10:J:6:ILE:HG13	10:J:72:VAL:HB	1.98	0.46
1:A:1532:U:O2	1:A:1532:U:C2'	2.62	0.46
19:S:6:LYS:CD	19:S:7:LYS:HE3	2.45	0.46
15:O:39:LEU:CD1	15:O:56:LEU:HB2	2.46	0.46
1:A:869:G:H5"	1:A:870:U:OP1	2.16	0.46
2:B:207:ALA:O	2:B:211:ILE:HG13	2.16	0.46
16:P:3:LYS:O	16:P:21:VAL:HA	2.16	0.46
13:M:23:TYR:HB3	13:M:67:GLU:HA	1.98	0.46
4:D:124:GLY:O	4:D:126:ILE:N	2.49	0.46
1:A:476:G:H2'	1:A:477:A:C8	2.51	0.46
1:A:1123:A:H4'	10:J:36:GLY:HA3	1.97	0.46
1:A:395:C:H2'	1:A:396:G:H5"	1.98	0.46
1:A:876:G:C6	1:A:877:C:N4	2.84	0.46
9:I:75:ASP:O	9:I:78:LYS:HB3	2.16	0.46
23:Y:34:I:O2'	23:Y:35:G:OP1	2.25	0.46
1:A:1032:G:H1'	1:A:1033:G:H5'	1.97	0.46
3:C:23:TYR:O	3:C:24:ALA:CB	2.63	0.46
20:T:45:GLN:HG2	20:T:91:LEU:CD2	2.44	0.46
5:E:45:PHE:CE2	5:E:47:LYS:CE	2.98	0.46
3:C:195:VAL:HG12	3:C:196:LEU:O	2.16	0.46
1:A:858:G:N7	1:A:869:G:N7	2.64	0.46
2:B:184:VAL:H	2:B:198:ASP:HB2	1.81	0.46
16:P:55:ARG:HD2	16:P:55:ARG:HA	1.79	0.46
3:C:10:PHE:CE2	3:C:178:LEU:HD13	2.51	0.46
11:K:67:ASP:OD1	11:K:67:ASP:C	2.54	0.46
1:A:1366:C:H2'	1:A:1367:C:C5	2.51	0.46
3:C:15:THR:HG23	3:C:181:ASN:HA	1.97	0.46
5:E:105:VAL:HB	5:E:106:PRO:HD3	1.97	0.46
10:J:64:GLU:HG2	14:N:59:ALA:HB2	1.97	0.46
1:A:273:A:H2'	1:A:274:A:O5'	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:199:ASN:ND2	4:D:202:LEU:HG	2.30	0.46
2:B:73:THR:OG1	2:B:170:GLU:OE1	2.30	0.46
17:Q:85:VAL:HG12	17:Q:89:LEU:HD12	1.97	0.46
1:A:90:U:O5'	1:A:90:U:H6	1.98	0.46
1:A:1306:A:H61	1:A:1331:G:H1'	1.82	0.45
1:A:623:C:N4	1:A:624:C:C4	2.84	0.45
1:A:544:G:OP1	4:D:62:GLN:NE2	2.40	0.45
1:A:878:G:H1'	8:H:3:THR:HG21	1.98	0.45
1:A:559:A:OP1	5:E:126:ARG:NH2	2.49	0.45
18:R:40:LEU:HB3	18:R:79:LEU:HD11	1.98	0.45
1:A:1338:G:H2'	1:A:1339:A:C8	2.51	0.45
3:C:126:ARG:O	3:C:128:PHE:N	2.50	0.45
1:A:1319:A:OP1	19:S:70:LYS:NZ	2.48	0.45
4:D:13:ARG:HD2	4:D:38:TYR:O	2.16	0.45
17:Q:68:ARG:N	17:Q:70:ARG:HH11	2.14	0.45
1:A:1031:G:H1'	1:A:1032:G:N1	2.31	0.45
1:A:1181:G:O2'	1:A:1182:G:N7	2.49	0.45
2:B:105:PHE:HE1	2:B:155:LEU:HD12	1.80	0.45
17:Q:80:GLY:O	17:Q:82:MET:N	2.49	0.45
1:A:488:C:H6	1:A:488:C:O5'	1.98	0.45
14:N:24:CYS:HB3	14:N:29:ARG:HB3	1.96	0.45
1:A:1368:G:OP2	9:I:112:LYS:HG3	2.17	0.45
1:A:686:U:HO2'	1:A:687:A:H8	1.63	0.45
1:A:1098:C:C2'	1:A:1099:G:O5'	2.65	0.45
1:A:1014:A:C2	1:A:1219:U:H1'	2.51	0.45
1:A:568:G:N2	1:A:883:C:C2	2.85	0.45
1:A:361:G:O5'	1:A:361:G:H8	1.99	0.45
15:O:74:ASP:O	15:O:76:GLU:N	2.49	0.45
1:A:448:A:C4	1:A:487:A:C2	3.04	0.45
1:A:1039:C:H6	1:A:1040:U:C5	2.34	0.45
2:B:98:LEU:N	2:B:98:LEU:HD23	2.32	0.45
5:E:28:PHE:O	5:E:47:LYS:HA	2.16	0.45
10:J:38:ILE:CD1	10:J:71:LEU:HD23	2.47	0.45
6:F:23:LYS:O	6:F:27:GLN:HG2	2.17	0.45
19:S:51:VAL:O	19:S:57:HIS:HA	2.17	0.45
1:A:936:C:H2'	1:A:937:A:O5'	2.16	0.45
13:M:11:ARG:HG2	13:M:12:ASN:N	2.32	0.45
1:A:684:A:N6	1:A:685:G:C6	2.85	0.45
1:A:622:A:C8	1:A:623:C:C6	3.04	0.45
1:A:1320:C:O2'	1:A:1321:C:H5'	2.16	0.45
1:A:1228:C:H2'	1:A:1229:A:C8	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:510:A:N3	1:A:543:C:H1'	2.31	0.45
8:H:39:LEU:HD11	8:H:137:VAL:HG21	1.98	0.45
1:A:513:C:C2'	1:A:514:C:O5'	2.65	0.45
1:A:1375:A:C5	1:A:1376:U:C5	3.04	0.45
1:A:922:G:N3	1:A:1398:A:H2	2.15	0.45
1:A:1226:C:H41	13:M:104:ARG:HG3	1.75	0.45
8:H:1:MET:O	8:H:2:LEU:CB	2.64	0.45
9:I:10:ARG:CD	9:I:75:ASP:HB3	2.46	0.45
9:I:8:GLY:HA2	9:I:79:LEU:HB3	1.98	0.45
1:A:1004:A:H2'	1:A:1038:C:O2	2.17	0.45
1:A:1072:G:H2'	1:A:1073:U:O4'	2.16	0.45
1:A:1281:U:O2	1:A:1281:U:O4'	2.34	0.45
1:A:1018:C:H6	1:A:1018:C:O5'	2.00	0.45
1:A:690:G:H2'	1:A:691:G:O4'	2.16	0.45
23:Y:34:I:H2'	23:Y:35:G:H8	1.81	0.45
9:I:40:LEU:HD13	9:I:70:LYS:HG2	1.99	0.45
1:A:1032:G:O2'	1:A:1033:G:O5'	2.30	0.45
13:M:82:MET:SD	13:M:83:ASP:N	2.90	0.45
4:D:184:LYS:HD2	4:D:186:LEU:HD12	1.97	0.45
3:C:39:ILE:HG22	3:C:40:ARG:N	2.32	0.45
16:P:59:TRP:O	16:P:60:LEU:C	2.55	0.45
2:B:130:ARG:NE	2:B:130:ARG:HA	2.32	0.45
6:F:100:ASN:O	6:F:101:ALA:HB3	2.16	0.45
1:A:1250:A:O4'	1:A:1250:A:P	2.74	0.45
3:C:11:ARG:CG	3:C:11:ARG:NH1	2.77	0.45
1:A:969:A:C2'	1:A:970:C:H5'	2.47	0.45
12:L:81:SER:O	12:L:82:VAL:HB	2.17	0.45
1:A:243:A:C2	1:A:246:A:C8	3.05	0.45
1:A:1507:A:C2	1:A:1508:G:C4	3.05	0.45
18:R:43:PHE:CD1	18:R:56:THR:HG22	2.50	0.44
1:A:1342:C:O2'	1:A:1343:G:H5'	2.16	0.44
14:N:53:LEU:HB3	14:N:56:VAL:CG2	2.47	0.44
1:A:1063:C:H3'	1:A:1064:G:H2'	2.00	0.44
19:S:50:ALA:HA	19:S:58:VAL:O	2.18	0.44
15:O:74:ASP:OD1	15:O:76:GLU:HB3	2.17	0.44
1:A:1249:C:C6	9:I:69:GLY:HA2	2.52	0.44
1:A:1032:G:HO2'	1:A:1033:G:C5'	2.29	0.44
1:A:624:C:H2'	1:A:625:G:C8	2.52	0.44
9:I:3:GLN:O	9:I:4:TYR:CD1	2.70	0.44
1:A:300:A:H8	1:A:300:A:O5'	2.00	0.44
2:B:236:TYR:HA	2:B:239:VAL:CG2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:24:GLU:OE2	17:Q:37:LYS:HD2	2.17	0.44
10:J:28:ARG:CG	10:J:34:VAL:HG21	2.47	0.44
18:R:53:ARG:HA	18:R:56:THR:OG1	2.17	0.44
1:A:376:G:P	16:P:67:THR:HG21	2.57	0.44
3:C:86:VAL:O	3:C:89:GLU:HB3	2.16	0.44
6:F:92:LYS:HZ2	6:F:92:LYS:HB2	1.82	0.44
2:B:17:PHE:HB3	2:B:44:LEU:HD21	1.99	0.44
12:L:90:VAL:HG11	12:L:93:LEU:HG	1.99	0.44
1:A:1207:G:H2'	1:A:1208:C:C6	2.52	0.44
1:A:1349:A:H2'	1:A:1350:A:O5'	2.18	0.44
1:A:1350:A:C5	1:A:1351:U:N3	2.85	0.44
3:C:11:ARG:HD2	3:C:15:THR:HG21	2.00	0.44
6:F:24:GLU:HG3	6:F:25:ILE:N	2.32	0.44
8:H:77:GLU:CG	8:H:78:GLN:N	2.80	0.44
4:D:5:ILE:H	4:D:115:ARG:HH12	1.64	0.44
4:D:148:VAL:HG12	4:D:149:ALA:N	2.32	0.44
1:A:817:C:N3	1:A:1529:G:O6	2.50	0.44
9:I:108:VAL:O	9:I:109:VAL:C	2.56	0.44
1:A:1055:A:C8	1:A:1206:G:N2	2.85	0.44
3:C:23:TYR:CE1	3:C:24:ALA:O	2.70	0.44
1:A:938:A:N6	1:A:939:G:C6	2.86	0.44
1:A:428:G:O4'	1:A:430:A:C8	2.71	0.44
1:A:414:A:C5	1:A:431:A:C2	3.06	0.44
2:B:77:ALA:O	2:B:79:ASP:N	2.49	0.44
1:A:1206:G:H4'	3:C:192:THR:O	2.17	0.44
1:A:1363(A):A:C4	1:A:1365:G:C6	3.06	0.44
1:A:1003:G:C2	1:A:1004:A:H1'	2.51	0.44
1:A:975:A:H4'	1:A:976:G:H5"	2.00	0.44
3:C:13:GLY:HA2	14:N:57:ARG:HE	1.82	0.44
1:A:985:C:O2	1:A:985:C:H2'	2.16	0.44
13:M:11:ARG:O	13:M:13:LYS:N	2.51	0.44
2:B:133:LYS:NZ	2:B:134:GLU:HG3	2.33	0.44
1:A:162:A:C5	1:A:163:C:H1'	2.53	0.44
11:K:52:GLY:O	11:K:55:LYS:HG3	2.17	0.44
1:A:714:G:H2'	1:A:715:A:C8	2.53	0.44
10:J:81:THR:O	10:J:83:GLU:N	2.46	0.44
1:A:1128:C:H2'	1:A:1139:G:O6	2.18	0.44
2:B:86:GLU:C	2:B:88:ALA:H	2.21	0.44
1:A:1030(C):G:C8	1:A:1030(C):G:C3'	3.00	0.44
8:H:44:PHE:CE2	8:H:109:ILE:HD12	2.50	0.44
13:M:68:GLY:HA2	13:M:71:ARG:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1148:U:O3'	9:I:14:VAL:HG11	2.18	0.44
1:A:1162:C:H2'	1:A:1163:C:H6	1.81	0.44
3:C:126:ARG:O	3:C:128:PHE:HD1	2.01	0.44
15:O:71:GLN:HB2	15:O:78:TYR:CD1	2.53	0.44
1:A:46:G:O2'	1:A:365:U:H1'	2.18	0.44
1:A:1137:C:O2'	1:A:1138:G:N2	2.49	0.44
15:O:61:GLY:O	15:O:62:GLN:C	2.55	0.44
1:A:982:U:H5"	14:N:6:LEU:HD21	2.00	0.44
1:A:1372:U:H2'	1:A:1373:G:C5'	2.48	0.44
1:A:973:G:O5'	1:A:973:G:H8	2.01	0.44
1:A:1197:G:OP1	1:A:1198:G:OP2	2.36	0.44
12:L:25:PRO:C	12:L:27:LEU:H	2.21	0.44
1:A:170:U:O2'	1:A:171:A:C5'	2.64	0.44
8:H:103:VAL:HG12	8:H:108:GLY:HA3	2.00	0.44
9:I:9:ARG:HB3	9:I:104:ARG:NH1	2.32	0.44
4:D:108:LEU:HB3	4:D:110:PHE:CE1	2.52	0.44
1:A:1236:A:O2'	1:A:1304:G:H4'	2.18	0.44
7:G:94:ARG:NH1	7:G:97:GLN:HG2	2.32	0.44
1:A:1015:A:N3	1:A:1218:C:O2'	2.49	0.44
13:M:56:LEU:O	13:M:57:ARG:C	2.56	0.44
1:A:1499:A:H2'	1:A:1500:A:H5'	2.00	0.43
15:O:87:ILE:HG22	15:O:88:ARG:H	1.81	0.43
7:G:17:VAL:HG12	7:G:18:TYR:CD1	2.53	0.43
1:A:1087:G:H2'	1:A:1088:G:C8	2.53	0.43
1:A:1392:G:N2	1:A:1502:A:C8	2.82	0.43
1:A:975:A:C5'	1:A:975:A:C8	3.00	0.43
8:H:87:SER:OG	8:H:92:ARG:HD2	2.18	0.43
1:A:815:A:O2'	1:A:1527:C:C1'	2.63	0.43
12:L:126:LYS:CA	12:L:129:ALA:O	2.66	0.43
11:K:108:ILE:HG22	11:K:109:VAL:N	2.33	0.43
1:A:1097:C:H2'	1:A:1098:C:C6	2.53	0.43
3:C:175:LEU:HD11	3:C:201:TYR:CE2	2.53	0.43
3:C:182:ILE:HA	3:C:202:ILE:O	2.18	0.43
3:C:156:ARG:O	3:C:159:GLY:N	2.51	0.43
1:A:653:A:P	8:H:56:LYS:NZ	2.91	0.43
7:G:60:LYS:O	7:G:64:GLN:HB2	2.18	0.43
1:A:1055:A:N6	1:A:1206:G:C5	2.86	0.43
1:A:1055:A:N6	1:A:1206:G:C6	2.86	0.43
11:K:48:ILE:HD13	11:K:48:ILE:N	2.32	0.43
2:B:115:LEU:HD21	2:B:153:ARG:CZ	2.48	0.43
6:F:21:LEU:HD12	6:F:24:GLU:OE2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:11:ARG:CG	13:M:12:ASN:N	2.82	0.43
17:Q:65:ILE:N	17:Q:65:ILE:HD12	2.33	0.43
10:J:90:LEU:H	10:J:91:PRO:CD	2.31	0.43
1:A:1327:C:OP1	21:U:20:LYS:N	2.51	0.43
1:A:1055:A:C5	1:A:1206:G:C2	3.07	0.43
1:A:84:U:C1'	1:A:88:A:OP2	2.56	0.43
4:D:5:ILE:O	4:D:5:ILE:CG2	2.66	0.43
3:C:108:ASN:ND2	3:C:144:SER:HB3	2.34	0.43
1:A:416:G:C5	1:A:417:C:C4	3.07	0.43
9:I:99:LEU:HB3	9:I:101:PHE:CE1	2.53	0.43
6:F:99:ALA:O	6:F:100:ASN:HB2	2.18	0.43
1:A:602:A:C2	1:A:637:G:C2	3.06	0.43
1:A:108:G:O4'	1:A:108:G:N3	2.50	0.43
1:A:1039:C:C5	1:A:1040:U:C5	3.06	0.43
3:C:134:ILE:HG23	3:C:151:VAL:HB	2.00	0.43
2:B:71:VAL:HG23	2:B:164:VAL:HG13	2.01	0.43
1:A:540:G:H2'	1:A:541:G:O4'	2.19	0.43
10:J:6:ILE:HA	10:J:97:GLU:O	2.17	0.43
2:B:130:ARG:O	2:B:131:PRO:C	2.57	0.43
20:T:48:LYS:HB2	20:T:52:ALA:HB2	1.99	0.43
2:B:75:LYS:HB3	2:B:76:GLN:HE21	1.82	0.43
1:A:1091:U:O2	1:A:1093:A:H8	1.97	0.43
1:A:803:G:C5	1:A:804:U:C4	3.06	0.43
1:A:815:A:OP2	1:A:816:A:H5'	2.19	0.43
8:H:104:ARG:O	8:H:105:ARG:C	2.57	0.43
17:Q:59:ILE:HD13	17:Q:59:ILE:HA	1.67	0.43
1:A:252:U:C4	1:A:253:U:O4	2.71	0.43
17:Q:90:ILE:O	17:Q:94:ASN:N	2.45	0.43
8:H:55:GLY:C	8:H:56:LYS:HD2	2.39	0.43
7:G:72:ARG:HD2	7:G:142:GLU:OE1	2.17	0.43
2:B:62:ALA:O	2:B:65:GLY:N	2.49	0.43
1:A:1285:A:O4'	1:A:1285:A:OP1	2.37	0.43
2:B:86:GLU:C	2:B:88:ALA:N	2.72	0.43
1:A:1481:U:H2'	1:A:1482:G:O4'	2.19	0.43
5:E:102:ALA:HB2	5:E:120:THR:HG21	2.01	0.43
1:A:1069:C:HO2'	1:A:1192:C:H1'	1.83	0.43
3:C:188:LEU:HD13	3:C:195:VAL:CG1	2.47	0.43
1:A:429:U:O2	1:A:430:A:C8	2.71	0.43
1:A:1281:U:OP2	1:A:1282:C:N4	2.52	0.43
10:J:5:ARG:O	10:J:99:LYS:HB2	2.19	0.43
4:D:57:ARG:NH2	4:D:205:GLU:OE2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:53:LEU:HA	17:Q:53:LEU:HD13	1.67	0.43
1:A:461:A:O5'	1:A:461:A:H2'	2.19	0.43
13:M:20:THR:C	13:M:22:ILE:H	2.21	0.43
1:A:1499:A:H5'	1:A:1499:A:C8	2.53	0.43
1:A:1140:C:O2'	1:A:1141:C:OP2	2.33	0.43
1:A:1168:A:H2'	1:A:1169:A:C8	2.54	0.43
4:D:150:GLU:HA	4:D:153:ARG:NE	2.33	0.43
15:O:74:ASP:C	15:O:76:GLU:H	2.22	0.43
4:D:104:VAL:HG21	4:D:140:VAL:HG21	2.01	0.43
14:N:23:ARG:O	14:N:24:CYS:C	2.57	0.43
1:A:1280:A:C5'	10:J:40:LEU:HD13	2.49	0.43
1:A:623:C:N4	1:A:624:C:N4	2.67	0.43
1:A:975:A:H4'	1:A:976:G:C5'	2.49	0.43
1:A:537:G:H2'	1:A:538:G:C8	2.53	0.43
1:A:942:G:N3	1:A:942:G:H2'	2.34	0.43
9:I:111:ARG:O	9:I:113:LYS:HD2	2.18	0.43
1:A:676:A:H1'	11:K:115:PRO:HB3	2.01	0.43
6:F:1:MET:HB2	6:F:67:MET:C	2.39	0.43
4:D:154:ASN:N	4:D:154:ASN:OD1	2.52	0.43
1:A:1033:G:O2'	1:A:1034:G:OP1	2.34	0.43
2:B:129:GLU:O	2:B:130:ARG:HB2	2.19	0.43
7:G:113:GLU:HG2	7:G:119:ARG:HG2	2.01	0.43
3:C:117:ALA:HB1	3:C:187:ALA:HB2	2.01	0.43
23:Y:34:I:O2'	23:Y:35:G:P	2.77	0.42
1:A:1365:G:C6	1:A:1366:C:C4	3.06	0.42
2:B:61:LEU:CD2	2:B:66:GLY:HA3	2.46	0.42
1:A:1133:G:H2'	1:A:1134:G:C8	2.53	0.42
1:A:33:A:O2'	1:A:363:A:H1'	2.19	0.42
1:A:457:C:H2'	1:A:458:C:C6	2.52	0.42
3:C:111:LEU:CD2	3:C:144:SER:HB2	2.49	0.42
1:A:1161:C:H2'	1:A:1162:C:C6	2.54	0.42
1:A:653:A:P	8:H:56:LYS:HZ2	2.42	0.42
1:A:278:G:OP2	17:Q:41:LYS:NZ	2.42	0.42
13:M:39:ILE:HD13	13:M:52:GLU:HB3	2.01	0.42
9:I:36:TYR:HD2	9:I:37:PHE:CE1	2.37	0.42
1:A:1309:G:H5'	13:M:78:ILE:HD11	2.01	0.42
6:F:72:VAL:CG2	6:F:90:VAL:HG11	2.49	0.42
1:A:664:G:N2	1:A:741:G:H1	2.06	0.42
3:C:72:LYS:HG3	3:C:75:VAL:CG2	2.46	0.42
4:D:111:ALA:HB1	4:D:116:GLN:OE1	2.18	0.42
1:A:415:A:N6	1:A:416:G:C6	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:11:ARG:HG2	13:M:12:ASN:HB2	2.01	0.42
5:E:8:GLU:OE2	5:E:63:ARG:NH2	2.46	0.42
13:M:78:ILE:HA	13:M:81:LEU:HD12	2.01	0.42
11:K:61:ALA:HB2	11:K:90:GLY:HA3	2.00	0.42
1:A:659:U:OP2	15:O:8:LYS:NZ	2.46	0.42
1:A:942:G:C4	1:A:943:U:C5	3.07	0.42
1:A:597:G:H5"	1:A:598:U:OP2	2.19	0.42
1:A:613:C:C2	1:A:628:G:N2	2.87	0.42
1:A:485:G:HO2'	1:A:486:U:P	2.40	0.42
1:A:530:G:H1'	23:Y:35:G:O2'	2.20	0.42
1:A:62:U:H5"	1:A:385:C:H1'	2.00	0.42
2:B:98:LEU:N	2:B:98:LEU:CD2	2.81	0.42
1:A:1416:G:H2'	1:A:1417:G:H5'	2.00	0.42
2:B:107:THR:C	2:B:109:SER:N	2.72	0.42
15:O:86:GLY:C	15:O:87:ILE:HG13	2.39	0.42
1:A:1134:G:H8	1:A:1134:G:O5'	2.02	0.42
1:A:1134:G:C5	1:A:1135:U:C5	3.08	0.42
1:A:936:C:C2'	1:A:937:A:O5'	2.67	0.42
16:P:4:ILE:N	16:P:4:ILE:CD1	2.82	0.42
7:G:28:ASN:O	7:G:31:MET:HB3	2.19	0.42
2:B:208:ILE:H	2:B:208:ILE:HD12	1.84	0.42
1:A:1306:A:N6	1:A:1331:G:H1'	2.34	0.42
1:A:1145:C:C4'	1:A:1146:A:OP1	2.68	0.42
19:S:6:LYS:HD2	19:S:7:LYS:HE3	2.01	0.42
10:J:96:ILE:N	10:J:96:ILE:CD1	2.83	0.42
1:A:1492:A:H1'	22:X:5:A:HO2'	1.85	0.42
4:D:196:LEU:HD23	4:D:197:PRO:HD2	2.00	0.42
14:N:26:ARG:NH1	14:N:47:LEU:CD2	2.83	0.42
2:B:9:GLU:CG	2:B:10:LEU:N	2.82	0.42
12:L:60:LEU:HD11	12:L:85:ILE:HD12	2.01	0.42
1:A:819:A:H5"	1:A:819:A:C8	2.55	0.42
20:T:24:LEU:HD22	20:T:24:LEU:HA	1.70	0.42
1:A:1203:C:H6	1:A:1203:C:O5'	2.02	0.42
4:D:18:LYS:HD3	4:D:31:CYS:CB	2.46	0.42
1:A:458:C:C2	1:A:460:G:C8	3.07	0.42
10:J:8:LEU:CD1	10:J:20:ALA:CB	2.98	0.42
8:H:9:MET:O	8:H:10:LEU:C	2.58	0.42
1:A:502:G:C6	1:A:503:C:C4	3.07	0.42
1:A:173:U:H6	1:A:198:G:HO2'	1.61	0.42
2:B:9:GLU:HG3	2:B:10:LEU:N	2.33	0.42
1:A:885:G:N3	1:A:914:A:C2	2.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:113:ALA:N	3:C:114:PRO:CD	2.82	0.42
9:I:65:VAL:HG22	9:I:73:GLN:HG2	2.02	0.42
7:G:21:VAL:HG23	7:G:22:LEU:N	2.35	0.42
16:P:23:ASP:OD1	16:P:24:ALA:N	2.52	0.42
16:P:26:ARG:HD3	16:P:31:LYS:N	2.35	0.42
4:D:145:GLU:OE1	4:D:182:LYS:HD2	2.20	0.42
12:L:33:ARG:HA	12:L:33:ARG:HD3	1.91	0.42
1:A:1057:G:C5	1:A:1204:A:C2	3.08	0.42
1:A:1349:A:C6	1:A:1374:A:C8	3.08	0.42
1:A:1240:U:H4'	1:A:1241:G:OP2	2.19	0.42
1:A:1031:G:H1'	1:A:1032:G:C2	2.55	0.42
20:T:67:ALA:O	20:T:73:HIS:CE1	2.72	0.42
2:B:153:ARG:CG	2:B:154:LEU:HD23	2.49	0.42
1:A:255:G:O6	1:A:266:G:O6	2.37	0.42
1:A:968:A:H4'	1:A:969:A:OP2	2.19	0.42
9:I:48:GLU:N	9:I:49:PRO:HD3	2.35	0.42
1:A:1067:A:O4'	1:A:1068:G:O4'	2.38	0.42
4:D:113:SER:HB3	4:D:116:GLN:H	1.84	0.42
1:A:639:G:H2'	1:A:640:A:H5'	2.01	0.42
9:I:10:ARG:HD3	9:I:75:ASP:HB3	2.02	0.42
9:I:108:VAL:O	9:I:110:GLU:N	2.53	0.42
1:A:1332:A:C2	1:A:1333:A:C4	3.08	0.42
11:K:74:ALA:C	11:K:76:GLY:H	2.23	0.42
1:A:189(D):C:O5'	1:A:189(D):C:H6	2.03	0.42
14:N:36:PHE:CG	14:N:36:PHE:O	2.72	0.42
1:A:1145:C:O2'	1:A:1146:A:H5'	2.20	0.42
1:A:401:C:C2'	1:A:402:G:H5'	2.49	0.42
10:J:55:LYS:O	10:J:56:HIS:CG	2.72	0.42
17:Q:27:PHE:O	17:Q:35:VAL:HA	2.19	0.42
9:I:99:LEU:CB	9:I:101:PHE:CE1	3.03	0.42
1:A:738:C:P	6:F:92:LYS:HZ3	2.42	0.42
10:J:13:HIS:HB3	10:J:68:HIS:CE1	2.55	0.42
1:A:1435:G:H2'	1:A:1436:U:C6	2.55	0.42
1:A:743:U:H2'	1:A:744:C:C6	2.55	0.42
2:B:90:MET:CE	2:B:90:MET:HA	2.50	0.42
10:J:49:VAL:HG22	14:N:41:ARG:HB2	2.02	0.42
5:E:143:ARG:NH1	8:H:77:GLU:OE2	2.53	0.42
5:E:122:GLU:O	5:E:123:LEU:HD23	2.20	0.42
1:A:353:A:H8	1:A:353:A:C5'	2.33	0.42
1:A:1175:G:C6	1:A:1176:A:N7	2.88	0.42
1:A:799:G:H2'	1:A:800:G:H5'	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:A:OP2	20:T:70:SER:OG	2.32	0.42
1:A:1186:G:H21	14:N:61:TRP:C	2.23	0.42
2:B:72:GLY:HA2	2:B:165:VAL:HG22	2.02	0.42
2:B:216:SER:O	2:B:219:VAL:N	2.48	0.41
1:A:1092:A:C6	1:A:1093:A:C6	3.08	0.41
3:C:11:ARG:O	3:C:13:GLY:N	2.53	0.41
5:E:9:LYS:HD2	5:E:10:MET:N	2.35	0.41
5:E:91:LEU:HA	5:E:91:LEU:HD12	1.96	0.41
2:B:223:ILE:O	2:B:225:ALA:N	2.52	0.41
2:B:142:LEU:HD23	2:B:142:LEU:O	2.20	0.41
16:P:58:TYR:O	16:P:61:SER:OG	2.21	0.41
6:F:28:ARG:O	6:F:32:ASN:HB2	2.19	0.41
2:B:21:ARG:HD2	2:B:39:ILE:HG23	2.01	0.41
1:A:1386:G:H2'	1:A:1387:G:H8	1.85	0.41
3:C:66:VAL:O	3:C:66:VAL:HG12	2.20	0.41
12:L:47:LYS:HG3	12:L:48:PRO:HD3	2.02	0.41
9:I:58:ARG:CZ	9:I:58:ARG:HB2	2.50	0.41
3:C:94:LEU:HD12	3:C:95:THR:N	2.35	0.41
1:A:89:C:O5'	1:A:89:C:H6	2.03	0.41
1:A:1056:U:O4	1:A:1200:C:C2	2.73	0.41
14:N:20:ALA:O	14:N:21:TYR:HB3	2.21	0.41
1:A:1353:G:O2'	1:A:1354:C:H5'	2.21	0.41
1:A:1321:C:C6	1:A:1322:C:C6	3.08	0.41
1:A:992:U:O2'	1:A:993:G:OP2	2.30	0.41
17:Q:5:VAL:HG22	17:Q:60:ILE:HD12	2.02	0.41
1:A:1095:U:H5"	1:A:1109:C:O2	2.20	0.41
1:A:1016:A:H2'	1:A:1017:G:O4'	2.20	0.41
10:J:8:LEU:HD13	10:J:20:ALA:CB	2.50	0.41
5:E:60:TYR:CE1	5:E:64:ARG:HD2	2.55	0.41
1:A:658:G:O2'	15:O:22:THR:HG21	2.20	0.41
1:A:1034:G:N3	1:A:1034:G:C2'	2.84	0.41
1:A:9:G:H2'	1:A:9:G:N3	2.35	0.41
3:C:11:ARG:C	3:C:13:GLY:H	2.23	0.41
3:C:14:ILE:CG2	3:C:15:THR:N	2.78	0.41
1:A:1417:G:N2	1:A:1482:G:H2'	2.36	0.41
16:P:55:ARG:O	16:P:58:TYR:HB3	2.20	0.41
1:A:883:C:O2'	1:A:884:U:H5'	2.20	0.41
17:Q:48:GLU:O	17:Q:49:GLU:C	2.59	0.41
9:I:11:LYS:O	9:I:11:LYS:CG	2.68	0.41
1:A:1495:U:H2'	1:A:1496:C:C6	2.56	0.41
12:L:110:VAL:H	12:L:122:THR:HG22	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1356:G:N2	1:A:1367:C:C2	2.89	0.41
7:G:88:PRO:HB3	7:G:145:ALA:HB1	2.02	0.41
1:A:1416:G:C2'	1:A:1417:G:H5'	2.51	0.41
5:E:88:LYS:HB3	5:E:123:LEU:HB2	2.02	0.41
1:A:1181:G:C2	1:A:1182:G:N2	2.88	0.41
10:J:8:LEU:CD1	10:J:20:ALA:HB1	2.51	0.41
3:C:114:PRO:O	3:C:118:GLN:HG3	2.20	0.41
1:A:56:U:H2'	1:A:57:G:C8	2.55	0.41
1:A:1030(C):G:C8	1:A:1030(C):G:H3'	2.55	0.41
3:C:72:LYS:CA	3:C:72:LYS:HE3	2.51	0.41
3:C:4:LYS:HB2	3:C:4:LYS:HE2	1.89	0.41
2:B:15:VAL:C	2:B:16:HIS:CG	2.93	0.41
1:A:407:G:H2'	1:A:408:A:C8	2.55	0.41
1:A:1160:G:O2'	1:A:1161:C:H5'	2.21	0.41
5:E:135:THR:O	5:E:139:LEU:HG	2.21	0.41
9:I:33:PHE:CZ	9:I:37:PHE:HD2	2.39	0.41
1:A:23:C:O2'	1:A:24:U:H5'	2.20	0.41
1:A:106:C:H2'	1:A:107:G:O4'	2.20	0.41
1:A:1392:G:O2'	1:A:1393:U:H5'	2.20	0.41
9:I:19:LEU:N	9:I:19:LEU:HD23	2.35	0.41
9:I:4:TYR:CD1	9:I:88:TYR:CD1	3.08	0.41
8:H:77:GLU:HG3	8:H:78:GLN:H	1.86	0.41
1:A:382:A:N1	1:A:383:A:C5	2.89	0.41
3:C:36:ASP:O	3:C:40:ARG:HG3	2.21	0.41
1:A:282:A:C4	1:A:283:C:C6	3.08	0.41
12:L:35:GLY:HA3	12:L:58:VAL:HG11	2.03	0.41
11:K:33:THR:HB	11:K:38:ASN:O	2.20	0.41
16:P:59:TRP:O	16:P:62:VAL:N	2.49	0.41
9:I:85:LEU:HB2	9:I:92:TYR:HD2	1.86	0.41
1:A:584:G:H5'	17:Q:91:ARG:NH2	2.35	0.41
13:M:66:LEU:O	13:M:69:GLU:N	2.54	0.41
15:O:44:LYS:O	15:O:47:LYS:NZ	2.37	0.41
14:N:42:ILE:O	14:N:44:LEU:N	2.54	0.41
1:A:1130:A:C4	1:A:1146:A:C2	3.09	0.41
17:Q:81:ARG:H	17:Q:81:ARG:HD2	1.86	0.41
20:T:73:HIS:O	20:T:74:LYS:HG3	2.20	0.41
1:A:266:G:C8	1:A:266:G:H5'	2.56	0.41
8:H:63:LEU:N	8:H:63:LEU:HD13	2.36	0.41
1:A:687:A:C2	1:A:700:G:N3	2.88	0.41
1:A:283:C:O2	1:A:283:C:H2'	2.20	0.41
1:A:864:A:C2	1:A:917:G:N3	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:123:GLN:O	3:C:128:PHE:HB2	2.20	0.41
2:B:129:GLU:CD	2:B:130:ARG:HE	2.24	0.41
3:C:113:ALA:HB3	3:C:114:PRO:HD3	2.01	0.41
4:D:70:ILE:HD12	4:D:100:ARG:CZ	2.51	0.41
1:A:244:U:O4	1:A:906:G:H1'	2.21	0.41
12:L:83:VAL:CG2	12:L:100:ILE:HG23	2.51	0.41
12:L:77:LEU:HD21	12:L:107:ALA:HA	2.02	0.41
13:M:106:ASN:O	13:M:107:ALA:HB3	2.20	0.41
1:A:620:C:C2	4:D:135:LEU:HG	2.55	0.41
1:A:813:U:H5"	1:A:903:G:O3'	2.20	0.41
1:A:911:U:H2'	1:A:912:C:C6	2.56	0.41
13:M:40:ASN:HA	13:M:41:PRO:HD3	1.91	0.41
4:D:9:CYS:HA	4:D:12:CYS:CB	2.50	0.41
1:A:1328:C:H2'	1:A:1329:A:O4'	2.20	0.41
1:A:1069:C:O3'	5:E:25:ARG:NH1	2.54	0.41
5:E:80:ILE:HG23	8:H:104:ARG:HH22	1.86	0.41
6:F:64:GLN:O	6:F:65:VAL:HG12	2.21	0.41
1:A:1195:C:H5"	1:A:1196:U:P	2.61	0.41
4:D:110:PHE:CD1	4:D:110:PHE:N	2.89	0.41
15:O:53:HIS:O	15:O:57:LEU:HD23	2.21	0.41
2:B:124:SER:OG	2:B:126:GLU:OE1	2.39	0.41
10:J:87:THR:O	10:J:88:LEU:HB2	2.21	0.41
4:D:78:LEU:CD2	4:D:96:LEU:HB3	2.51	0.41
1:A:1394:A:H4'	1:A:1395:C:OP2	2.22	0.41
1:A:1054:C:OP2	1:A:1197:G:OP2	2.38	0.40
2:B:51:LEU:CD2	2:B:55:PHE:CE2	3.01	0.40
2:B:209:ARG:HG2	2:B:209:ARG:H	1.70	0.40
1:A:298:A:H2'	1:A:299:G:O4'	2.21	0.40
19:S:7:LYS:HA	19:S:7:LYS:HD3	1.75	0.40
2:B:118:LEU:HB2	2:B:142:LEU:HD12	2.03	0.40
3:C:48:TYR:HE1	3:C:118:GLN:NE2	2.20	0.40
7:G:101:LEU:O	7:G:105:VAL:HG23	2.21	0.40
9:I:41:VAL:O	9:I:41:VAL:HG12	2.20	0.40
1:A:1129:C:O3'	1:A:1131:G:OP2	2.39	0.40
1:A:1030(B):C:C2	1:A:1031:G:C2	3.08	0.40
4:D:62:GLN:HA	4:D:62:GLN:OE1	2.21	0.40
1:A:980:C:H5'	1:A:980:C:H6	1.86	0.40
6:F:27:GLN:O	6:F:31:GLU:HB2	2.21	0.40
20:T:98:PRO:HD2	20:T:99:LEU:HG	2.04	0.40
1:A:938:A:C6	1:A:939:G:C5	3.09	0.40
1:A:107:G:N7	20:T:15:ARG:NH2	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:G:N3	1:A:196:A:H2	2.20	0.40
6:F:60:PHE:CZ	18:R:78:LEU:HD21	2.56	0.40
12:L:119:LYS:C	12:L:121:GLY:H	2.25	0.40
10:J:82:ILE:O	10:J:82:ILE:HG22	2.20	0.40
1:A:59:A:N3	1:A:59:A:H2'	2.36	0.40
1:A:1029:C:O2	1:A:1033:G:O6	2.40	0.40
1:A:623:C:C4	1:A:624:C:C5	3.09	0.40
19:S:4:SER:C	19:S:5:LEU:HD22	2.41	0.40
14:N:53:LEU:O	14:N:56:VAL:HG23	2.21	0.40
10:J:26:ALA:CB	10:J:85:LEU:HD21	2.50	0.40
9:I:78:LYS:HE3	9:I:101:PHE:HD2	1.86	0.40
9:I:33:PHE:CE1	9:I:47:LEU:HD11	2.57	0.40
11:K:61:ALA:CB	11:K:90:GLY:HA3	2.52	0.40
1:A:786:G:C2	1:A:797:C:C2	3.09	0.40
20:T:14:LYS:HA	20:T:17:ARG:CZ	2.51	0.40
20:T:34:LYS:O	20:T:36:LEU:N	2.54	0.40
6:F:22:GLU:OE2	6:F:22:GLU:HA	2.21	0.40
21:U:25:LYS:HD3	21:U:25:LYS:HA	1.93	0.40
18:R:84:LYS:HD3	18:R:84:LYS:N	2.37	0.40
14:N:41:ARG:HG3	14:N:42:ILE:N	2.37	0.40
1:A:1207:G:H2'	1:A:1208:C:H6	1.86	0.40
1:A:84:U:C2'	1:A:84:U:O2	2.69	0.40
1:A:1029:C:H6	1:A:1029:C:O5'	2.05	0.40
3:C:64:VAL:HG23	3:C:99:VAL:HA	2.02	0.40
1:A:538:G:H5"	12:L:114:LYS:HB2	2.04	0.40
1:A:1162:C:C2	1:A:1175:G:N2	2.90	0.40
5:E:139:LEU:O	5:E:141:GLN:N	2.55	0.40
1:A:1131:G:C6	1:A:1132:C:N4	2.90	0.40
6:F:80:ARG:NH1	6:F:88:VAL:HB	2.35	0.40
2:B:42:ILE:HD11	2:B:203:GLY:HA2	2.04	0.40
1:A:483:C:O5'	1:A:483:C:H6	2.05	0.40
1:A:1223:C:H5"	1:A:1224:G:H5"	2.03	0.40
1:A:1251:A:OP2	1:A:1251:A:H3'	2.21	0.40
1:A:1306:A:C5	1:A:1307:U:C5	3.09	0.40
1:A:974:A:H8	1:A:974:A:OP1	2.05	0.40
1:A:926:G:C6	1:A:1505:G:C6	3.10	0.40
1:A:1055:A:N7	1:A:1206:G:C2	2.89	0.40
1:A:1206:G:C4	1:A:1207:G:C8	3.10	0.40
1:A:975:A:H5'	1:A:975:A:C8	2.55	0.40
1:A:1531:A:O2'	1:A:1532:U:P	2.79	0.40
20:T:72:LEU:O	20:T:72:LEU:HD13	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:789:U:O2'	1:A:791:G:N7	2.37	0.40
2:B:223:ILE:C	2:B:225:ALA:N	2.75	0.40
1:A:382:A:O2'	1:A:383:A:H5'	2.22	0.40
2:B:9:GLU:N	2:B:12:GLU:OE1	2.55	0.40
14:N:13:THR:HA	14:N:14:PRO:HD3	1.92	0.40
3:C:165:THR:HG22	3:C:165:THR:O	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:G:O2'	1:A:1340:A:O2'[3_445]	2.15	0.05

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	232/234 (99%)	167 (72%)	51 (22%)	14 (6%)	2 14
3	C	204/206 (99%)	139 (68%)	45 (22%)	20 (10%)	1 4
4	D	206/208 (99%)	164 (80%)	26 (13%)	16 (8%)	1 7
5	E	148/150 (99%)	135 (91%)	9 (6%)	4 (3%)	6 37
6	F	99/101 (98%)	83 (84%)	13 (13%)	3 (3%)	5 34
7	G	153/155 (99%)	113 (74%)	29 (19%)	11 (7%)	1 9
8	H	136/138 (99%)	117 (86%)	14 (10%)	5 (4%)	4 27
9	I	125/127 (98%)	86 (69%)	29 (23%)	10 (8%)	1 7
10	J	96/98 (98%)	78 (81%)	11 (12%)	7 (7%)	1 9
11	K	117/119 (98%)	95 (81%)	17 (14%)	5 (4%)	3 23
12	L	123/125 (98%)	96 (78%)	14 (11%)	13 (11%)	0 3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
13	M	118/120 (98%)	85 (72%)	22 (19%)	11 (9%)	1 4
14	N	58/60 (97%)	31 (53%)	18 (31%)	9 (16%)	0 1
15	O	86/88 (98%)	75 (87%)	9 (10%)	2 (2%)	8 42
16	P	81/83 (98%)	68 (84%)	12 (15%)	1 (1%)	16 58
17	Q	97/99 (98%)	86 (89%)	8 (8%)	3 (3%)	5 32
18	R	68/70 (97%)	63 (93%)	4 (6%)	1 (2%)	13 53
19	S	76/78 (97%)	53 (70%)	16 (21%)	7 (9%)	1 4
20	T	97/99 (98%)	66 (68%)	16 (16%)	15 (16%)	0 1
21	U	22/24 (92%)	19 (86%)	2 (9%)	1 (4%)	3 22
All	All	2342/2382 (98%)	1819 (78%)	365 (16%)	158 (7%)	1 11

All (158) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	17	PHE
2	B	20	GLU
2	B	78	GLN
2	B	130	ARG
2	B	226	ARG
3	C	24	ALA
3	C	36	ASP
3	C	47	LEU
3	C	67	THR
3	C	127	ARG
3	C	154	SER
3	C	189	ALA
3	C	206	GLU
4	D	3	ARG
4	D	10	ARG
4	D	14	ARG
4	D	26	CYS
4	D	29	PRO
4	D	30	LYS
4	D	32	ALA
7	G	33	ASP
7	G	155	ARG
8	H	97	VAL
8	H	105	ARG
9	I	56	LEU

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Mol	Chain	Res	Type
9	I	81	ILE
9	I	109	VAL
9	I	118	LYS
10	J	88	LEU
12	L	27	LEU
12	L	28	LYS
12	L	29	GLY
12	L	30	ALA
12	L	47	LYS
13	M	46	LYS
13	M	83	ASP
13	M	91	ARG
13	M	113	PRO
14	N	3	ARG
14	N	26	ARG
14	N	28	GLY
17	Q	49	GLU
17	Q	81	ARG
19	S	6	LYS
19	S	10	PHE
19	S	46	GLY
20	T	49	ALA
20	T	73	HIS
20	T	74	LYS
20	T	75	ASN
20	T	87	LYS
20	T	98	PRO
20	T	100	ILE
2	B	15	VAL
2	B	105	PHE
2	B	131	PRO
2	B	224	GLN
2	B	239	VAL
3	C	12	LEU
3	C	53	ALA
3	C	96	GLY
3	C	101	LEU
3	C	157	ILE
4	D	58	LEU
4	D	59	ARG
5	E	22	GLY
5	E	73	ASN

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Mol	Chain	Res	Type
5	E	140	ARG
7	G	7	ALA
7	G	52	GLU
7	G	81	GLY
7	G	137	LYS
8	H	2	LEU
9	I	40	LEU
9	I	89	ASN
9	I	93	ARG
9	I	119	ALA
9	I	125	TYR
10	J	59	SER
10	J	82	ILE
11	K	12	ARG
11	K	91	ARG
11	K	103	LEU
12	L	91	LYS
12	L	109	GLY
13	M	12	ASN
13	M	67	GLU
14	N	44	LEU
15	O	88	ARG
19	S	30	LEU
19	S	42	PRO
19	S	45	VAL
20	T	47	GLY
20	T	72	LEU
20	T	77	ALA
20	T	99	LEU
2	B	9	GLU
2	B	195	ASP
2	B	232	PRO
3	C	20	SER
4	D	4	TYR
4	D	12	CYS
4	D	102	ASP
4	D	125	HIS
4	D	168	ARG
6	F	38	GLU
7	G	136	LYS
8	H	70	GLN
10	J	57	LYS

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Mol	Chain	Res	Type
12	L	48	PRO
12	L	79	GLU
13	M	89	GLY
14	N	14	PRO
14	N	23	ARG
17	Q	34	LYS
20	T	97	ALA
21	U	3	LYS
2	B	132	LYS
3	C	4	LYS
3	C	81	GLY
7	G	152	ALA
9	I	55	ALA
10	J	36	GLY
10	J	55	LYS
10	J	90	LEU
11	K	27	ASN
11	K	109	VAL
12	L	45	PRO
12	L	51	ALA
13	M	4	ILE
13	M	120	LYS
14	N	16	PHE
14	N	41	ARG
18	R	36	ASN
20	T	50	GLU
20	T	86	ARG
3	C	16	ARG
12	L	82	VAL
13	M	6	GLY
14	N	46	GLU
16	P	78	GLY
19	S	67	VAL
20	T	45	GLN
4	D	5	ILE
4	D	92	VAL
5	E	8	GLU
6	F	70	ASP
8	H	73	ASP
13	M	10	PRO
3	C	39	ILE
3	C	80	GLY

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Mol	Chain	Res	Type
7	G	112	PRO
7	G	17	VAL
15	O	75	PRO
6	F	56	PRO
7	G	42	ILE
12	L	121	GLY
3	C	14	ILE

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
2	B	202/202 (100%)	153 (76%)	49 (24%)	1 3
3	C	160/160 (100%)	126 (79%)	34 (21%)	1 6
4	D	180/180 (100%)	141 (78%)	39 (22%)	1 6
5	E	115/115 (100%)	94 (82%)	21 (18%)	2 10
6	F	90/90 (100%)	76 (84%)	14 (16%)	3 14
7	G	126/126 (100%)	101 (80%)	25 (20%)	1 8
8	H	119/119 (100%)	97 (82%)	22 (18%)	2 10
9	I	98/98 (100%)	78 (80%)	20 (20%)	1 7
10	J	88/88 (100%)	66 (75%)	22 (25%)	1 3
11	K	90/90 (100%)	73 (81%)	17 (19%)	2 10
12	L	104/104 (100%)	81 (78%)	23 (22%)	1 6
13	M	96/96 (100%)	64 (67%)	32 (33%)	0 0
14	N	49/49 (100%)	41 (84%)	8 (16%)	3 13
15	O	79/79 (100%)	72 (91%)	7 (9%)	12 42
16	P	72/72 (100%)	57 (79%)	15 (21%)	1 7
17	Q	94/94 (100%)	81 (86%)	13 (14%)	4 20
18	R	61/61 (100%)	53 (87%)	8 (13%)	5 23
19	S	69/69 (100%)	54 (78%)	15 (22%)	1 6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
20	T	76/76 (100%)	64 (84%)	12 (16%)	3 14
21	U	19/19 (100%)	16 (84%)	3 (16%)	3 14
All	All	1987/1987 (100%)	1588 (80%)	399 (20%)	1 8

All (399) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	7	VAL
2	B	8	LYS
2	B	9	GLU
2	B	11	LEU
2	B	15	VAL
2	B	17	PHE
2	B	22	LYS
2	B	24	TRP
2	B	27	LYS
2	B	44	LEU
2	B	45	GLN
2	B	48	MET
2	B	67	THR
2	B	74	LYS
2	B	80	ILE
2	B	86	GLU
2	B	90	MET
2	B	96	ARG
2	B	97	TRP
2	B	98	LEU
2	B	102	LEU
2	B	103	THR
2	B	108	ILE
2	B	110	GLN
2	B	112	VAL
2	B	115	LEU
2	B	119	GLU
2	B	127	ILE
2	B	133	LYS
2	B	144	ARG
2	B	145	LEU
2	B	154	LEU
2	B	155	LEU
2	B	156	LYS

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Mol	Chain	Res	Type
2	B	157	ARG
2	B	164	VAL
2	B	168	THR
2	B	172	ILE
2	B	175	ARG
2	B	179	LYS
2	B	185	ILE
2	B	187	LEU
2	B	196	LEU
2	B	208	ILE
2	B	209	ARG
2	B	210	SER
2	B	212	GLN
2	B	221	LEU
2	B	238	LEU
3	C	3	ASN
3	C	11	ARG
3	C	16	ARG
3	C	17	ASP
3	C	26	LYS
3	C	27	LYS
3	C	28	GLN
3	C	36	ASP
3	C	38	ARG
3	C	40	ARG
3	C	54	ARG
3	C	62	ASP
3	C	64	VAL
3	C	72	LYS
3	C	79	ARG
3	C	93	LYS
3	C	98	ASN
3	C	101	LEU
3	C	122	GLU
3	C	127	ARG
3	C	128	PHE
3	C	130	VAL
3	C	131	ARG
3	C	139	GLN
3	C	143	GLU
3	C	166	GLU
3	C	167	TRP

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Mol	Chain	Res	Type
3	C	175	LEU
3	C	178	LEU
3	C	188	LEU
3	C	191	THR
3	C	192	THR
3	C	196	LEU
3	C	204	LEU
4	D	3	ARG
4	D	10	ARG
4	D	11	LEU
4	D	19	LEU
4	D	24	GLU
4	D	27	TYR
4	D	30	LYS
4	D	33	MET
4	D	49	ARG
4	D	50	ARG
4	D	58	LEU
4	D	73	ARG
4	D	76	ARG
4	D	83	SER
4	D	84	LYS
4	D	86	LYS
4	D	96	LEU
4	D	103	ASN
4	D	106	TYR
4	D	108	LEU
4	D	113	SER
4	D	119	GLN
4	D	127	THR
4	D	131	ARG
4	D	135	LEU
4	D	139	ARG
4	D	150	GLU
4	D	154	ASN
4	D	162	LEU
4	D	168	ARG
4	D	170	VAL
4	D	182	LYS
4	D	184	LYS
4	D	186	LEU
4	D	187	ARG

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Mol	Chain	Res	Type
4	D	188	LEU
4	D	194	LEU
4	D	200	GLU
4	D	209	ARG
5	E	10	MET
5	E	12	LEU
5	E	16	THR
5	E	18	ARG
5	E	27	ARG
5	E	31	LEU
5	E	33	VAL
5	E	41	VAL
5	E	57	LYS
5	E	64	ARG
5	E	68	GLU
5	E	71	LEU
5	E	79	GLU
5	E	80	ILE
5	E	87	SER
5	E	91	LEU
5	E	92	LYS
5	E	120	THR
5	E	137	GLU
5	E	147	ASP
5	E	153	LYS
6	F	17	SER
6	F	31	GLU
6	F	45	LEU
6	F	47	ARG
6	F	54	LYS
6	F	65	VAL
6	F	69	GLU
6	F	79	LEU
6	F	80	ARG
6	F	83	ASP
6	F	84	ASN
6	F	92	LYS
6	F	95	GLU
6	F	98	LEU
7	G	5	ARG
7	G	8	GLU
7	G	11	GLN

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Mol	Chain	Res	Type
7	G	13	GLN
7	G	24	THR
7	G	27	ILE
7	G	32	ARG
7	G	38	LEU
7	G	49	ILE
7	G	50	ILE
7	G	54	THR
7	G	69	VAL
7	G	72	ARG
7	G	79	ARG
7	G	89	MET
7	G	94	ARG
7	G	95	ARG
7	G	98	SER
7	G	104	LEU
7	G	114	ARG
7	G	122	HIS
7	G	138	LYS
7	G	144	MET
7	G	149	ARG
7	G	156	TRP
8	H	3	THR
8	H	18	ARG
8	H	26	VAL
8	H	39	LEU
8	H	50	ARG
8	H	56	LYS
8	H	63	LEU
8	H	64	LYS
8	H	70	GLN
8	H	75	ARG
8	H	83	ILE
8	H	85	ARG
8	H	87	SER
8	H	91	ARG
8	H	98	LYS
8	H	99	GLU
8	H	107	LEU
8	H	109	ILE
8	H	112	LEU
8	H	121	ASP

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Mol	Chain	Res	Type
8	H	126	LYS
8	H	127	LEU
9	I	4	TYR
9	I	10	ARG
9	I	11	LYS
9	I	14	VAL
9	I	19	LEU
9	I	31	GLN
9	I	42	ARG
9	I	47	LEU
9	I	54	ASP
9	I	58	ARG
9	I	60	ASP
9	I	66	ARG
9	I	70	LYS
9	I	79	LEU
9	I	85	LEU
9	I	91	ASP
9	I	104	ARG
9	I	108	VAL
9	I	125	TYR
9	I	128	ARG
10	J	14	LYS
10	J	21	GLN
10	J	33	GLN
10	J	35	SER
10	J	38	ILE
10	J	46	ARG
10	J	50	ILE
10	J	55	LYS
10	J	58	ASP
10	J	66	ARG
10	J	70	ARG
10	J	76	ASN
10	J	78	ASN
10	J	79	ARG
10	J	80	LYS
10	J	84	GLN
10	J	86	MET
10	J	87	THR
10	J	92	THR
10	J	95	GLU

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Mol	Chain	Res	Type
10	J	96	ILE
10	J	98	ILE
11	K	18	ARG
11	K	29	ILE
11	K	31	THR
11	K	43	SER
11	K	57	THR
11	K	67	ASP
11	K	70	LYS
11	K	84	VAL
11	K	92	GLU
11	K	93	GLN
11	K	104	GLN
11	K	114	VAL
11	K	117	ASN
11	K	120	ARG
11	K	122	LYS
11	K	126	ARG
11	K	127	LYS
12	L	18	VAL
12	L	20	LYS
12	L	21	LYS
12	L	24	VAL
12	L	34	ARG
12	L	38	THR
12	L	46	LYS
12	L	47	LYS
12	L	52	LEU
12	L	55	VAL
12	L	59	ARG
12	L	60	LEU
12	L	62	SER
12	L	67	THR
12	L	79	GLU
12	L	83	VAL
12	L	104	VAL
12	L	111	LYS
12	L	113	ARG
12	L	114	LYS
12	L	117	ARG
12	L	122	THR
12	L	123	LYS

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Mol	Chain	Res	Type
13	M	7	VAL
13	M	8	GLU
13	M	15	VAL
13	M	16	ASP
13	M	19	LEU
13	M	20	THR
13	M	34	LEU
13	M	35	GLU
13	M	47	ASP
13	M	48	LEU
13	M	49	THR
13	M	57	ARG
13	M	58	GLU
13	M	61	GLU
13	M	64	TRP
13	M	66	LEU
13	M	79	LYS
13	M	82	MET
13	M	84	ILE
13	M	88	ARG
13	M	90	LEU
13	M	91	ARG
13	M	93	ARG
13	M	94	ARG
13	M	101	GLN
13	M	102	ARG
13	M	104	ARG
13	M	108	ARG
13	M	115	LYS
13	M	117	VAL
13	M	120	LYS
13	M	121	LYS
14	N	3	ARG
14	N	4	LYS
14	N	7	ILE
14	N	18	VAL
14	N	24	CYS
14	N	33	VAL
14	N	53	LEU
14	N	56	VAL
15	O	3	ILE
15	O	13	GLN

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Mol	Chain	Res	Type
15	O	31	LEU
15	O	41	GLU
15	O	44	LYS
15	O	65	ARG
15	O	82	ILE
16	P	2	VAL
16	P	5	ARG
16	P	19	ILE
16	P	21	VAL
16	P	27	LYS
16	P	28	ARG
16	P	33	ILE
16	P	36	ILE
16	P	43	LYS
16	P	45	THR
16	P	53	VAL
16	P	54	GLU
16	P	67	THR
16	P	69	THR
16	P	74	LEU
17	Q	7	THR
17	Q	9	VAL
17	Q	14	LYS
17	Q	25	ARG
17	Q	38	ARG
17	Q	52	LYS
17	Q	53	LEU
17	Q	59	ILE
17	Q	78	GLU
17	Q	87	LYS
17	Q	89	LEU
17	Q	97	SER
17	Q	100	LYS
18	R	28	GLU
18	R	46	GLU
18	R	47	THR
18	R	59	SER
18	R	76	LEU
18	R	82	THR
18	R	83	GLU
18	R	84	LYS
19	S	4	SER

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Mol	Chain	Res	Type
19	S	6	LYS
19	S	7	LYS
19	S	13	ASP
19	S	22	LEU
19	S	31	ILE
19	S	33	THR
19	S	37	ARG
19	S	44	MET
19	S	47	HIS
19	S	62	ILE
19	S	64	GLU
19	S	65	ASN
19	S	79	THR
19	S	80	TYR
20	T	10	LEU
20	T	11	SER
20	T	24	LEU
20	T	33	ILE
20	T	38	LYS
20	T	50	GLU
20	T	54	LYS
20	T	70	SER
20	T	73	HIS
20	T	84	LEU
20	T	87	LYS
20	T	104	LEU
21	U	8	THR
21	U	15	ARG
21	U	25	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	76	GLN
2	B	78	GLN
2	B	94	ASN
2	B	95	GLN
2	B	224	GLN
3	C	108	ASN
3	C	123	GLN
4	D	42	GLN
6	F	7	ASN

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Mol	Chain	Res	Type
8	H	82	HIS
9	I	124	GLN
10	J	62	HIS
11	K	104	GLN
13	M	12	ASN
14	N	49	HIS
15	O	13	GLN
19	S	47	HIS

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1510/1517 (99%)	437 (28%)	98 (6%)
22	X	4/5 (80%)	2 (50%)	0
23	Y	9/10 (90%)	3 (33%)	1 (11%)
All	All	1523/1532 (99%)	442 (29%)	99 (6%)

All (442) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	9	G
1	A	14	U
1	A	20	U
1	A	22	G
1	A	28	G
1	A	31	G
1	A	32	A
1	A	35	G
1	A	39	G
1	A	44	G
1	A	45	U
1	A	47	C
1	A	48	C
1	A	50	A
1	A	51	A
1	A	54	C
1	A	62	U
1	A	73	G
1	A	79	G
1	A	81	U
1	A	82	U

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Mol	Chain	Res	Type
1	A	83	U
1	A	84	U
1	A	88	A
1	A	90	U
1	A	98	G
1	A	101	A
1	A	105	G
1	A	107	G
1	A	108	G
1	A	110	C
1	A	116	A
1	A	121	C
1	A	131	C
1	A	142	G
1	A	144	G
1	A	149	A
1	A	156	G
1	A	163	C
1	A	165	C
1	A	166	G
1	A	179	A
1	A	182	U
1	A	189(F)	U
1	A	189(I)	G
1	A	191	G
1	A	195	A
1	A	197	A
1	A	201	C
1	A	202	U
1	A	203	U
1	A	204	U
1	A	216	G
1	A	217	C
1	A	220	G
1	A	221	C
1	A	226	G
1	A	231	G
1	A	247	G
1	A	250	A
1	A	251	G
1	A	260	G
1	A	266	G

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Mol	Chain	Res	Type
1	A	267	C
1	A	274	A
1	A	275	G
1	A	280	C
1	A	289	G
1	A	306	G
1	A	312	C
1	A	317	G
1	A	321	A
1	A	328	C
1	A	329	A
1	A	330	C
1	A	332	G
1	A	341	C
1	A	345	C
1	A	348	G
1	A	350	G
1	A	352	C
1	A	353	A
1	A	354	G
1	A	355	C
1	A	367	U
1	A	372	C
1	A	373	A
1	A	374	A
1	A	378	G
1	A	382	A
1	A	388	G
1	A	389	A
1	A	393	A
1	A	396	G
1	A	397	A
1	A	398	C
1	A	406	G
1	A	412	A
1	A	413	G
1	A	414	A
1	A	419	C
1	A	421	U
1	A	422	C
1	A	423	G
1	A	424	G

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Mol	Chain	Res	Type
1	A	429	U
1	A	430	A
1	A	434	U
1	A	439	A
1	A	441	A
1	A	452	A
1	A	453	A
1	A	461	A
1	A	470	C
1	A	484	G
1	A	485	G
1	A	495	A
1	A	496	A
1	A	498	U
1	A	499	A
1	A	504	C
1	A	505	G
1	A	507	C
1	A	508	C
1	A	509	A
1	A	510	A
1	A	511	C
1	A	514	C
1	A	517	G
1	A	518	C
1	A	519	C
1	A	522	C
1	A	527	G
1	A	529	G
1	A	531	U
1	A	532	A
1	A	533	A
1	A	539	A
1	A	547	A
1	A	550	G
1	A	561	U
1	A	562	C
1	A	566	G
1	A	567	G
1	A	570	G
1	A	571	U
1	A	572	A

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Mol	Chain	Res	Type
1	A	573	A
1	A	575	G
1	A	576	G
1	A	577	G
1	A	582	U
1	A	587	G
1	A	588	G
1	A	597	G
1	A	602	A
1	A	607	A
1	A	619	U
1	A	630	G
1	A	632	A
1	A	633	G
1	A	640	A
1	A	645	C
1	A	650	G
1	A	651	C
1	A	652	U
1	A	653	A
1	A	665	A
1	A	687	A
1	A	688	G
1	A	693	G
1	A	702	A
1	A	703	G
1	A	721	G
1	A	722	A
1	A	723	U
1	A	724	G
1	A	729	A
1	A	731	G
1	A	736	C
1	A	755	G
1	A	761	G
1	A	769	G
1	A	777	A
1	A	782	A
1	A	793	U
1	A	794	A
1	A	801	U
1	A	804	U

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Mol	Chain	Res	Type
1	A	805	C
1	A	814	A
1	A	815	A
1	A	816	A
1	A	817	C
1	A	819	A
1	A	820	U
1	A	828	A
1	A	832	C
1	A	836	G
1	A	839	U
1	A	840	C
1	A	841	U
1	A	848	C
1	A	851	G
1	A	853	G
1	A	859	A
1	A	867	G
1	A	869	G
1	A	877	C
1	A	882	C
1	A	900	A
1	A	902	G
1	A	913	A
1	A	914	A
1	A	919	A
1	A	926	G
1	A	927	G
1	A	934	C
1	A	935	A
1	A	937	A
1	A	938	A
1	A	943	U
1	A	955	U
1	A	958	A
1	A	960	U
1	A	961	U
1	A	963	G
1	A	965	A
1	A	966	G
1	A	969	A
1	A	971	G

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Mol	Chain	Res	Type
1	A	972	C
1	A	974	A
1	A	975	A
1	A	976	G
1	A	977	A
1	A	978	A
1	A	980	C
1	A	984	C
1	A	985	C
1	A	988	G
1	A	991	U
1	A	992	U
1	A	993	G
1	A	994	A
1	A	1001(A)	G
1	A	1003	G
1	A	1004	A
1	A	1005	A
1	A	1006	C
1	A	1010	G
1	A	1016	A
1	A	1024	G
1	A	1025	U
1	A	1026	G
1	A	1030	C
1	A	1030(A)	G
1	A	1030(C)	G
1	A	1030(D)	A
1	A	1031	G
1	A	1032	G
1	A	1033	G
1	A	1034	G
1	A	1035	A
1	A	1041	A
1	A	1042	G
1	A	1046	A
1	A	1049	U
1	A	1053	G
1	A	1054	C
1	A	1055	A
1	A	1057	G
1	A	1060	C

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Mol	Chain	Res	Type
1	A	1061	G
1	A	1064	G
1	A	1065	U
1	A	1067	A
1	A	1068	G
1	A	1094	G
1	A	1095	U
1	A	1096	C
1	A	1099	G
1	A	1101	A
1	A	1108	G
1	A	1112	C
1	A	1113	C
1	A	1117	G
1	A	1119	C
1	A	1123	A
1	A	1124	G
1	A	1125	U
1	A	1126	U
1	A	1127	G
1	A	1128	C
1	A	1129	C
1	A	1130	A
1	A	1131	G
1	A	1133	G
1	A	1134	G
1	A	1136	U
1	A	1137	C
1	A	1138	G
1	A	1139	G
1	A	1140	C
1	A	1141	C
1	A	1142	G
1	A	1145	C
1	A	1146	A
1	A	1151	A
1	A	1152	A
1	A	1159	U
1	A	1160	G
1	A	1171	G
1	A	1174	G
1	A	1181	G

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Mol	Chain	Res	Type
1	A	1182	G
1	A	1184	G
1	A	1185	G
1	A	1186	G
1	A	1187	G
1	A	1192	C
1	A	1194	U
1	A	1196	U
1	A	1197	G
1	A	1199	U
1	A	1202	G
1	A	1206	G
1	A	1211	U
1	A	1212	U
1	A	1213	A
1	A	1214	C
1	A	1216	G
1	A	1217	C
1	A	1218	C
1	A	1225	A
1	A	1226	C
1	A	1227	A
1	A	1230	C
1	A	1238	A
1	A	1241	G
1	A	1242	C
1	A	1244	C
1	A	1246	C
1	A	1248	A
1	A	1249	C
1	A	1250	A
1	A	1251	A
1	A	1252	A
1	A	1253	G
1	A	1255	G
1	A	1256	A
1	A	1257	U
1	A	1258	G
1	A	1259	C
1	A	1262	C
1	A	1272	G
1	A	1273	G

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Mol	Chain	Res	Type
1	A	1278	U
1	A	1280	A
1	A	1281	U
1	A	1282	C
1	A	1285	A
1	A	1286	A
1	A	1287	A
1	A	1289	A
1	A	1297	C
1	A	1299	A
1	A	1300	G
1	A	1302	U
1	A	1305	G
1	A	1312	G
1	A	1317	C
1	A	1319	A
1	A	1320	C
1	A	1322	C
1	A	1324	A
1	A	1325	C
1	A	1327	C
1	A	1329	A
1	A	1331	G
1	A	1332	A
1	A	1335	C
1	A	1336	C
1	A	1337	G
1	A	1338	G
1	A	1346	A
1	A	1347	G
1	A	1348	U
1	A	1350	A
1	A	1352	C
1	A	1354	C
1	A	1363	C
1	A	1363(A)	A
1	A	1369	C
1	A	1370	G
1	A	1373	G
1	A	1379	G
1	A	1381	U
1	A	1382	C

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Mol	Chain	Res	Type
1	A	1383	C
1	A	1391	U
1	A	1392	G
1	A	1397	C
1	A	1398	A
1	A	1401	G
1	A	1404	C
1	A	1419	G
1	A	1420	C
1	A	1427	U
1	A	1433	A
1	A	1434	A
1	A	1442	G
1	A	1442(A)	G
1	A	1443	G
1	A	1452	C
1	A	1456	G
1	A	1475	G
1	A	1487	G
1	A	1492	A
1	A	1497	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	1507	A
1	A	1514	C
1	A	1517	G
1	A	1522	U
1	A	1529	G
1	A	1530	G
1	A	1531	A
1	A	1532	U
1	A	1533	C
1	A	1541	U
1	A	1544	U
22	X	6	G
22	X	8	A
23	Y	34	I
23	Y	35	G

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Mol	Chain	Res	Type
23	Y	40	C

All (99) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	65	U
1	A	82	U
1	A	83	U
1	A	84	U
1	A	105	G
1	A	106	C
1	A	108	G
1	A	109	A
1	A	115	G
1	A	119	A
1	A	139	G
1	A	202	U
1	A	203	U
1	A	204	U
1	A	246	A
1	A	250	A
1	A	266	G
1	A	274	A
1	A	279	A
1	A	329	A
1	A	344	A
1	A	353	A
1	A	405	U
1	A	412	A
1	A	421	U
1	A	422	C
1	A	428	G
1	A	429	U
1	A	461	A
1	A	484	G
1	A	495	A
1	A	508	C
1	A	509	A
1	A	530	G
1	A	532	A
1	A	560	U
1	A	561	U

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Mol	Chain	Res	Type
1	A	570	G
1	A	575	G
1	A	587	G
1	A	595	G
1	A	687	A
1	A	702	A
1	A	722	A
1	A	723	U
1	A	748	C
1	A	760	G
1	A	793	U
1	A	811	C
1	A	814	A
1	A	819	A
1	A	840	C
1	A	866	C
1	A	913	A
1	A	960	U
1	A	962	C
1	A	968	A
1	A	971	G
1	A	992	U
1	A	993	G
1	A	1003	G
1	A	1005	A
1	A	1025	U
1	A	1030(B)	C
1	A	1030(C)	G
1	A	1044	A
1	A	1046	A
1	A	1048	G
1	A	1049	U
1	A	1054	C
1	A	1064	G
1	A	1067	A
1	A	1124	G
1	A	1125	U
1	A	1126	U
1	A	1128	C
1	A	1139	G
1	A	1145	C
1	A	1151	A

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Mol	Chain	Res	Type
1	A	1181	G
1	A	1201	A
1	A	1211	U
1	A	1225	A
1	A	1248	A
1	A	1256	A
1	A	1280	A
1	A	1285	A
1	A	1319	A
1	A	1331	G
1	A	1335	C
1	A	1353	G
1	A	1380	U
1	A	1414	U
1	A	1499	A
1	A	1504	G
1	A	1505	G
1	A	1532	U
1	A	1540	U
23	Y	34	I

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	$\#\|Z\| > 2$
22	PSU	X	4	22,23	14,18,22	2.22	2 (14%)	18,26,33	4.23	12 (66%)

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
22	PSU	X	4	22,23	-	0/6/22/26	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	X	4	PSU	C5-C1'	-6.59	1.46	1.52
22	X	4	PSU	C2'-C1'	-3.98	1.50	1.53

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	X	4	PSU	N1-C2-N3	-10.36	121.72	128.33
22	X	4	PSU	C5-C1'-C2'	-5.50	105.75	115.52
22	X	4	PSU	C5-C6-N1	-3.68	119.20	124.39
22	X	4	PSU	O4'-C4'-C3'	-2.88	99.34	105.15
22	X	4	PSU	C3'-C2'-C1'	-2.11	99.35	101.79
22	X	4	PSU	O5'-C5'-C4'	3.93	124.33	111.33
22	X	4	PSU	C6-N1-C2	4.02	121.93	115.47
22	X	4	PSU	C4'-O4'-C1'	4.05	113.71	109.58
22	X	4	PSU	O4'-C1'-C2'	4.16	108.98	104.73
22	X	4	PSU	O4'-C4'-C5'	4.35	118.59	109.17
22	X	4	PSU	C2'-C3'-C4'	4.54	111.94	102.61
22	X	4	PSU	C4-N3-C2	7.01	121.31	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	X	4	PSU	3	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 18 ligands modelled in this entry, 18 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	1511/1517 (99%)	-0.30	12 (0%) 87 79	37, 75, 144, 237	0
2	B	234/234 (100%)	-0.09	8 (3%) 49 32	55, 108, 168, 190	0
3	C	206/206 (100%)	-0.25	3 (1%) 76 62	67, 102, 146, 182	0
4	D	208/208 (100%)	-0.27	4 (1%) 70 54	61, 92, 129, 145	0
5	E	150/150 (100%)	-0.40	1 (0%) 89 82	50, 72, 97, 154	0
6	F	101/101 (100%)	-0.38	1 (0%) 84 74	76, 108, 133, 147	0
7	G	155/155 (100%)	-0.30	4 (2%) 59 44	67, 99, 144, 204	0
8	H	138/138 (100%)	-0.47	2 (1%) 78 64	48, 67, 94, 113	0
9	I	127/127 (100%)	-0.26	0 100 100	61, 113, 140, 170	0
10	J	98/98 (100%)	0.10	4 (4%) 41 25	65, 135, 176, 194	0
11	K	119/119 (100%)	-0.35	3 (2%) 61 45	50, 80, 118, 140	0
12	L	125/125 (100%)	-0.32	3 (2%) 62 45	42, 81, 119, 162	0
13	M	120/120 (100%)	-0.04	5 (4%) 40 24	56, 96, 141, 171	0
14	N	60/60 (100%)	-0.20	0 100 100	72, 94, 123, 130	0
15	O	88/88 (100%)	-0.52	0 100 100	54, 82, 120, 160	0
16	P	83/83 (100%)	-0.39	0 100 100	53, 72, 94, 127	0
17	Q	99/99 (100%)	-0.51	0 100 100	45, 71, 101, 113	0
18	R	70/70 (100%)	-0.39	0 100 100	63, 89, 122, 137	0
19	S	78/78 (100%)	-0.20	2 (2%) 59 44	77, 117, 151, 176	0
20	T	99/99 (100%)	-0.46	0 100 100	51, 77, 124, 145	0
21	U	24/24 (100%)	0.04	1 (4%) 40 24	67, 80, 113, 139	0
22	X	4/5 (80%)	-0.19	0 100 100	78, 91, 109, 125	0
23	Y	9/10 (90%)	0.42	0 100 100	73, 84, 116, 137	0
All	All	3906/3914 (99%)	-0.29	53 (1%) 78 64	37, 85, 145, 237	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	M	119	GLY	7.5
13	M	120	LYS	6.1
1	A	1034	G	5.2
1	A	1540	U	5.1
7	G	81	GLY	5.1
2	B	7	VAL	4.7
12	L	127	GLU	4.4
19	S	81	ARG	4.3
13	M	7	VAL	4.2
11	K	129	SER	4.0
5	E	154	GLY	3.8
1	A	1541	U	3.7
19	S	30	LEU	3.4
7	G	5	ARG	3.1
3	C	2	GLY	3.1
1	A	1250	A	3.1
7	G	156	TRP	3.1
2	B	231	GLU	3.0
21	U	25	LYS	3.0
11	K	127	LYS	3.0
10	J	34	VAL	2.9
1	A	1138	G	2.9
1	A	630	G	2.8
1	A	1129	C	2.8
10	J	33	GLN	2.7
6	F	101	ALA	2.7
13	M	121	LYS	2.6
1	A	841	U	2.6
12	L	128	ALA	2.6
7	G	82	GLY	2.6
13	M	117	VAL	2.5
2	B	132	LYS	2.5
3	C	78	GLY	2.5
2	B	15	VAL	2.5
4	D	209	ARG	2.4
1	A	470	C	2.4
2	B	237	ALA	2.3
4	D	23	GLY	2.3
2	B	128	GLU	2.3
11	K	128	ALA	2.2
2	B	133	LYS	2.2
8	H	1	MET	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	36	ARG	2.2
3	C	194	GLY	2.2
1	A	1030(C)	G	2.2
1	A	202	U	2.1
4	D	2	GLY	2.1
10	J	89	ASP	2.1
10	J	74	ILE	2.1
4	D	37	PRO	2.1
8	H	54	ASP	2.0
12	L	129	ALA	2.0
1	A	1144	G	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
22	PSU	X	4	17/21	0.90	0.17	-	37,57,73,75	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
24	MG	A	1608	1/1	0.98	0.68	43.40	48,48,48,48	0
24	MG	A	1607	1/1	0.91	0.30	16.20	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
24	MG	A	1614	1/1	0.93	0.29	12.74	36,36,36,36	0
24	MG	A	1610	1/1	0.97	0.27	10.66	39,39,39,39	0
25	ZN	D	301	1/1	0.98	0.21	-1.14	119,119,119,119	0
24	MG	X	101	1/1	0.99	0.09	-2.80	43,43,43,43	0
24	MG	A	1611	1/1	0.94	0.26	-	48,48,48,48	0
24	MG	A	1603	1/1	0.83	0.39	-	60,60,60,60	0
24	MG	A	1606	1/1	0.87	0.22	-	52,52,52,52	0
24	MG	A	1605	1/1	0.93	0.43	-	35,35,35,35	0
24	MG	A	1615	1/1	0.98	0.44	-	43,43,43,43	0
24	MG	Y	101	1/1	0.95	0.30	-	70,70,70,70	0
24	MG	A	1609	1/1	0.93	0.33	-	47,47,47,47	0
24	MG	A	1604	1/1	0.96	0.65	-	35,35,35,35	0
24	MG	A	1602	1/1	0.96	0.57	-	36,36,36,36	0
24	MG	A	1613	1/1	0.94	0.48	-	48,48,48,48	0
24	MG	A	1601	1/1	0.95	0.52	-	59,59,59,59	0
24	MG	A	1612	1/1	0.96	0.41	-	41,41,41,41	0

6.5 Other polymers (i)

There are no such residues in this entry.