Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:04 PM GMT

PDB ID	:	4K0K
Title	:	Crystal structure of the Thermus thermophilus 30S ribosomal subunit complexed with a serine-ASL and mRNA containing a stop codon
Authors	:	Fernandez, I.S.; Ng, C.L.; Kelley, A.C.; Guowei, W.; Yu, Y.T.; Ramakrishnan, V.
Deposited on	:	2013-04-04
Resolution	:	3.40 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:

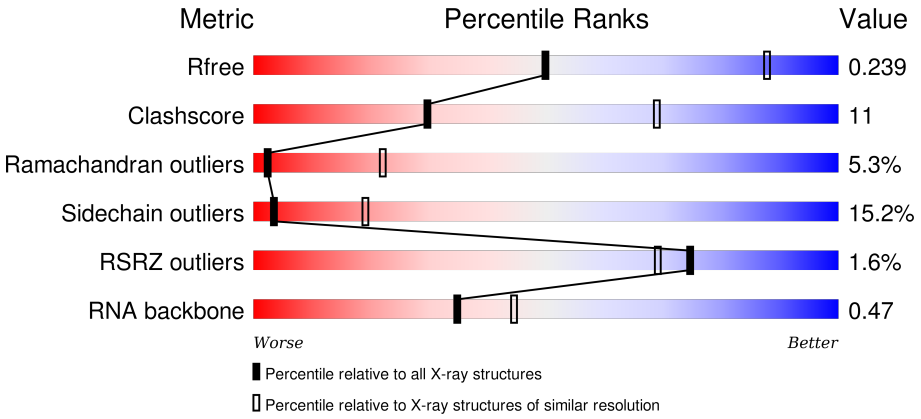
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.40 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	1476 (3.50-3.30)
Clashscore	102246	1611 (3.50-3.30)
Ramachandran outliers	100387	1571 (3.50-3.30)
Sidechain outliers	100360	1571 (3.50-3.30)
RSRZ outliers	91569	1485 (3.50-3.30)
RNA backbone	2183	1041 (4.00-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	2% 54% 35% 10%
2	B	235	2% 49% 40% 10%
3	C	207	54% 37% 8%
4	D	208	% 54% 32% 13%

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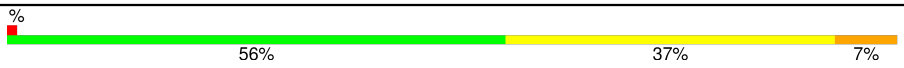
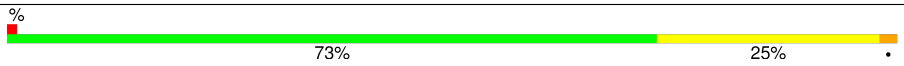
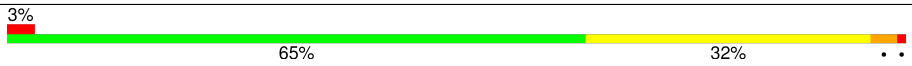
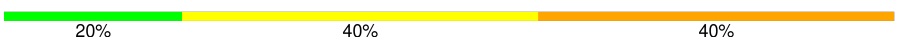
Mol	Chain	Length	Quality of chain
5	E	151	
6	F	101	
7	G	155	
8	H	138	
9	I	127	
10	J	99	
11	K	119	
12	L	126	
13	M	121	
14	N	60	
15	O	88	
16	P	84	
17	Q	100	
18	R	70	
19	S	79	
20	T	99	
21	U	25	
22	X	5	
23	Y	11	

2 Entry composition

There are 23 unique types of molecules in this entry. The entry contains 51915 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	79	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	235	1901	1213	342	341	5	0	0	1

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	207	1613	1016	315	281	1	0	0	1

- 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	151	1147	724	218	201	4	0	0	1

- 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	99	Total	C	N	O	S	0	0	1
			795	499	157	138	1			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	126	Total	C	N	O	S	0	0	1
			976	614	197	164	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	121	Total	C	N	O	S	0	0	1
			956	591	198	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	84	Total	C	N	O	S	0	0	1
			701	443	140	117	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	100	Total	C	N	O	S	0	0	1
			824	528	152	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	79	Total	C	N	O	S	0	0	1
			630	403	115	110	2			

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	U	25	Total	C	N	O	0	0	1
			209	128	51	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 RNA-ASL.

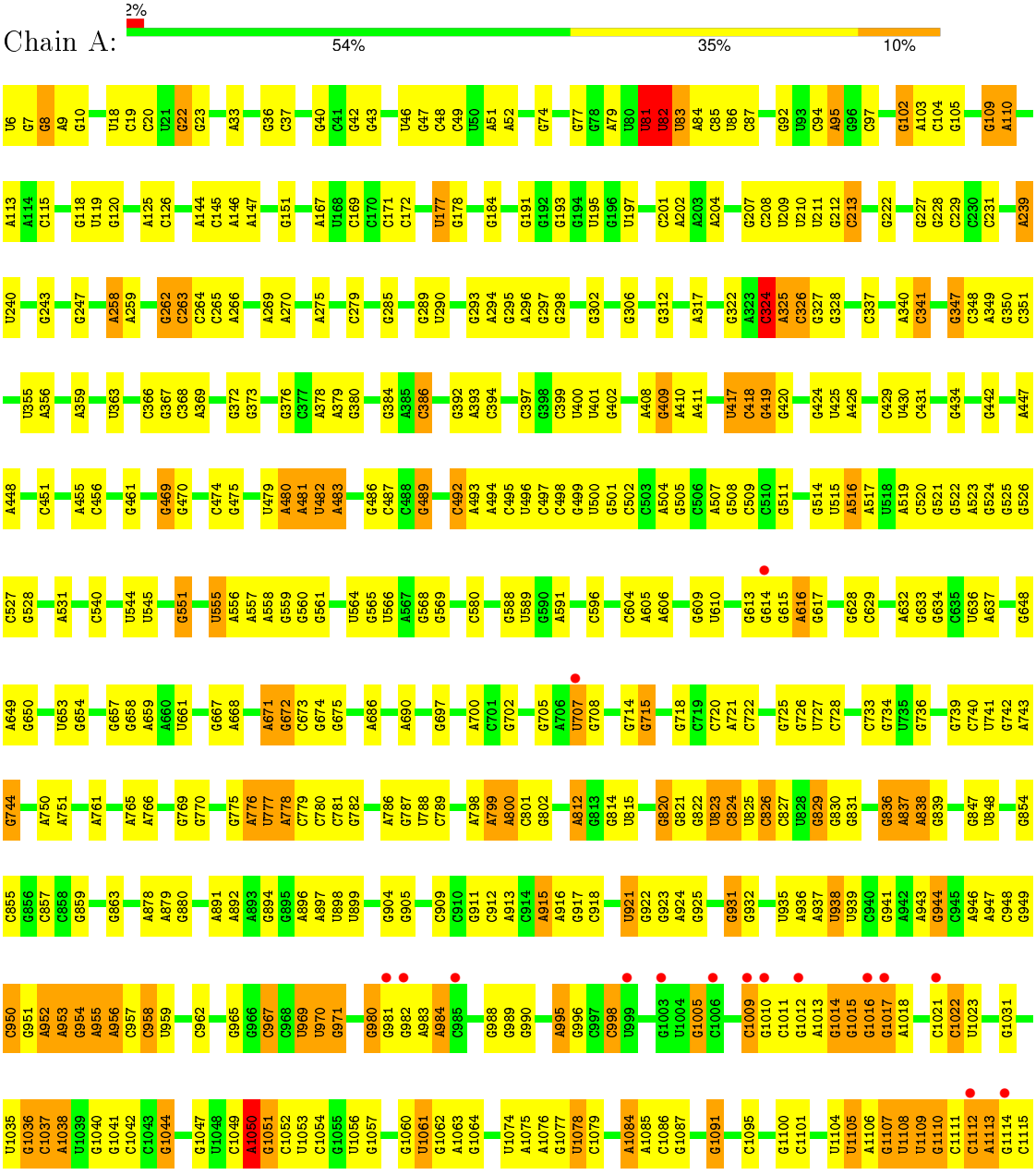
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	Y	10	Total	C	N	O	P	0	0	0
			213	96	38	69	10			

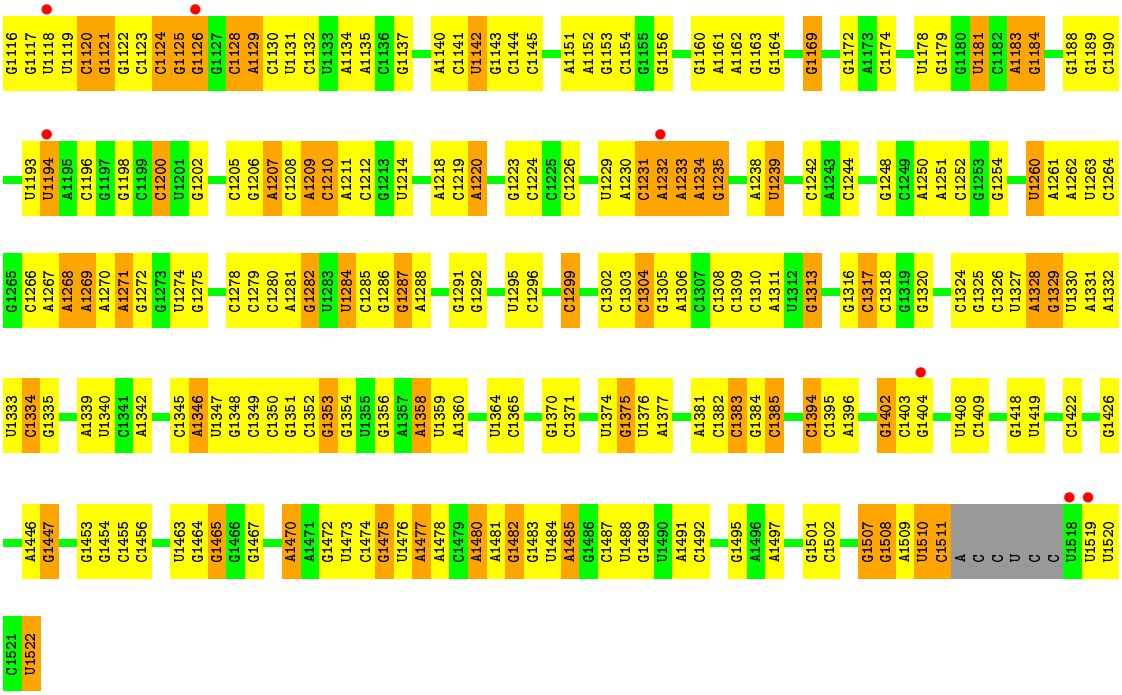
3 Residue-property plots (i)

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

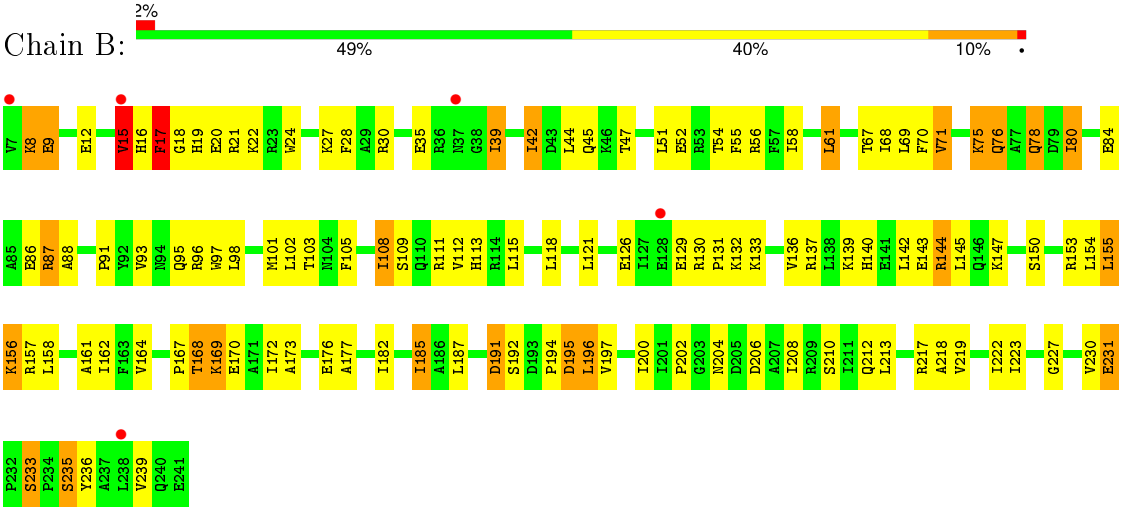
Chain A:





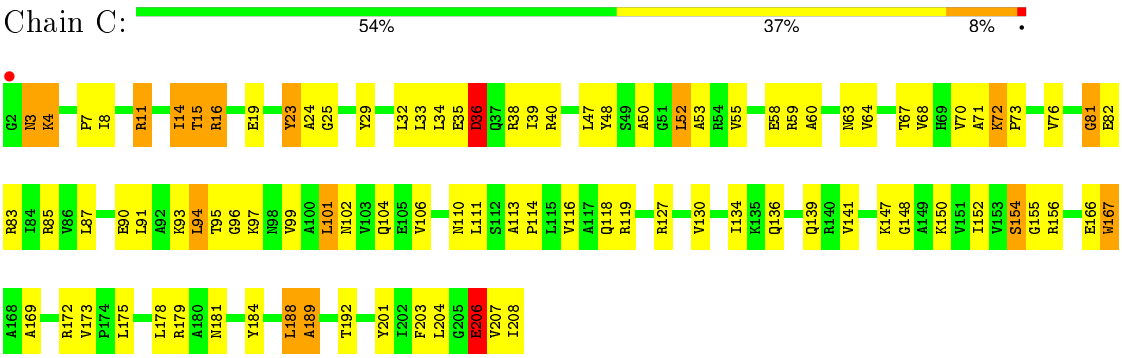
• Molecule 2: 30S ribosomal protein S2

Chain B:



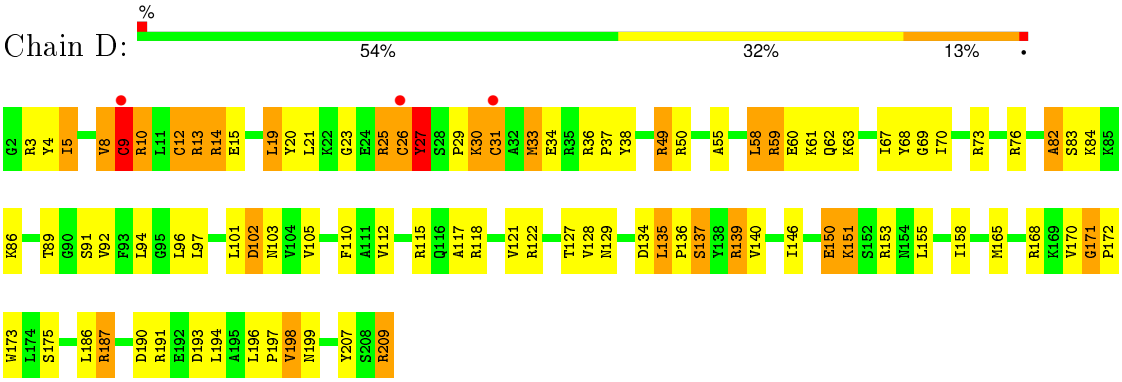
• Molecule 3: 30S ribosomal protein S3

Chain C:



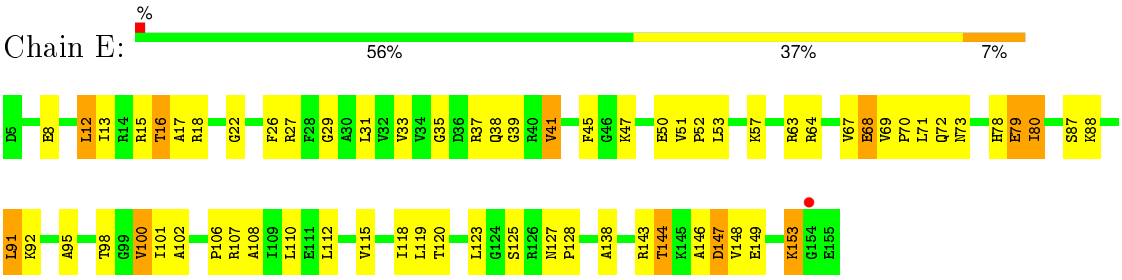
- Molecule 4: 30S ribosomal protein S4

Chain D:



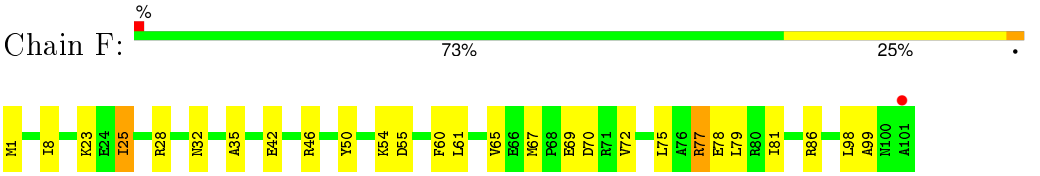
- Molecule 5: 30S ribosomal protein S5

Chain E:



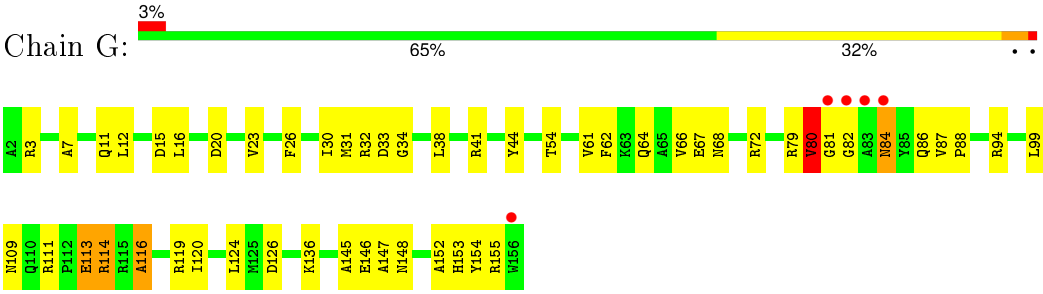
- Molecule 6: 30S ribosomal protein S6

Chain F:



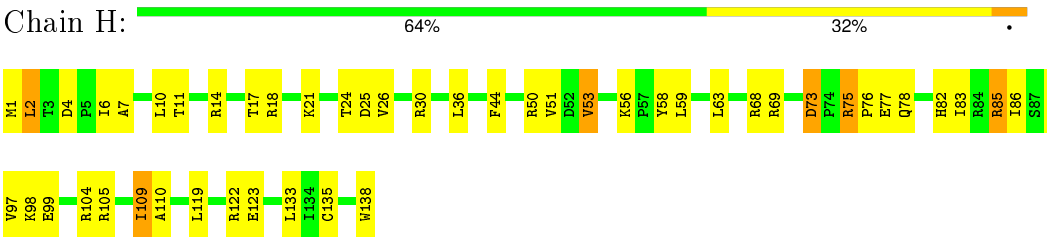
- Molecule 7: 30S ribosomal protein S7

Chain G:



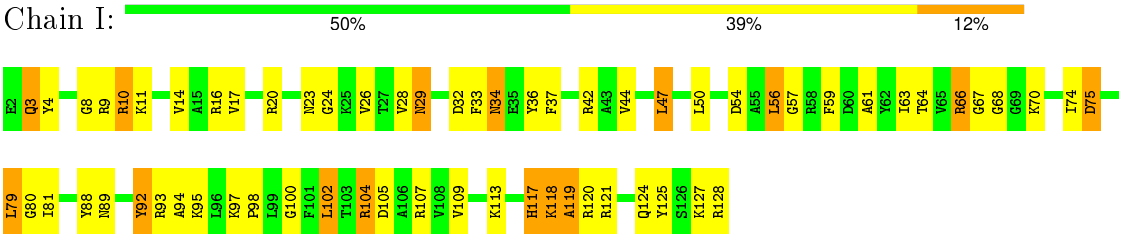
- Molecule 8: 30S ribosomal protein S8

Chain H:



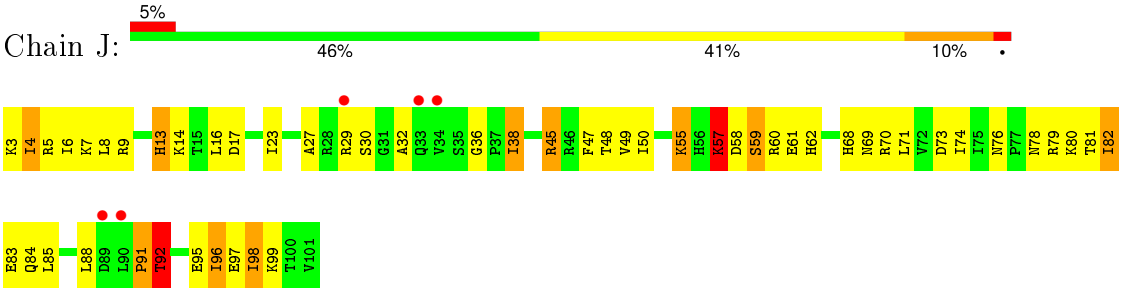
• Molecule 9: 30S ribosomal protein S9

Chain I:



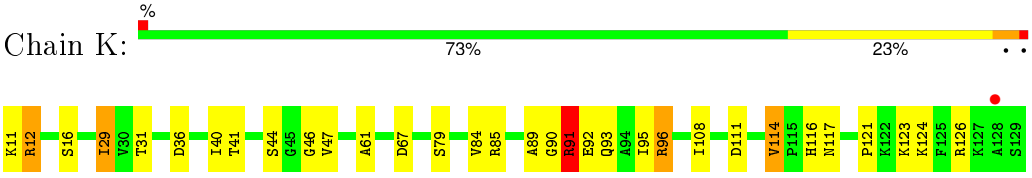
• Molecule 10: 30S ribosomal protein S10

Chain J:



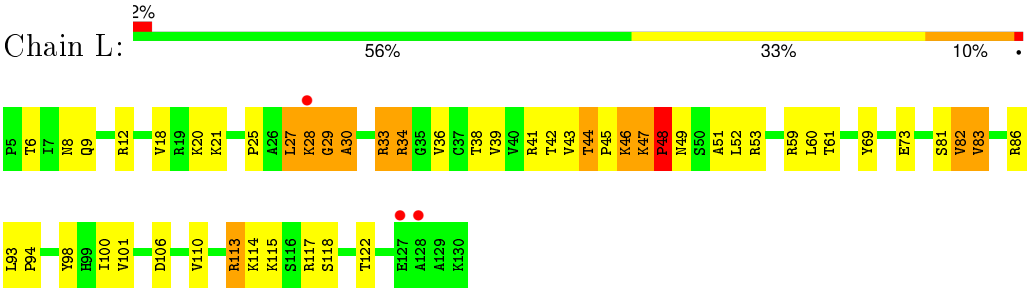
• Molecule 11: 30S ribosomal protein S11

Chain K:



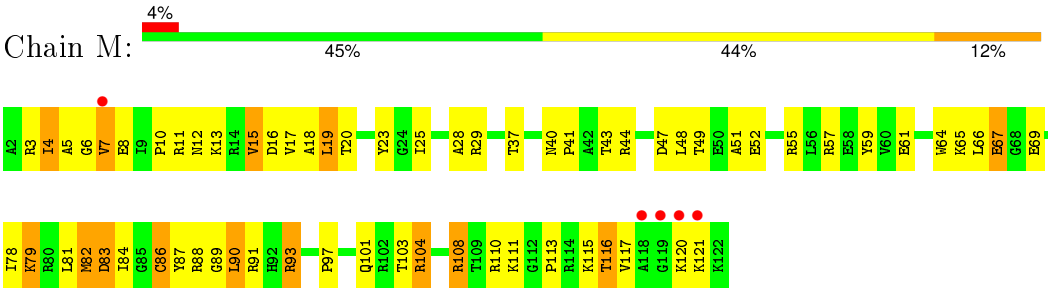
• Molecule 12: 30S ribosomal protein S12

Chain L:



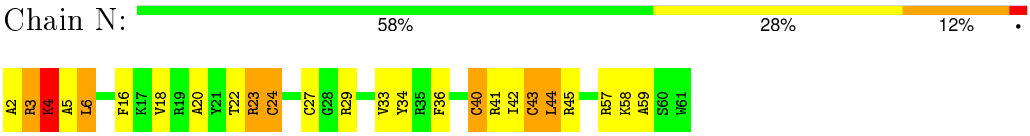
• Molecule 13: 30S ribosomal protein S13

Chain M:



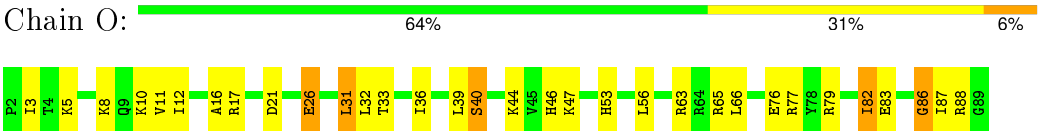
• Molecule 14: 30S ribosomal protein S14

Chain N:



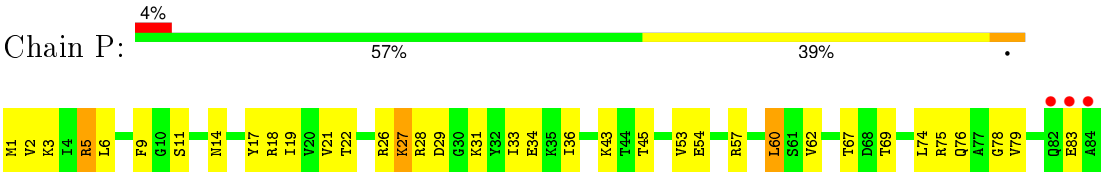
- Molecule 15: 30S ribosomal protein S15

Chain O:



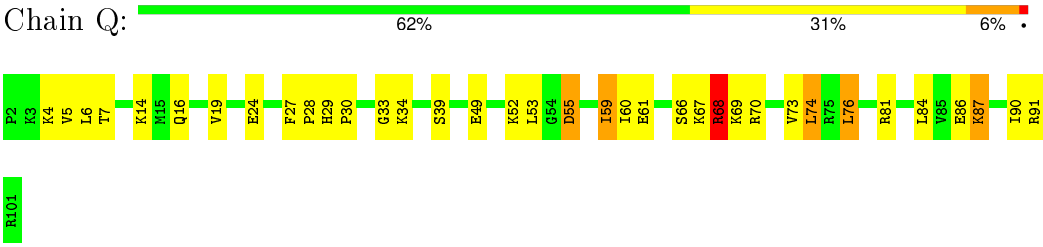
- Molecule 16: 30S ribosomal protein S16

Chain P:



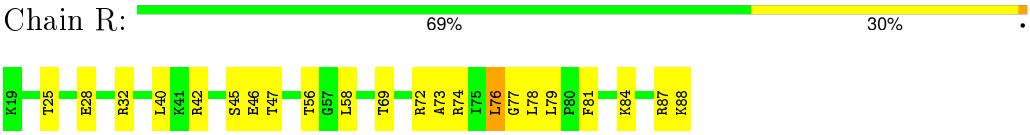
- Molecule 17: 30S ribosomal protein S17

Chain Q:



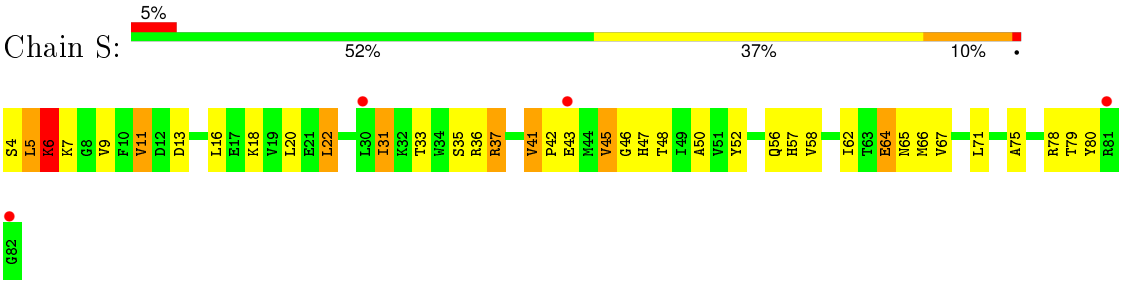
- Molecule 18: 30S ribosomal protein S18

Chain R:



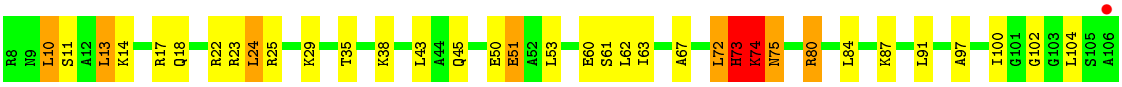
- Molecule 19: 30S ribosomal protein S19

Chain S:

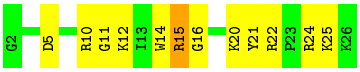


- Molecule 20: 30S ribosomal protein S20

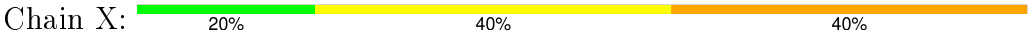
Chain T:



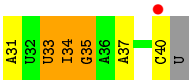
• Molecule 21: 30S ribosomal protein THX



• Molecule 22: mRNA



• Molecule 23: RNA-ASL



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	401.30Å 401.30Å 173.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.40 20.00 – 3.40	Depositor EDS
% Data completeness (in resolution range)	98.1 (20.00-3.40) 98.7 (20.00-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.34 (at 3.36Å)	Xtriage
Refinement program	REFMAC 5.8.0033	Depositor
R, R_{free}	0.187 , 0.242 0.189 , 0.239	Depositor DCC
R_{free} test set	9471 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	95.3	Xtriage
Anisotropy	0.007	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 64.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Outliers	0 of 189418 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	51915	wwPDB-VP
Average B, all atoms (Å^2)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.54% 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

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	0.45	3/36342 (0.0%)	0.74	17/56718 (0.0%)
2	B	0.46	0/1936	0.74	0/2611
3	C	0.51	0/1637	0.77	1/2207 (0.0%)
4	D	0.54	1/1733 (0.1%)	0.83	2/2318 (0.1%)
5	E	0.58	0/1163	0.84	1/1566 (0.1%)
6	F	0.41	0/856	0.65	0/1154
7	G	0.43	0/1276	0.71	0/1709
8	H	0.57	0/1136	0.81	0/1527
9	I	0.47	0/1029	0.73	0/1378
10	J	0.50	0/808	0.75	0/1087
11	K	0.51	0/900	0.75	0/1213
12	L	0.57	0/992	0.87	1/1329 (0.1%)
13	M	0.50	0/966	0.79	0/1294
14	N	0.66	1/501 (0.2%)	0.94	1/664 (0.2%)
15	O	0.45	0/745	0.73	0/992
16	P	0.55	0/717	0.83	1/965 (0.1%)
17	Q	0.55	0/837	0.81	1/1119 (0.1%)
18	R	0.45	0/579	0.73	0/768
19	S	0.47	0/643	0.73	0/867
20	T	0.51	0/765	0.81	0/1007
21	U	0.55	0/213	0.83	0/279
22	X	1.72	3/116 (2.6%)	1.95	5/179 (2.8%)
23	Y	2.48	1/237 (0.4%)	1.39	4/364 (1.1%)
All	All	0.51	9/56127 (0.0%)	0.76	34/83315 (0.0%)

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
3	C	0	1
9	I	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
20	T	0	2
23	Y	1	0
All	All	1	4

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	Y	34	I	O3'-P	37.06	2.05	1.61
22	X	4	U	C4-C5	-10.47	1.34	1.43
22	X	4	U	N1-C2	10.39	1.47	1.38
1	A	82	U	O3'-P	7.11	1.69	1.61
1	A	81	U	O3'-P	6.22	1.68	1.61
1	A	799	A	O3'-P	-5.96	1.54	1.61
22	X	4	U	C2-N3	-5.65	1.33	1.37
14	N	24	CYS	CB-SG	5.19	1.91	1.82
4	D	12	CYS	CA-CB	5.17	1.65	1.53

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	Y	34	I	OP1-P-O3'	13.34	134.54	105.20
22	X	4	U	C5-C4-O4	-13.18	117.99	125.90
22	X	4	U	N3-C4-C5	10.84	121.10	114.60
23	Y	34	I	P-O3'-C3'	-10.75	106.80	119.70
23	Y	34	I	OP2-P-O3'	-10.19	82.79	105.20
22	X	4	U	C2-N3-C4	-9.11	121.53	127.00
1	A	1206	G	O5'-P-OP2	-8.15	98.36	105.70
1	A	1206	G	O5'-P-OP1	7.78	120.03	110.70
1	A	6	U	C5'-C4'-O4'	7.52	118.12	109.10
4	D	9	CYS	CA-CB-SG	7.26	127.08	114.00
1	A	83	U	N1-C1'-C2'	7.05	123.16	114.00
14	N	40	CYS	CA-CB-SG	7.03	126.65	114.00
17	Q	68	ARG	NE-CZ-NH1	6.68	123.64	120.30
22	X	4	U	C5-C6-N1	-6.60	119.40	122.70
1	A	22	G	O5'-P-OP1	6.55	118.56	110.70
3	C	11	ARG	NE-CZ-NH1	6.41	123.51	120.30
1	A	22	G	O5'-P-OP2	-6.22	100.10	105.70
1	A	324	C	N1-C1'-C2'	6.07	121.89	114.00
4	D	31	CYS	CA-CB-SG	6.05	124.89	114.00
1	A	558	A	O5'-P-OP1	-5.96	100.34	105.70
1	A	948	C	O5'-P-OP2	5.86	117.73	110.70
12	L	34	ARG	NE-CZ-NH1	5.70	123.15	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	558	A	O5'-P-OP2	5.69	117.53	110.70
22	X	4	U	N1-C1'-C2'	-5.47	105.98	112.00
5	E	12	LEU	CA-CB-CG	5.41	127.75	115.30
1	A	492	C	C2'-C3'-O3'	5.40	122.35	113.70
1	A	469	G	C2'-C3'-O3'	5.32	122.20	113.70
23	Y	37	A	O5'-P-OP2	-5.30	100.93	105.70
1	A	1480	A	N9-C1'-C2'	5.27	120.85	114.00
1	A	551	G	O5'-P-OP1	-5.26	100.97	105.70
1	A	686	A	O4'-C1'-C2'	-5.22	100.58	105.80
1	A	1050	A	C2'-C3'-O3'	5.19	122.01	113.70
1	A	1507	G	C4-N9-C1'	-5.18	119.77	126.50
16	P	60	LEU	CA-CB-CG	-5.03	103.72	115.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	Y	34	I	C4'

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	206	GLU	Peptide
9	I	117	HIS	Peptide
20	T	74	LYS	Peptide
20	T	75	ASN	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	481	0
2	B	1901	0	1951	66	0
3	C	1613	0	1677	58	0
4	D	1703	0	1763	55	0
5	E	1147	0	1207	44	0
6	F	843	0	857	15	0
7	G	1257	0	1296	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	H	1116	0	1177	29	0
9	I	1011	0	1043	49	0
10	J	795	0	840	38	0
11	K	885	0	904	20	0
12	L	976	0	1062	38	0
13	M	956	0	1021	36	0
14	N	492	0	529	18	0
15	O	734	0	771	12	0
16	P	701	0	720	18	0
17	Q	824	0	891	24	0
18	R	574	0	644	12	0
19	S	630	0	652	25	0
20	T	763	0	861	18	0
21	U	209	0	221	7	0
22	X	104	0	55	5	0
23	Y	213	0	109	18	0
All	All	51915	0	36642	984	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (984) 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:O3'	23:Y:35:G:P	2.05	1.15
1:A:1231:C:N4	1:A:1269:A:N7	2.00	1.07
1:A:1522:U:O3'	22:X:4:U:O5'	1.72	1.05
1:A:951:G:OP1	10:J:57:LYS:NZ	1.99	0.95
3:C:154:SER:OG	3:C:155:GLY:N	1.96	0.93
17:Q:66:SER:O	17:Q:70:ARG:NH1	2.04	0.91
4:D:19:LEU:HD11	4:D:67:ILE:HG12	1.50	0.91
1:A:77:G:H1	1:A:87:C:H5	1.20	0.89
1:A:1014:G:N3	1:A:1015:G:N1	2.22	0.87
1:A:1120:C:O2'	1:A:1121:G:N2	2.07	0.87
1:A:1287:G:N2	1:A:1313:G:H2'	1.90	0.86
13:M:49:THR:HG22	13:M:51:ALA:H	1.42	0.84
4:D:63:LYS:HD2	4:D:198:VAL:HG23	1.57	0.84
23:Y:33:U:H3'	23:Y:34:I:OP1	1.78	0.84
1:A:953:A:H5'	1:A:953:A:H8	1.43	0.83
19:S:6:LYS:HG2	19:S:7:LYS:HE3	1.63	0.81
20:T:67:ALA:O	20:T:73:HIS:ND1	2.13	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1288:A:H61	1:A:1313:G:H1'	1.46	0.81
1:A:855:C:OP1	8:H:88:LYS:HE2	1.80	0.81
3:C:14:ILE:O	3:C:16:ARG:N	2.14	0.79
2:B:84:GLU:HB3	2:B:219:VAL:HG21	1.63	0.79
14:N:29:ARG:HD3	14:N:40:CYS:HB2	1.65	0.79
1:A:565:G:H8	1:A:565:G:O5'	1.66	0.78
1:A:1328:A:OP1	9:I:120:ARG:NH1	2.16	0.77
1:A:565:G:C6	1:A:742:G:N7	2.53	0.77
1:A:957:C:H3'	1:A:958:C:H5"	1.66	0.77
1:A:1349:C:H2'	1:A:1350:C:H6	1.50	0.76
7:G:16:LEU:HD12	9:I:42:ARG:HA	1.67	0.76
1:A:836:G:C6	1:A:847:G:N7	2.54	0.76
12:L:90:VAL:O	12:L:91:LYS:HB3	1.85	0.75
19:S:45:VAL:O	19:S:47:HIS:N	2.16	0.75
1:A:1501:G:OP1	11:K:123:LYS:NZ	2.16	0.75
1:A:952:A:OP2	14:N:41:ARG:NH1	2.20	0.74
1:A:1382:C:H4'	1:A:1383:C:H5"	1.67	0.74
1:A:690:A:O4'	11:K:29:ILE:HD11	1.88	0.74
5:E:68:GLU:HG3	5:E:70:PRO:HD3	1.69	0.73
23:Y:31:A:N3	23:Y:31:A:H2'	2.02	0.73
1:A:1110:G:O2'	9:I:16:ARG:NH2	2.21	0.73
5:E:80:ILE:HD12	5:E:91:LEU:HB2	1.68	0.73
4:D:13:ARG:O	4:D:15:GLU:N	2.22	0.72
5:E:143:ARG:NH1	8:H:77:GLU:OE2	2.22	0.72
1:A:1374:U:H2'	1:A:1375:G:C8	2.24	0.72
2:B:115:LEU:HD13	2:B:145:LEU:HB3	1.71	0.72
1:A:1040:G:H5"	3:C:154:SER:HB2	1.72	0.72
11:K:40:ILE:HG22	11:K:41:THR:HG23	1.71	0.71
17:Q:81:ARG:HB3	17:Q:84:LEU:HD12	1.72	0.71
1:A:184:G:H1	1:A:195:U:H3	1.38	0.71
1:A:231:C:H5'	17:Q:70:ARG:HG2	1.71	0.71
7:G:145:ALA:O	7:G:147:ALA:N	2.22	0.71
13:M:90:LEU:HA	13:M:93:ARG:HB2	1.73	0.70
10:J:6:ILE:HG22	10:J:98:ILE:HA	1.72	0.70
1:A:372:G:H5"	16:P:5:ARG:HD3	1.72	0.70
12:L:47:LYS:HB3	12:L:48:PRO:HD3	1.73	0.70
23:Y:34:I:C3'	23:Y:35:G:P	2.80	0.70
1:A:822:G:H1	1:A:826:C:N4	1.89	0.70
1:A:516:A:N6	1:A:1188:G:O2'	2.25	0.69
7:G:15:ASP:OD1	7:G:44:TYR:OH	2.11	0.69
1:A:1037:C:N4	23:Y:34:I:C8	2.61	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1037:C:N3	23:Y:34:I:O4'	2.27	0.68
1:A:386:C:O3'	16:P:28:ARG:NH2	2.26	0.68
1:A:1208:C:OP2	13:M:103:THR:HG21	1.93	0.68
1:A:79:A:H61	1:A:85:C:H42	1.40	0.68
2:B:71:VAL:HG12	2:B:93:VAL:HB	1.75	0.68
1:A:648:G:H22	1:A:725:G:H1	1.42	0.68
18:R:56:THR:HB	18:R:58:LEU:HD13	1.76	0.67
19:S:64:GLU:O	19:S:66:MET:N	2.28	0.67
1:A:1310:C:OP1	21:U:21:TYR:OH	2.12	0.67
16:P:57:ARG:NH1	16:P:79:VAL:O	2.28	0.67
1:A:1349:C:H2'	1:A:1350:C:C6	2.29	0.67
12:L:28:LYS:O	12:L:30:ALA:N	2.29	0.66
1:A:9:A:C6	4:D:209:ARG:HB3	2.30	0.66
16:P:28:ARG:HG2	16:P:29:ASP:OD1	1.95	0.66
1:A:1052:C:O2'	1:A:1174:C:H1'	1.95	0.66
23:Y:33:U:H3'	23:Y:34:I:P	2.35	0.66
2:B:17:PHE:HB3	2:B:44:LEU:HD21	1.78	0.66
1:A:924:A:H2'	1:A:925:G:C8	2.30	0.66
5:E:144:THR:O	5:E:148:VAL:HG23	1.95	0.66
2:B:140:HIS:HA	2:B:143:GLU:HG2	1.76	0.66
4:D:4:TYR:HD2	4:D:115:ARG:HH12	1.44	0.66
5:E:71:LEU:O	5:E:73:ASN:N	2.29	0.66
8:H:10:LEU:HD22	8:H:83:ILE:HD11	1.78	0.65
1:A:950:C:O3'	10:J:57:LYS:HG2	1.95	0.65
1:A:812:A:N6	1:A:836:G:O2'	2.30	0.65
14:N:24:CYS:HB2	14:N:40:CYS:HB3	1.79	0.65
12:L:47:LYS:HB3	12:L:48:PRO:CD	2.27	0.65
2:B:91:PRO:HG3	2:B:154:LEU:HB2	1.79	0.65
7:G:26:PHE:CE2	7:G:30:ILE:HD11	2.31	0.65
17:Q:66:SER:HB3	17:Q:69:LYS:HB2	1.79	0.64
1:A:1375:G:N2	1:A:1480:A:H8	1.95	0.64
1:A:1207:A:OP1	13:M:103:THR:HG22	1.97	0.64
1:A:821:G:H1	1:A:827:C:H42	1.43	0.64
2:B:158:LEU:HD23	2:B:182:ILE:HD11	1.77	0.64
4:D:8:VAL:O	4:D:10:ARG:N	2.22	0.64
1:A:778:A:H2'	1:A:779:C:C6	2.32	0.64
1:A:1418:G:H2'	1:A:1419:U:C6	2.31	0.64
1:A:295:G:H2'	1:A:296:A:C8	2.33	0.64
1:A:1169:G:OP1	9:I:113:LYS:HE2	1.97	0.64
1:A:1473:U:H2'	1:A:1474:C:H6	1.62	0.64
1:A:1287:G:H22	1:A:1313:G:H2'	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:17:VAL:O	13:M:20:THR:HB	1.98	0.64
1:A:1261:A:O2'	1:A:1263:U:OP2	2.14	0.64
1:A:144:A:H2'	1:A:145:C:C6	2.33	0.64
1:A:1107:G:O2'	1:A:1128:C:N4	2.29	0.64
1:A:1269:A:C8	1:A:1270:A:N7	2.66	0.63
4:D:36:ARG:O	4:D:38:TYR:N	2.30	0.63
1:A:1288:A:N6	1:A:1313:G:H1'	2.13	0.63
14:N:29:ARG:HD3	14:N:40:CYS:CB	2.29	0.63
1:A:715:G:OP1	1:A:750:A:H1'	1.99	0.63
1:A:1509:A:O2'	1:A:1510:U:O5'	2.17	0.63
3:C:114:PRO:O	3:C:118:GLN:HB2	1.99	0.63
4:D:165:MET:HA	4:D:168:ARG:HB2	1.79	0.63
1:A:1037:C:C2	23:Y:34:I:O4'	2.52	0.62
1:A:953:A:C8	1:A:953:A:H5'	2.30	0.62
9:I:10:ARG:HD3	9:I:75:ASP:HB3	1.81	0.62
15:O:16:ALA:HB1	15:O:21:ASP:HB3	1.79	0.62
4:D:9:CYS:HA	4:D:12:CYS:HB2	1.81	0.62
1:A:521:G:OP1	12:L:113:ARG:NH2	2.32	0.62
1:A:36:G:O2'	12:L:118:SER:O	2.13	0.62
2:B:76:GLN:HB3	2:B:208:ILE:HG13	1.81	0.62
23:Y:34:I:C8	23:Y:34:I:H4'	2.35	0.62
20:T:60:GLU:HA	20:T:63:ILE:HD12	1.82	0.62
1:A:77:G:N1	1:A:87:C:H5	1.95	0.61
1:A:609:G:H2'	1:A:610:U:C6	2.36	0.61
4:D:25:ARG:O	4:D:27:TYR:N	2.33	0.61
1:A:1014:G:H1'	1:A:1015:G:N2	2.16	0.61
1:A:1232:A:H2'	1:A:1232:A:N3	2.14	0.61
1:A:954:G:H5'	1:A:1340:U:O2'	2.00	0.61
12:L:90:VAL:HG11	12:L:93:LEU:HG	1.82	0.61
11:K:85:ARG:NH1	11:K:111:ASP:OD1	2.33	0.61
1:A:1309:C:OP2	21:U:12:LYS:NZ	2.31	0.61
7:G:113:GLU:HG2	7:G:119:ARG:HG2	1.82	0.61
1:A:81:U:OP2	1:A:81:U:H6	1.84	0.61
1:A:1134:A:HO2'	1:A:1135:A:H8	1.46	0.61
1:A:1124:C:H2'	1:A:1125:G:H8	1.66	0.61
19:S:18:LYS:O	19:S:22:LEU:HB2	2.01	0.61
7:G:88:PRO:HG2	7:G:152:ALA:HB2	1.82	0.61
5:E:51:VAL:HB	5:E:52:PRO:HD3	1.82	0.61
10:J:45:ARG:HH11	10:J:45:ARG:HB3	1.65	0.61
1:A:1040:G:H5"	3:C:154:SER:CB	2.31	0.60
1:A:524:G:H2'	1:A:525:G:O4'	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1130:C:O2	9:I:16:ARG:CZ	2.49	0.60
3:C:52:LEU:H	3:C:52:LEU:HD23	1.67	0.60
1:A:822:G:H1	1:A:826:C:H42	1.48	0.60
3:C:15:THR:HG23	3:C:181:ASN:HA	1.82	0.60
1:A:1295:U:OP1	19:S:6:LYS:HG3	2.01	0.60
2:B:231:GLU:HG3	2:B:233:SER:H	1.65	0.60
1:A:1198:G:OP1	14:N:2:ALA:HB1	2.01	0.60
1:A:1035:U:O2'	1:A:1038:A:OP2	2.12	0.60
13:M:10:PRO:HB2	13:M:18:ALA:HB1	1.83	0.60
13:M:5:ALA:O	13:M:7:VAL:N	2.35	0.60
1:A:955:A:H2'	1:A:956:A:H5'	1.84	0.60
2:B:191:ASP:N	2:B:191:ASP:OD1	2.35	0.60
2:B:136:VAL:O	2:B:140:HIS:N	2.34	0.60
9:I:17:VAL:HG11	9:I:81:ILE:HD13	1.83	0.60
1:A:1299:C:N3	19:S:37:ARG:NH2	2.50	0.60
1:A:969:U:O4	1:A:1194:U:O2'	2.15	0.59
17:Q:59:ILE:HD13	17:Q:73:VAL:HA	1.84	0.59
16:P:34:GLU:HG2	16:P:36:ILE:HG23	1.83	0.59
16:P:11:SER:H	16:P:14:ASN:HB3	1.67	0.59
20:T:43:LEU:HD13	20:T:51:GLU:HG2	1.83	0.59
1:A:951:G:H3'	1:A:952:A:H5"	1.84	0.59
9:I:16:ARG:HB2	9:I:64:THR:HG23	1.85	0.59
1:A:1248:G:N2	1:A:1251:A:OP2	2.35	0.59
1:A:1476:U:OP2	1:A:1520:U:O2'	2.20	0.59
4:D:12:CYS:SG	4:D:19:LEU:O	2.61	0.59
1:A:896:A:H2'	1:A:897:A:C8	2.37	0.59
2:B:195:ASP:O	8:H:68:ARG:NH2	2.36	0.59
10:J:6:ILE:HD11	10:J:23:ILE:HG21	1.85	0.59
5:E:147:ASP:OD1	5:E:147:ASP:N	2.35	0.59
1:A:103:A:H2'	1:A:322:G:N2	2.18	0.59
4:D:23:GLY:HA3	4:D:112:VAL:HG22	1.84	0.58
1:A:417:U:O2'	1:A:419:G:O6	2.19	0.58
1:A:700:A:N3	11:K:117:ASN:O	2.36	0.58
1:A:514:G:H1'	23:Y:35:G:O2'	2.04	0.58
4:D:49:ARG:HD3	4:D:50:ARG:H	1.68	0.58
1:A:1480:A:H2	1:A:1483:G:H1	1.50	0.58
8:H:1:MET:O	8:H:2:LEU:HB2	2.03	0.58
3:C:32:LEU:O	3:C:36:ASP:HB2	2.04	0.58
12:L:41:ARG:HG2	12:L:42:THR:H	1.68	0.58
1:A:690:A:N3	11:K:31:THR:HG21	2.20	0.57
15:O:39:LEU:HD12	15:O:56:LEU:HD13	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1135:A:OP1	10:J:68:HIS:ND1	2.33	0.57
1:A:97:C:P	20:T:17:ARG:HH21	2.26	0.57
2:B:88:ALA:HB2	2:B:219:VAL:HG13	1.86	0.57
2:B:168:THR:HG23	2:B:192:SER:HA	1.85	0.57
1:A:1205:C:P	19:S:78:ARG:HH21	2.27	0.57
7:G:62:PHE:HA	7:G:124:LEU:HD22	1.86	0.57
1:A:702:G:C8	11:K:116:HIS:HB3	2.39	0.57
1:A:1056:U:OP2	5:E:57:LYS:NZ	2.32	0.57
1:A:1231:C:N4	1:A:1270:A:H62	2.03	0.57
17:Q:68:ARG:H	17:Q:70:ARG:NH1	2.02	0.57
1:A:1375:G:H21	1:A:1480:A:H8	1.50	0.57
1:A:81:U:O2	1:A:82:U:O2	2.23	0.57
3:C:130:VAL:O	3:C:134:ILE:HG12	2.04	0.57
1:A:661:U:H3	1:A:697:G:H22	1.53	0.57
1:A:1087:G:OP1	2:B:144:ARG:NH1	2.38	0.57
1:A:1522:U:O3'	22:X:4:U:C5'	2.53	0.56
1:A:1112:C:O2'	1:A:1114:G:H8	1.88	0.56
1:A:1113:A:H4'	9:I:3:GLN:HE22	1.71	0.56
3:C:34:LEU:O	3:C:38:ARG:HG3	2.04	0.56
2:B:80:ILE:HD11	2:B:212:GLN:HA	1.87	0.56
1:A:1031:G:OP1	14:N:4:LYS:HB2	2.04	0.56
5:E:95:ALA:O	5:E:98:THR:OG1	2.21	0.56
1:A:400:U:H2'	1:A:401:U:H6	1.68	0.56
1:A:262:G:H5'	1:A:264:C:H41	1.69	0.56
1:A:1120:C:HO2'	1:A:1121:G:N2	2.01	0.56
1:A:1084:A:H4'	1:A:1085:A:O5'	2.04	0.56
1:A:1488:U:H2'	1:A:1489:G:C8	2.41	0.56
1:A:1064:G:P	5:E:16:THR:HG1	2.28	0.56
1:A:636:U:O4	1:A:736:G:O2'	2.16	0.56
1:A:653:U:H2'	1:A:654:G:C8	2.40	0.56
5:E:16:THR:OG1	5:E:17:ALA:N	2.35	0.56
9:I:70:LYS:O	9:I:74:ILE:HG13	2.05	0.56
2:B:61:LEU:HD21	2:B:68:ILE:HD11	1.88	0.56
1:A:1384:G:C2	1:A:1385:C:H1'	2.41	0.56
1:A:1111:C:O2'	1:A:1112:C:H5"	2.05	0.56
1:A:262:G:H5"	1:A:263:C:C5	2.41	0.56
4:D:150:GLU:HA	4:D:153:ARG:HG3	1.86	0.56
1:A:526:G:H2'	1:A:527:C:H6	1.71	0.56
1:A:982:G:N2	1:A:1022:C:N3	2.52	0.55
6:F:1:MET:HA	6:F:69:GLU:OE1	2.07	0.55
9:I:9:ARG:HG2	9:I:14:VAL:HG22	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:21:VAL:HG22	16:P:33:ILE:HB	1.87	0.55
1:A:1078:U:P	1:A:1091:G:H1	2.29	0.55
1:A:657:G:H2'	1:A:658:G:C8	2.42	0.55
6:F:70:ASP:N	6:F:70:ASP:OD1	2.35	0.55
5:E:15:ARG:HD2	5:E:26:PHE:CD2	2.41	0.55
1:A:836:G:C5'	1:A:836:G:H8	2.18	0.55
1:A:836:G:C6	1:A:847:G:C8	2.94	0.55
4:D:155:LEU:HB2	4:D:158:ILE:HG12	1.89	0.55
10:J:38:ILE:HG12	10:J:71:LEU:HB3	1.88	0.55
1:A:1309:C:OP1	21:U:20:LYS:HB3	2.06	0.55
1:A:1144:C:H2'	1:A:1145:C:C6	2.41	0.55
1:A:340:A:H5"	1:A:341:C:C5	2.42	0.55
1:A:1280:C:H4'	1:A:1281:A:O4'	2.06	0.55
11:K:44:SER:H	11:K:47:VAL:HB	1.72	0.55
3:C:81:GLY:O	3:C:83:ARG:N	2.39	0.55
1:A:1061:U:H5"	1:A:1062:G:OP2	2.07	0.55
13:M:13:LYS:HA	13:M:44:ARG:HH11	1.70	0.55
1:A:523:A:H2'	1:A:524:G:H8	1.71	0.55
1:A:258:A:C6	1:A:259:A:C6	2.95	0.55
15:O:12:ILE:HG12	15:O:31:LEU:HD21	1.88	0.55
1:A:671:A:H4'	1:A:672:G:O5'	2.07	0.55
1:A:1130:C:O2	9:I:16:ARG:NE	2.41	0.54
13:M:97:PRO:HA	13:M:110:ARG:HD3	1.90	0.54
13:M:37:THR:O	13:M:55:ARG:NH2	2.39	0.54
9:I:4:TYR:CZ	9:I:88:TYR:HD1	2.26	0.54
1:A:779:C:H5"	1:A:780:C:OP2	2.07	0.54
2:B:126:GLU:HG3	2:B:129:GLU:OE2	2.08	0.54
10:J:5:ARG:HA	10:J:73:ASP:OD1	2.07	0.54
12:L:53:ARG:HG2	12:L:69:TYR:HE1	1.73	0.54
1:A:765:A:H5'	1:A:766:A:OP2	2.07	0.54
1:A:855:C:H5"	8:H:88:LYS:HD3	1.88	0.54
1:A:1183:A:H4'	1:A:1184:G:O5'	2.07	0.54
1:A:1510:U:O2	1:A:1511:C:H5"	2.07	0.54
20:T:18:GLN:O	20:T:22:ARG:HG3	2.08	0.54
18:R:73:ALA:HB3	18:R:79:LEU:HD12	1.90	0.54
10:J:50:ILE:HG22	10:J:60:ARG:HG2	1.89	0.54
10:J:91:PRO:O	10:J:92:THR:HG23	2.07	0.54
1:A:1482:G:OP1	1:A:1485:A:H4'	2.08	0.54
1:A:372:G:OP2	16:P:67:THR:HG21	2.07	0.54
1:A:604:C:C2	4:D:135:LEU:HG	2.43	0.54
19:S:50:ALA:HB1	19:S:57:HIS:HB3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1268:A:C8	1:A:1269:A:H4'	2.43	0.53
1:A:1303:C:H3'	1:A:1304:C:H5"	1.89	0.53
1:A:836:G:N2	1:A:848:U:OP2	2.41	0.53
1:A:648:G:H22	1:A:725:G:H22	1.56	0.53
4:D:101:LEU:O	4:D:103:ASN:N	2.41	0.53
5:E:8:GLU:OE2	5:E:63:ARG:NH2	2.41	0.53
5:E:92:LYS:HB3	5:E:119:LEU:HB2	1.90	0.53
20:T:53:LEU:HD23	20:T:102:GLY:HA3	1.89	0.53
3:C:110:ASN:O	3:C:111:LEU:HD23	2.07	0.53
8:H:17:THR:HB	8:H:78:GLN:OE1	2.08	0.53
1:A:1009:C:H4'	1:A:1010:G:H5'	1.90	0.53
15:O:82:ILE:O	15:O:86:GLY:N	2.42	0.53
4:D:82:ALA:O	4:D:84:LYS:N	2.40	0.53
1:A:1101:C:H1'	1:A:1161:A:C4	2.42	0.53
1:A:775:G:C6	1:A:776:A:N7	2.76	0.53
7:G:84:ASN:N	7:G:84:ASN:OD1	2.42	0.53
7:G:26:PHE:O	7:G:30:ILE:HG13	2.09	0.53
10:J:4:ILE:HG22	10:J:74:ILE:HG13	1.91	0.53
21:U:5:ASP:O	21:U:11:GLY:HA3	2.09	0.53
2:B:197:VAL:HG12	2:B:200:ILE:HG12	1.90	0.53
1:A:720:C:H2'	1:A:721:A:C8	2.44	0.53
3:C:11:ARG:HH11	3:C:11:ARG:HG2	1.74	0.53
1:A:1311:A:P	13:M:28:ALA:HB3	2.49	0.53
10:J:30:SER:HB2	10:J:80:LYS:O	2.08	0.53
1:A:1477:A:O2'	1:A:1478:A:H5'	2.08	0.53
1:A:1144:C:H2'	1:A:1145:C:H6	1.72	0.53
2:B:142:LEU:O	2:B:142:LEU:HD23	2.09	0.53
12:L:6:THR:OG1	12:L:9:GLN:HG3	2.09	0.53
2:B:21:ARG:HB2	2:B:39:ILE:HG23	1.90	0.53
17:Q:67:LYS:HA	17:Q:70:ARG:HH12	1.74	0.52
1:A:1480:A:H2	1:A:1483:G:N1	2.07	0.52
1:A:239:A:H4'	1:A:240:U:H5"	1.90	0.52
3:C:87:LEU:HA	3:C:90:GLU:HB2	1.90	0.52
19:S:50:ALA:HA	19:S:58:VAL:O	2.10	0.52
5:E:80:ILE:HD13	5:E:138:ALA:HB1	1.89	0.52
4:D:8:VAL:C	4:D:10:ARG:H	2.08	0.52
1:A:324:C:O2	1:A:324:C:C2'	2.57	0.52
10:J:50:ILE:CG2	10:J:60:ARG:HG2	2.39	0.52
4:D:173:TRP:HB2	4:D:187:ARG:HG3	1.90	0.52
3:C:19:GLU:O	3:C:40:ARG:NH2	2.34	0.52
8:H:119:LEU:HD22	8:H:123:GLU:HB3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:507:A:H61	12:L:92:ASP:HB2	1.74	0.52
1:A:965:G:H1	1:A:1200:C:H42	1.58	0.52
1:A:938:U:H1'	1:A:1205:C:H5'	1.92	0.52
1:A:1233:A:H8	9:I:68:GLY:H	1.56	0.52
1:A:931:G:C5'	1:A:943:A:H61	2.23	0.52
1:A:409:G:N2	1:A:424:G:H1'	2.23	0.52
20:T:72:LEU:HD11	20:T:80:ARG:HD2	1.91	0.52
1:A:37:C:O2'	12:L:117:ARG:NH2	2.42	0.52
16:P:26:ARG:HD2	16:P:31:LYS:O	2.10	0.52
1:A:1351:G:O2'	1:A:1352:C:H5'	2.10	0.52
5:E:39:GLY:HA2	5:E:69:VAL:HB	1.91	0.52
13:M:73:GLU:O	13:M:77:ASN:N	2.39	0.52
2:B:112:VAL:HG11	2:B:153:ARG:HA	1.92	0.52
10:J:27:ALA:HB2	10:J:85:LEU:HD11	1.90	0.52
1:A:1063:A:H5"	5:E:16:THR:HG21	1.92	0.52
5:E:8:GLU:HA	5:E:33:VAL:O	2.10	0.52
1:A:306:G:OP2	16:P:27:LYS:NZ	2.42	0.52
1:A:1172:G:OP1	3:C:4:LYS:HA	2.10	0.52
1:A:954:G:C8	1:A:1340:U:O2	2.63	0.52
2:B:75:LYS:HD3	2:B:76:GLN:HG3	1.91	0.52
2:B:21:ARG:HH21	2:B:39:ILE:HG12	1.75	0.52
2:B:101:MET:HA	2:B:108:ILE:HD12	1.92	0.52
1:A:1078:U:OP1	1:A:1091:G:N2	2.43	0.51
4:D:91:SER:OG	4:D:92:VAL:N	2.44	0.51
1:A:1394:C:H42	1:A:1467:G:H1	1.56	0.51
1:A:1042:C:O3'	14:N:45:ARG:NH2	2.43	0.51
1:A:1330:U:H2'	1:A:1331:A:H8	1.75	0.51
7:G:66:VAL:O	7:G:68:ASN:N	2.42	0.51
1:A:953:A:H4'	1:A:954:G:H5"	1.91	0.51
1:A:1160:G:N2	1:A:1162:A:H3'	2.25	0.51
3:C:206:GLU:O	3:C:208:ILE:N	2.44	0.51
4:D:128:VAL:HG12	4:D:129:ASN:ND2	2.24	0.51
1:A:207:G:H2'	1:A:208:C:O4'	2.10	0.51
1:A:1239:U:H4'	1:A:1239:U:OP2	2.10	0.51
1:A:1060:G:O6	5:E:47:LYS:NZ	2.44	0.51
5:E:110:LEU:HD13	5:E:118:ILE:HG21	1.91	0.51
23:Y:34:I:C8	23:Y:34:I:C4'	2.93	0.51
1:A:565:G:C8	1:A:565:G:O5'	2.56	0.51
6:F:8:ILE:HD11	6:F:79:LEU:HD21	1.92	0.51
9:I:26:VAL:HG13	9:I:61:ALA:HB3	1.93	0.51
1:A:911:G:O6	7:G:3:ARG:NH2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1473:U:H2'	1:A:1474:C:C6	2.44	0.51
4:D:60:GLU:OE1	4:D:199:ASN:N	2.27	0.51
6:F:60:PHE:CZ	18:R:78:LEU:HD21	2.46	0.51
1:A:46:U:H2'	1:A:47:G:C8	2.46	0.51
8:H:36:LEU:HD12	8:H:59:LEU:HD13	1.93	0.51
1:A:714:G:C5	1:A:715:G:H1'	2.45	0.51
1:A:400:U:H2'	1:A:401:U:C6	2.44	0.51
1:A:1172:G:O2'	3:C:3:ASN:CB	2.58	0.51
1:A:1140:A:H4'	1:A:1141:C:O5'	2.10	0.51
1:A:372:G:P	16:P:67:THR:HG21	2.51	0.51
4:D:15:GLU:HG2	4:D:63:LYS:HG3	1.92	0.50
12:L:47:LYS:CB	12:L:48:PRO:HD3	2.39	0.50
3:C:148:GLY:HA3	3:C:172:ARG:O	2.10	0.50
1:A:1210:C:H4'	13:M:116:THR:HA	1.93	0.50
3:C:70:VAL:HG12	3:C:72:LYS:H	1.76	0.50
20:T:25:ARG:O	20:T:29:LYS:HG3	2.11	0.50
2:B:52:GLU:HB2	2:B:56:ARG:NH2	2.26	0.50
18:R:46:GLU:OE2	18:R:46:GLU:N	2.35	0.50
1:A:366:C:C2	1:A:367:G:C8	2.99	0.50
1:A:1508:G:OP1	1:A:1508:G:H4'	2.11	0.50
2:B:86:GLU:C	2:B:88:ALA:H	2.14	0.50
12:L:90:VAL:O	12:L:91:LYS:CB	2.59	0.50
1:A:1207:A:H2'	1:A:1208:C:C5	2.45	0.50
1:A:1124:C:H2'	1:A:1125:G:C8	2.45	0.50
20:T:45:GLN:HA	20:T:91:LEU:HD22	1.91	0.50
15:O:17:ARG:HD3	15:O:26:GLU:HG3	1.93	0.50
15:O:36:ILE:O	15:O:40:SER:OG	2.29	0.50
8:H:109:ILE:HG12	8:H:110:ALA:N	2.26	0.50
18:R:74:ARG:HB3	18:R:81:PHE:CE1	2.47	0.50
3:C:8:ILE:HG23	3:C:16:ARG:HG2	1.94	0.50
1:A:604:C:H2'	1:A:605:A:O4'	2.11	0.50
4:D:140:VAL:HG11	4:D:146:ILE:HD11	1.93	0.50
1:A:201:C:OP1	20:T:61:SER:OG	2.28	0.50
5:E:80:ILE:HA	8:H:104:ARG:HH22	1.77	0.50
1:A:932:G:H21	1:A:1209:A:H62	1.59	0.50
1:A:1280:C:H2'	7:G:114:ARG:NH1	2.27	0.50
1:A:265:C:H2'	1:A:266:A:C8	2.46	0.50
1:A:1453:G:H2'	1:A:1454:G:H8	1.77	0.50
4:D:15:GLU:OE2	4:D:59:ARG:NH1	2.45	0.50
2:B:15:VAL:H	2:B:16:HIS:CE1	2.30	0.50
13:M:57:ARG:O	13:M:61:GLU:HB2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:496:U:H2'	1:A:497:C:H6	1.77	0.50
1:A:1189:G:H2'	1:A:1190:C:C6	2.47	0.49
3:C:7:PRO:O	3:C:11:ARG:HG2	2.11	0.49
9:I:118:LYS:HB3	9:I:121:ARG:HB3	1.94	0.49
1:A:1086:C:H5"	2:B:98:LEU:HD13	1.93	0.49
1:A:1223:G:H2'	1:A:1224:C:C6	2.46	0.49
7:G:15:ASP:HB3	7:G:20:ASP:H	1.76	0.49
10:J:61:GLU:OE1	14:N:58:LYS:HE2	2.13	0.49
17:Q:86:GLU:O	17:Q:90:ILE:HG12	2.12	0.49
1:A:523:A:H2'	1:A:524:G:C8	2.48	0.49
3:C:150:LYS:HG3	3:C:169:ALA:HB2	1.94	0.49
13:M:40:ASN:HB3	13:M:43:THR:HG23	1.94	0.49
12:L:8:ASN:O	12:L:12:ARG:HG3	2.12	0.49
23:Y:33:U:C3'	23:Y:34:I:P	3.00	0.49
19:S:64:GLU:O	19:S:67:VAL:HG23	2.13	0.49
9:I:32:ASP:OD1	9:I:33:PHE:N	2.45	0.49
4:D:61:LYS:HD2	4:D:207:TYR:OH	2.12	0.49
1:A:659:A:O2'	11:K:114:VAL:O	2.29	0.49
1:A:836:G:H8	1:A:836:G:O5'	1.95	0.49
1:A:1135:A:H4'	10:J:13:HIS:HD2	1.77	0.49
12:L:25:PRO:C	12:L:27:LEU:H	2.16	0.49
1:A:989:G:O6	1:A:998:C:N4	2.44	0.49
12:L:43:VAL:HG12	12:L:44:THR:O	2.12	0.49
1:A:399:C:OP1	4:D:137:SER:OG	2.31	0.49
1:A:1364:U:H2'	1:A:1365:C:H6	1.77	0.49
1:A:1128:C:H4'	1:A:1129:A:O5'	2.13	0.49
16:P:22:THR:HA	16:P:33:ILE:HG13	1.94	0.49
12:L:86:ARG:NH1	12:L:87:GLY:O	2.45	0.49
1:A:777:U:H5'	1:A:778:A:H5"	1.95	0.49
1:A:921:U:C2'	1:A:922:G:H5'	2.43	0.49
8:H:4:ASP:OD2	8:H:85:ARG:NH1	2.46	0.49
9:I:104:ARG:O	9:I:104:ARG:HD2	2.13	0.49
1:A:955:A:C2'	1:A:956:A:H5'	2.43	0.49
21:U:12:LYS:HB3	21:U:22:ARG:HD2	1.94	0.49
1:A:410:A:H2'	1:A:411:A:O4'	2.13	0.49
9:I:34:ASN:N	9:I:34:ASN:OD1	2.46	0.49
23:Y:34:I:H3'	23:Y:35:G:OP2	2.13	0.49
1:A:1057:G:O3'	2:B:103:THR:CG2	2.61	0.49
1:A:1274:U:P	7:G:41:ARG:HH22	2.36	0.49
1:A:1278:C:H4'	1:A:1284:U:C5	2.47	0.49
3:C:58:GLU:O	3:C:64:VAL:HA	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:80:ILE:HD13	5:E:91:LEU:HD23	1.94	0.48
1:A:1021:C:H2'	1:A:1022:C:O2	2.13	0.48
5:E:41:VAL:O	5:E:67:VAL:HG12	2.13	0.48
1:A:1358:A:OP1	7:G:12:LEU:HD21	2.13	0.48
1:A:1261:A:O2'	1:A:1264:C:N4	2.46	0.48
2:B:194:PRO:O	2:B:196:LEU:N	2.46	0.48
1:A:1470:A:H1'	22:X:5:A:O2'	2.13	0.48
1:A:707:U:H2'	1:A:707:U:O2	2.12	0.48
1:A:1113:A:OP2	9:I:20:ARG:NH2	2.36	0.48
11:K:44:SER:OG	11:K:46:GLY:N	2.36	0.48
1:A:1331:A:H2'	1:A:1332:A:H8	1.78	0.48
12:L:38:THR:HG22	12:L:39:VAL:HG23	1.94	0.48
1:A:1238:A:H62	1:A:1260:U:C5'	2.26	0.48
1:A:359:A:OP1	12:L:33:ARG:HD2	2.13	0.48
7:G:16:LEU:CD1	9:I:42:ARG:HA	2.42	0.48
1:A:1188:G:C6	1:A:1189:G:C5	3.01	0.48
1:A:725:G:H2'	1:A:726:G:O4'	2.14	0.48
3:C:34:LEU:HG	3:C:38:ARG:HD2	1.94	0.48
1:A:765:A:C5	1:A:786:A:C2	3.02	0.48
1:A:397:C:O2'	1:A:605:A:N3	2.33	0.48
4:D:101:LEU:HD23	4:D:121:VAL:HG13	1.95	0.48
3:C:90:GLU:O	3:C:93:LYS:HB3	2.13	0.48
1:A:1408:U:H2'	1:A:1409:C:H6	1.78	0.48
1:A:954:G:C8	1:A:1340:U:C2	3.01	0.48
2:B:71:VAL:HG23	2:B:164:VAL:HA	1.95	0.48
1:A:340:A:H5"	1:A:341:C:H5	1.77	0.48
1:A:1234:A:H2	1:A:1235:G:C5	2.31	0.48
1:A:1331:A:H2'	1:A:1332:A:C8	2.48	0.48
1:A:1316:G:H5"	1:A:1317:C:OP2	2.12	0.48
1:A:1037:C:N3	23:Y:34:I:C1'	2.77	0.48
1:A:1205:C:P	19:S:78:ARG:NH2	2.86	0.48
9:I:118:LYS:O	9:I:119:ALA:HB3	2.13	0.48
9:I:28:VAL:HA	9:I:63:ILE:O	2.13	0.48
1:A:898:U:H2'	1:A:899:U:C6	2.49	0.48
1:A:967:C:HO2'	1:A:996:G:HO2'	1.47	0.48
20:T:10:LEU:O	20:T:13:LEU:HD23	2.13	0.48
14:N:43:CYS:O	14:N:44:LEU:HB2	2.13	0.48
3:C:55:VAL:HG12	3:C:55:VAL:O	2.14	0.48
1:A:1510:U:O2	1:A:1510:U:H2'	2.14	0.48
12:L:27:LEU:O	12:L:29:GLY:N	2.47	0.48
10:J:9:ARG:HG2	10:J:69:ASN:OD1	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:91:ARG:O	11:K:95:ILE:HG13	2.13	0.48
1:A:568:G:OP2	17:Q:87:LYS:NZ	2.34	0.48
3:C:23:TYR:C	3:C:23:TYR:CD1	2.87	0.48
1:A:1040:G:H2'	1:A:1041:G:O4'	2.14	0.48
20:T:14:LYS:HA	20:T:17:ARG:HG3	1.95	0.48
1:A:1211:A:C2	1:A:1212:C:C4	3.01	0.48
2:B:156:LYS:HD2	2:B:157:ARG:N	2.29	0.48
1:A:118:G:C6	1:A:119:U:C4	3.02	0.48
10:J:5:ARG:HG2	10:J:99:LYS:HB2	1.96	0.47
12:L:45:PRO:HD3	12:L:51:ALA:O	2.14	0.47
1:A:482:U:O2'	1:A:483:A:OP2	2.27	0.47
2:B:118:LEU:CB	2:B:142:LEU:HD12	2.44	0.47
1:A:42:G:H2'	1:A:43:G:C8	2.49	0.47
9:I:33:PHE:CZ	9:I:47:LEU:HD21	2.49	0.47
1:A:1358:A:C5	1:A:1359:U:C5	3.02	0.47
10:J:96:ILE:H	10:J:96:ILE:HD13	1.79	0.47
1:A:514:G:O6	22:X:6:G:H1'	2.14	0.47
1:A:1296:C:OP2	19:S:6:LYS:HE2	2.15	0.47
1:A:955:A:C8	1:A:1205:C:N3	2.82	0.47
1:A:1349:C:O2'	1:A:1350:C:H5'	2.14	0.47
13:M:20:THR:HA	13:M:25:ILE:HG22	1.96	0.47
2:B:208:ILE:HD12	2:B:208:ILE:H	1.78	0.47
2:B:167:PRO:HD2	2:B:192:SER:OG	2.15	0.47
2:B:55:PHE:HA	2:B:58:ILE:HG12	1.95	0.47
3:C:188:LEU:O	3:C:189:ALA:HB2	2.15	0.47
10:J:49:VAL:O	10:J:60:ARG:HB3	2.15	0.47
1:A:980:G:N1	1:A:981:G:O6	2.47	0.47
3:C:95:THR:O	3:C:97:LYS:N	2.47	0.47
6:F:50:TYR:CE1	18:R:77:GLY:HA2	2.50	0.47
4:D:121:VAL:O	4:D:134:ASP:HA	2.15	0.47
1:A:508:G:H2'	1:A:509:C:C6	2.50	0.47
2:B:95:GLN:HE21	2:B:147:LYS:HE2	1.79	0.47
1:A:1382:C:C2	1:A:1384:G:C5	3.02	0.47
1:A:690:A:C1'	11:K:29:ILE:HD11	2.44	0.47
1:A:1208:C:C4	13:M:104:ARG:HG2	2.49	0.47
1:A:1209:A:H3'	1:A:1209:A:C8	2.49	0.47
8:H:6:ILE:O	8:H:10:LEU:HG	2.14	0.47
1:A:1509:A:O2'	1:A:1510:U:P	2.72	0.47
5:E:50:GLU:OE2	5:E:51:VAL:HG23	2.14	0.47
1:A:397:C:OP1	4:D:73:ARG:NH1	2.47	0.47
6:F:35:ALA:HA	6:F:67:MET:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:486:G:C2	1:A:487:C:C2	3.03	0.47
5:E:13:ILE:HA	5:E:29:GLY:O	2.15	0.47
8:H:86:ILE:HG12	8:H:135:CYS:HA	1.96	0.47
5:E:107:ARG:HG2	5:E:108:ALA:N	2.29	0.47
14:N:6:LEU:HD23	14:N:23:ARG:HH22	1.79	0.47
4:D:196:LEU:HD23	4:D:197:PRO:HD2	1.97	0.47
10:J:57:LYS:HD2	10:J:60:ARG:NH2	2.30	0.47
1:A:231:C:C5'	17:Q:70:ARG:HG2	2.43	0.47
1:A:1107:G:H4'	10:J:38:ILE:HD12	1.97	0.47
1:A:1324:C:O2'	1:A:1325:G:H5'	2.15	0.47
19:S:33:THR:OG1	19:S:35:SER:OG	2.17	0.47
5:E:50:GLU:HG3	5:E:52:PRO:HD2	1.97	0.47
1:A:401:U:O2	1:A:482:U:O2'	2.33	0.47
9:I:8:GLY:HA2	9:I:79:LEU:HD12	1.97	0.47
10:J:48:THR:OG1	10:J:62:HIS:CD2	2.67	0.47
1:A:596:C:O2	1:A:613:G:N2	2.48	0.47
17:Q:4:LYS:HE2	17:Q:6:LEU:HD21	1.97	0.47
3:C:136:GLN:O	3:C:139:GLN:N	2.48	0.47
17:Q:5:VAL:HG22	17:Q:60:ILE:HG13	1.96	0.47
3:C:91:LEU:HB3	3:C:99:VAL:HG11	1.95	0.47
1:A:1403:C:H2'	1:A:1404:G:O4'	2.15	0.47
1:A:1209:A:H3'	1:A:1209:A:H8	1.80	0.47
4:D:8:VAL:HG12	4:D:21:LEU:HD13	1.96	0.47
1:A:1474:C:H2'	1:A:1475:G:O4'	2.15	0.47
1:A:970:U:H4'	1:A:971:G:O5'	2.14	0.47
1:A:1329:G:N2	1:A:1356:G:H2'	2.30	0.47
1:A:81:U:H4'	1:A:82:U:OP1	2.15	0.46
1:A:1113:A:H5"	9:I:20:ARG:NH2	2.30	0.46
6:F:69:GLU:O	6:F:72:VAL:HG12	2.14	0.46
3:C:179:ARG:O	3:C:206:GLU:HG3	2.16	0.46
13:M:3:ARG:HA	13:M:8:GLU:O	2.14	0.46
8:H:10:LEU:HB3	8:H:83:ILE:HG12	1.97	0.46
1:A:144:A:H2'	1:A:145:C:H6	1.79	0.46
1:A:1057:G:O3'	2:B:103:THR:HG21	2.16	0.46
1:A:1422:C:OP1	20:T:38:LYS:HE2	2.15	0.46
10:J:30:SER:O	10:J:81:THR:HG22	2.15	0.46
5:E:13:ILE:HD12	5:E:13:ILE:O	2.15	0.46
1:A:355:U:H2'	1:A:356:A:C8	2.50	0.46
4:D:31:CYS:C	4:D:33:MET:H	2.19	0.46
7:G:99:LEU:HD22	7:G:103:TRP:CZ2	2.50	0.46
1:A:931:G:H5'	1:A:943:A:H61	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:95:THR:C	3:C:97:LYS:H	2.18	0.46
17:Q:29:HIS:CG	17:Q:30:PRO:HD2	2.50	0.46
1:A:798:A:H2'	1:A:800:A:C5'	2.45	0.46
1:A:1333:U:H1'	7:G:33:ASP:HB3	1.97	0.46
12:L:34:ARG:O	12:L:61:THR:HG23	2.14	0.46
7:G:104:LEU:HD13	7:G:104:LEU:HA	1.69	0.46
23:Y:34:I:H2'	23:Y:35:G:C8	2.51	0.46
1:A:1232:A:H4'	9:I:67:GLY:H	1.80	0.46
2:B:109:SER:O	2:B:112:VAL:N	2.37	0.46
4:D:3:ARG:HG2	4:D:118:ARG:CZ	2.46	0.46
19:S:41:VAL:HB	19:S:42:PRO:HD2	1.97	0.46
20:T:74:LYS:HB3	20:T:74:LYS:HE3	1.76	0.46
1:A:42:G:H2'	1:A:43:G:H8	1.81	0.46
1:A:8:G:O2'	5:E:120:THR:O	2.33	0.46
16:P:60:LEU:HD23	16:P:60:LEU:HA	1.72	0.46
16:P:74:LEU:O	16:P:79:VAL:HG23	2.15	0.46
1:A:1470:A:H1'	22:X:5:A:HO2'	1.81	0.46
13:M:23:TYR:HB3	13:M:67:GLU:HA	1.98	0.46
1:A:733:C:OP2	1:A:734:G:OP2	2.34	0.46
1:A:1220:A:C8	1:A:1285:C:H1'	2.50	0.46
1:A:1395:C:H2'	1:A:1396:A:C8	2.50	0.46
1:A:915:A:H8	1:A:915:A:O5'	1.99	0.46
1:A:1017:G:H2'	1:A:1017:G:N3	2.31	0.46
9:I:100:GLY:C	9:I:102:LEU:H	2.17	0.46
1:A:1385:C:O2	1:A:1478:A:N1	2.49	0.46
1:A:1087:G:H4'	2:B:111:ARG:NH1	2.30	0.46
1:A:943:A:H4'	1:A:944:G:OP1	2.15	0.46
1:A:990:G:N2	1:A:998:C:O2	2.48	0.46
6:F:99:ALA:O	18:R:28:GLU:HA	2.16	0.46
9:I:93:ARG:C	9:I:95:LYS:H	2.18	0.46
1:A:177:U:C4	1:A:178:G:H1'	2.51	0.46
11:K:61:ALA:HB2	11:K:90:GLY:HA3	1.97	0.46
1:A:1044:G:OP1	10:J:59:SER:OG	2.32	0.46
23:Y:33:U:O2'	23:Y:35:G:N7	2.43	0.46
1:A:1015:G:HO2'	1:A:1016:G:C5'	2.28	0.46
1:A:373:G:OP1	16:P:3:LYS:HD3	2.16	0.46
4:D:102:ASP:HB3	4:D:136:PRO:HB3	1.97	0.46
12:L:36:VAL:HG22	12:L:82:VAL:HG22	1.97	0.46
8:H:14:ARG:O	8:H:18:ARG:HD3	2.15	0.46
1:A:632:A:H2'	1:A:633:G:O4'	2.15	0.46
2:B:235:SER:OG	2:B:235:SER:O	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:24:LEU:HD22	20:T:24:LEU:HA	1.78	0.46
20:T:72:LEU:HD21	20:T:80:ARG:NE	2.31	0.46
19:S:9:VAL:HG23	19:S:11:VAL:HG12	1.97	0.46
1:A:1214:U:OP1	9:I:124:GLN:HG2	2.16	0.46
5:E:102:ALA:HB1	5:E:106:PRO:HG2	1.96	0.46
6:F:55:ASP:OD2	6:F:86:ARG:NH1	2.48	0.46
4:D:139:ARG:HB2	4:D:139:ARG:NH1	2.30	0.46
1:A:770:G:C2	1:A:781:C:C2	3.04	0.46
1:A:878:A:H2'	1:A:879:A:C8	2.50	0.46
1:A:94:C:H2'	1:A:95:A:C8	2.50	0.46
1:A:1510:U:H2'	1:A:1511:C:H5"	1.98	0.45
1:A:207:G:H1	1:A:213:C:H42	1.64	0.45
3:C:70:VAL:HG12	3:C:71:ALA:N	2.30	0.45
5:E:127:ASN:HA	5:E:128:PRO:HD3	1.81	0.45
1:A:1104:U:C4	1:A:1105:U:C4	3.05	0.45
17:Q:100:LYS:HD2	17:Q:100:LYS:N	2.30	0.45
1:A:836:G:C5'	1:A:836:G:C8	3.00	0.45
1:A:372:G:H2'	1:A:373:G:H8	1.80	0.45
2:B:194:PRO:O	2:B:197:VAL:N	2.26	0.45
8:H:11:THR:HA	8:H:14:ARG:NH1	2.32	0.45
8:H:24:THR:HG22	8:H:25:ASP:O	2.16	0.45
9:I:29:ASN:N	9:I:29:ASN:OD1	2.49	0.45
8:H:73:ASP:OD1	8:H:75:ARG:HD3	2.15	0.45
5:E:68:GLU:CG	5:E:70:PRO:HD3	2.42	0.45
1:A:1402:G:C6	1:A:1403:C:N4	2.84	0.45
1:A:675:G:O2'	1:A:781:C:H4'	2.16	0.45
1:A:18:U:H2'	1:A:19:C:C6	2.51	0.45
13:M:86:CYS:SG	13:M:87:TYR:N	2.89	0.45
11:K:92:GLU:HB3	11:K:96:ARG:HH11	1.82	0.45
16:P:6:LEU:HD23	16:P:17:TYR:CG	2.50	0.45
16:P:9:PHE:CD1	16:P:18:ARG:HG3	2.51	0.45
1:A:1491:A:H2'	1:A:1492:C:C6	2.52	0.45
1:A:1210:C:H2'	1:A:1211:A:H8	1.81	0.45
15:O:26:GLU:OE2	15:O:77:ARG:HD2	2.16	0.45
1:A:561:G:H1'	1:A:800:A:N3	2.31	0.45
17:Q:55:ASP:N	17:Q:55:ASP:OD1	2.47	0.45
7:G:32:ARG:O	7:G:34:GLY:N	2.45	0.45
1:A:823:U:H5'	1:A:824:C:H5	1.82	0.45
9:I:57:GLY:C	9:I:59:PHE:H	2.19	0.45
1:A:312:G:OP2	1:A:347:G:O2'	2.33	0.45
1:A:125:A:N1	1:A:229:C:O2'	2.43	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1334:C:H2'	1:A:1335:G:C8	2.51	0.45
1:A:1125:G:H3'	1:A:1126:G:H8	1.81	0.45
4:D:82:ALA:O	4:D:84:LYS:HG2	2.16	0.45
1:A:1218:A:H4'	1:A:1286:G:H4'	1.98	0.45
2:B:19:HIS:HB2	2:B:204:ASN:ND2	2.32	0.45
1:A:1232:A:OP2	9:I:66:ARG:HA	2.17	0.45
19:S:58:VAL:HG23	19:S:58:VAL:O	2.16	0.45
2:B:21:ARG:HG3	2:B:22:LYS:HG2	1.98	0.45
1:A:324:C:H2'	1:A:324:C:O2	2.16	0.45
9:I:93:ARG:O	9:I:95:LYS:N	2.50	0.45
9:I:89:ASN:O	9:I:92:TYR:HB2	2.17	0.45
1:A:565:G:C6	1:A:742:G:C8	3.05	0.45
1:A:1208:C:N4	13:M:104:ARG:HG2	2.32	0.45
1:A:967:C:O2'	1:A:996:G:O2'	2.23	0.45
6:F:25:ILE:O	6:F:28:ARG:HB2	2.17	0.45
1:A:480:A:H4'	1:A:481:A:OP1	2.16	0.45
9:I:127:LYS:HB3	9:I:127:LYS:HE2	1.83	0.45
23:Y:34:I:H3'	23:Y:35:G:P	2.54	0.45
1:A:109:G:H1'	1:A:110:A:N7	2.32	0.45
1:A:1254:G:C8	1:A:1254:G:H5"	2.51	0.45
3:C:50:ALA:HB1	3:C:70:VAL:HG11	1.99	0.45
10:J:7:LYS:HB3	10:J:97:GLU:HB2	1.98	0.45
1:A:430:U:H2'	1:A:431:C:C6	2.52	0.45
1:A:1346:A:H1'	1:A:1348:G:N7	2.32	0.45
7:G:87:VAL:HG22	7:G:154:TYR:HD2	1.82	0.45
1:A:588:G:C5	1:A:589:U:C5	3.04	0.45
1:A:740:C:H2'	1:A:741:U:O4'	2.17	0.45
12:L:81:SER:O	12:L:106:ASP:HB2	2.16	0.45
15:O:33:THR:HG23	15:O:63:ARG:NH1	2.32	0.45
1:A:442:G:O5'	1:A:442:G:H8	2.00	0.45
19:S:47:HIS:O	19:S:62:ILE:HG22	2.17	0.45
1:A:982:G:H2'	1:A:983:A:O4'	2.16	0.45
7:G:79:ARG:HA	7:G:84:ASN:HA	1.99	0.45
12:L:49:ASN:ND2	12:L:92:ASP:OD2	2.39	0.45
5:E:110:LEU:O	5:E:115:VAL:HB	2.16	0.45
1:A:451:C:H42	1:A:461:G:H1	1.65	0.45
3:C:175:LEU:HD21	3:C:201:TYR:CE2	2.52	0.45
1:A:1291:G:H2'	1:A:1292:G:O4'	2.17	0.44
12:L:87:GLY:HA2	12:L:98:TYR:HA	1.99	0.44
1:A:1242:C:OP1	1:A:1266:C:O2'	2.31	0.44
1:A:616:A:H5'	1:A:617:G:OP2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Y:33:U:O3'	23:Y:34:I:P	2.75	0.44
4:D:19:LEU:HD13	4:D:19:LEU:HA	1.68	0.44
7:G:16:LEU:HD23	7:G:16:LEU:HA	1.75	0.44
5:E:69:VAL:O	5:E:71:LEU:HG	2.17	0.44
1:A:324:C:H4'	1:A:325:A:H5"	1.99	0.44
13:M:15:VAL:HG22	13:M:43:THR:O	2.17	0.44
3:C:35:GLU:HB3	3:C:59:ARG:HH22	1.81	0.44
3:C:23:TYR:CD1	3:C:24:ALA:N	2.85	0.44
1:A:1329:G:C6	9:I:107:ARG:NH2	2.85	0.44
2:B:218:ALA:O	2:B:222:ILE:HG13	2.18	0.44
1:A:289:G:H2'	1:A:290:U:H6	1.81	0.44
1:A:959:U:O5'	1:A:959:U:H6	2.00	0.44
1:A:1047:G:C2	1:A:1049:C:N4	2.85	0.44
1:A:648:G:N2	1:A:725:G:H22	2.15	0.44
1:A:109:G:H4'	1:A:110:A:O5'	2.17	0.44
10:J:58:ASP:O	10:J:59:SER:C	2.56	0.44
1:A:1446:A:H2'	1:A:1447:G:O4'	2.17	0.44
1:A:1342:A:H8	1:A:1342:A:OP1	2.00	0.44
10:J:8:LEU:HD11	10:J:23:ILE:HD12	1.98	0.44
1:A:1208:C:H4'	1:A:1209:A:OP1	2.18	0.44
1:A:673:C:OP1	11:K:44:SER:OG	2.25	0.44
1:A:859:G:P	12:L:12:ARG:HH22	2.41	0.44
1:A:1408:U:H2'	1:A:1409:C:C6	2.53	0.44
4:D:58:LEU:HD22	4:D:62:GLN:HG2	2.00	0.44
13:M:83:ASP:OD1	13:M:84:ILE:N	2.49	0.44
4:D:151:LYS:HD3	4:D:151:LYS:N	2.33	0.44
1:A:1151:A:C6	1:A:1152:A:C6	3.06	0.44
5:E:71:LEU:HD23	5:E:71:LEU:HA	1.88	0.44
1:A:1233:A:H1'	1:A:1353:G:H4'	1.99	0.44
13:M:11:ARG:HG2	13:M:12:ASN:N	2.33	0.44
1:A:1226:C:H42	1:A:1275:G:H1	1.64	0.44
6:F:77:ARG:NH1	6:F:78:GLU:HB2	2.33	0.44
1:A:522:G:H2'	1:A:523:A:C8	2.53	0.44
2:B:126:GLU:OE1	2:B:126:GLU:N	2.50	0.44
3:C:94:LEU:HD12	3:C:95:THR:H	1.82	0.44
5:E:37:ARG:O	5:E:38:GLN:HG3	2.17	0.44
5:E:88:LYS:HB3	5:E:123:LEU:HB2	2.00	0.44
1:A:667:G:H2'	1:A:668:A:O4'	2.18	0.44
1:A:980:G:C2	1:A:981:G:C6	3.05	0.44
21:U:12:LYS:O	21:U:16:GLY:N	2.48	0.44
1:A:1060:G:N2	1:A:1063:A:OP2	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:81:THR:C	10:J:83:GLU:H	2.21	0.44
1:A:486:G:H2'	1:A:487:C:O4'	2.18	0.44
1:A:1325:G:H2'	1:A:1326:C:C6	2.53	0.44
3:C:173:VAL:O	3:C:175:LEU:HD12	2.18	0.44
1:A:167:A:N7	1:A:169:C:C4	2.86	0.44
1:A:714:G:N7	1:A:715:G:H1'	2.33	0.43
18:R:32:ARG:HA	18:R:69:THR:HG21	2.00	0.43
1:A:787:G:C6	1:A:788:U:C4	3.06	0.43
1:A:956:A:H5"	1:A:957:C:OP2	2.18	0.43
9:I:16:ARG:HD2	9:I:64:THR:CG2	2.48	0.43
4:D:91:SER:O	4:D:94:LEU:N	2.50	0.43
1:A:727:U:H2'	1:A:728:C:C6	2.53	0.43
1:A:1036:G:O2'	1:A:1181:U:H5	2.01	0.43
3:C:152:ILE:HG13	3:C:167:TRP:HB2	2.00	0.43
1:A:1354:G:P	9:I:11:LYS:HD3	2.58	0.43
1:A:1270:A:H1'	1:A:1334:C:O2'	2.18	0.43
5:E:79:GLU:O	8:H:104:ARG:NH1	2.52	0.43
1:A:1375:G:C5	1:A:1376:U:C5	3.05	0.43
6:F:28:ARG:O	6:F:32:ASN:N	2.49	0.43
1:A:787:G:C5	1:A:788:U:C4	3.06	0.43
15:O:79:ARG:O	15:O:83:GLU:HG2	2.18	0.43
1:A:1250:A:N3	1:A:1308:C:O2'	2.43	0.43
10:J:16:LEU:HD23	10:J:16:LEU:HA	1.75	0.43
4:D:190:ASP:O	4:D:193:ASP:N	2.50	0.43
17:Q:55:ASP:HB3	17:Q:76:LEU:HD12	1.99	0.43
4:D:190:ASP:O	4:D:191:ARG:C	2.56	0.43
9:I:36:TYR:CD2	9:I:37:PHE:CE1	3.06	0.43
15:O:53:HIS:ND1	15:O:53:HIS:O	2.51	0.43
1:A:1477:A:H2'	1:A:1478:A:H8	1.84	0.43
1:A:1477:A:H5'	1:A:1477:A:H8	1.83	0.43
1:A:980:G:H2'	1:A:981:G:C8	2.54	0.43
3:C:7:PRO:HG2	3:C:184:TYR:HB2	2.00	0.43
1:A:1333:U:C1'	7:G:33:ASP:HB3	2.48	0.43
1:A:984:A:H2	1:A:1005:G:C5	2.36	0.43
2:B:47:THR:HA	2:B:202:PRO:HG2	1.99	0.43
1:A:1014:G:H1'	1:A:1015:G:C2	2.53	0.43
12:L:47:LYS:CB	12:L:48:PRO:CD	2.96	0.43
12:L:86:ARG:HB3	12:L:101:VAL:HG23	1.99	0.43
9:I:104:ARG:O	9:I:105:ASP:HB3	2.19	0.43
11:K:11:LYS:HE3	11:K:12:ARG:HB3	1.99	0.43
1:A:1135:A:H4'	10:J:13:HIS:CD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1135:A:O3'	10:J:13:HIS:NE2	2.50	0.43
1:A:722:C:H5"	6:F:69:GLU:HB2	2.01	0.43
9:I:4:TYR:CG	9:I:88:TYR:HB2	2.54	0.43
1:A:397:C:H1'	1:A:606:A:H1'	1.99	0.43
1:A:504:A:OP2	12:L:51:ALA:HB1	2.18	0.43
1:A:1305:G:H2'	1:A:1306:A:C8	2.53	0.43
10:J:84:GLN:HB3	10:J:88:LEU:HD22	2.01	0.43
1:A:474:C:H2'	1:A:475:G:H8	1.83	0.43
1:A:1382:C:O2	1:A:1384:G:C5	2.72	0.43
10:J:82:ILE:HA	10:J:85:LEU:HB2	2.00	0.43
3:C:59:ARG:HG2	3:C:64:VAL:HG12	2.01	0.43
1:A:561:G:H1'	1:A:800:A:C4	2.54	0.43
1:A:1327:U:C4	1:A:1360:A:C2	3.07	0.43
4:D:110:PHE:CD1	4:D:110:PHE:N	2.87	0.43
1:A:1349:C:C2	1:A:1350:C:C5	3.06	0.43
1:A:1509:A:C4	1:A:1510:U:H6	2.37	0.43
12:L:41:ARG:CG	12:L:42:THR:H	2.31	0.43
1:A:1172:G:O2'	3:C:3:ASN:HB2	2.19	0.43
9:I:47:LEU:HB3	9:I:50:LEU:HD12	2.01	0.43
10:J:62:HIS:HB3	14:N:59:ALA:HB3	2.01	0.43
1:A:429:C:O2'	1:A:430:U:H5'	2.19	0.43
1:A:146:A:H2'	1:A:147:A:O4'	2.19	0.43
1:A:1011:C:O5'	1:A:1011:C:H6	2.02	0.43
1:A:1375:G:N2	1:A:1480:A:C8	2.82	0.43
2:B:69:LEU:HD13	2:B:91:PRO:HB2	2.01	0.43
1:A:1311:A:OP1	13:M:28:ALA:HB3	2.19	0.43
8:H:75:ARG:HA	8:H:76:PRO:HD3	1.85	0.43
1:A:751:A:O2'	1:A:1502:C:O2	2.30	0.43
8:H:82:HIS:ND1	8:H:138:TRP:NE1	2.66	0.43
1:A:499:G:H2'	1:A:500:U:O4'	2.19	0.43
1:A:269:A:H1'	17:Q:16:GLN:NE2	2.34	0.43
1:A:820:G:C6	1:A:829:G:C5	3.06	0.43
8:H:53:VAL:HG12	8:H:58:TYR:CD1	2.53	0.43
1:A:566:U:C2	1:A:744:G:C6	3.07	0.42
4:D:105:VAL:HG12	4:D:117:ALA:HB1	2.01	0.42
1:A:1108:U:H5'	1:A:1109:U:H5	1.84	0.42
1:A:1202:G:O3'	19:S:36:ARG:HD3	2.18	0.42
8:H:122:ARG:NH1	8:H:122:ARG:HB2	2.34	0.42
7:G:20:ASP:HB3	7:G:23:VAL:HG23	2.01	0.42
13:M:4:ILE:HG22	13:M:5:ALA:N	2.34	0.42
9:I:17:VAL:HG21	9:I:80:GLY:HA3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:14:TRP:HZ3	21:U:15:ARG:NH1	2.17	0.42
1:A:836:G:O6	1:A:847:G:N7	2.51	0.42
5:E:53:LEU:O	5:E:57:LYS:HB2	2.18	0.42
1:A:1112:C:O5'	1:A:1113:A:H8	2.02	0.42
3:C:101:LEU:HD23	3:C:102:ASN:O	2.19	0.42
1:A:954:G:N7	1:A:1340:U:C2	2.87	0.42
1:A:721:A:O2'	6:F:72:VAL:HG13	2.20	0.42
4:D:173:TRP:O	4:D:186:LEU:HB2	2.19	0.42
1:A:727:U:H2'	1:A:728:C:H6	1.84	0.42
1:A:1022:C:C6	1:A:1023:U:C5	3.07	0.42
3:C:36:ASP:HA	3:C:39:ILE:HD12	2.01	0.42
2:B:118:LEU:HB3	2:B:142:LEU:HD12	2.01	0.42
9:I:28:VAL:HG22	9:I:63:ILE:HB	2.02	0.42
1:A:119:U:H2'	1:A:120:G:C8	2.55	0.42
3:C:147:LYS:HG3	3:C:204:LEU:O	2.19	0.42
2:B:173:ALA:O	2:B:176:GLU:HB2	2.19	0.42
1:A:417:U:H4'	1:A:418:C:OP2	2.20	0.42
2:B:58:ILE:O	2:B:61:LEU:HD23	2.19	0.42
1:A:1280:C:H2'	7:G:114:ARG:HH12	1.83	0.42
5:E:35:GLY:N	5:E:112:LEU:HD23	2.34	0.42
18:R:25:THR:HG21	18:R:42:ARG:HH11	1.85	0.42
1:A:171:C:H2'	1:A:172:C:H6	1.85	0.42
1:A:1311:A:H5'	13:M:29:ARG:HD2	2.01	0.42
1:A:921:U:H2'	1:A:922:G:H5'	2.00	0.42
1:A:568:G:H5'	17:Q:91:ARG:NH2	2.35	0.42
1:A:781:C:O2'	1:A:782:G:H5'	2.20	0.42
1:A:838:A:H2'	1:A:839:G:O4'	2.20	0.42
17:Q:69:LYS:O	17:Q:70:ARG:HD2	2.20	0.42
18:R:40:LEU:HB3	18:R:79:LEU:HD11	2.02	0.42
7:G:111:ARG:NH2	7:G:126:ASP:OD2	2.53	0.42
1:A:1142:U:C5	1:A:1164:G:C4	3.08	0.42
2:B:161:ALA:HB1	2:B:185:ILE:HD11	2.02	0.42
1:A:489:G:C6	1:A:519:A:C2	3.08	0.42
1:A:980:G:N2	1:A:1023:U:C2	2.87	0.42
1:A:1280:C:P	7:G:114:ARG:HH22	2.43	0.42
10:J:5:ARG:O	10:J:99:LYS:N	2.34	0.42
1:A:1095:C:O2	3:C:179:ARG:HG2	2.20	0.42
1:A:995:A:H2'	1:A:996:G:O4'	2.19	0.42
1:A:289:G:C4	1:A:290:U:C5	3.07	0.42
19:S:31:ILE:HG23	19:S:48:THR:O	2.20	0.42
1:A:1271:A:H5"	1:A:1272:G:OP2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1219:C:HO2'	1:A:1282:G:H1	1.67	0.42
1:A:104:C:H2'	1:A:105:G:O4'	2.19	0.42
12:L:83:VAL:HG21	12:L:100:ILE:HD13	2.02	0.42
2:B:42:ILE:HD13	2:B:42:ILE:HG21	1.84	0.42
2:B:121:LEU:C	2:B:139:LYS:HZ1	2.23	0.42
14:N:24:CYS:HB2	14:N:29:ARG:HB3	2.02	0.42
14:N:4:LYS:HA	14:N:4:LYS:HE3	2.01	0.42
2:B:54:THR:O	2:B:58:ILE:HG12	2.20	0.42
8:H:4:ASP:HB3	8:H:7:ALA:HB3	2.01	0.42
13:M:82:MET:SD	13:M:83:ASP:N	2.93	0.42
3:C:116:VAL:HG11	3:C:141:VAL:HG21	2.02	0.42
19:S:52:TYR:HA	19:S:56:GLN:O	2.20	0.42
3:C:25:GLY:O	3:C:29:TYR:HB2	2.19	0.42
13:M:52:GLU:HG2	13:M:55:ARG:NH1	2.35	0.41
19:S:5:LEU:HA	19:S:6:LYS:NZ	2.35	0.41
20:T:67:ALA:O	20:T:73:HIS:CE1	2.73	0.41
1:A:1477:A:H5'	1:A:1477:A:C8	2.54	0.41
20:T:51:GLU:OE2	20:T:51:GLU:N	2.53	0.41
1:A:1050:A:N3	1:A:1051:G:H1'	2.35	0.41
13:M:79:LYS:O	13:M:82:MET:HB3	2.20	0.41
3:C:29:TYR:O	3:C:33:LEU:HB2	2.20	0.41
1:A:917:G:C6	1:A:918:C:C4	3.07	0.41
1:A:1132:C:O5'	1:A:1132:C:H6	2.03	0.41
1:A:528:G:OP1	4:D:59:ARG:NH2	2.53	0.41
1:A:1234:A:O2'	1:A:1235:G:O4'	2.34	0.41
1:A:1074:U:O2	1:A:1076:A:C8	2.73	0.41
7:G:80:VAL:HB	7:G:81:GLY:H	1.75	0.41
13:M:65:LYS:HE2	13:M:69:GLU:HB3	2.02	0.41
1:A:1252:C:O2'	1:A:1296:C:H5'	2.20	0.41
1:A:1131:U:O3'	9:I:14:VAL:HG11	2.19	0.41
1:A:1161:A:H2'	1:A:1162:A:O4'	2.19	0.41
5:E:100:VAL:HA	5:E:118:ILE:HG22	2.03	0.41
3:C:70:VAL:O	3:C:106:VAL:HG23	2.20	0.41
8:H:44:PHE:CE2	8:H:109:ILE:HG21	2.56	0.41
11:K:95:ILE:HG21	11:K:108:ILE:HD13	2.02	0.41
7:G:31:MET:SD	7:G:34:GLY:HA2	2.60	0.41
1:A:837:A:H2'	1:A:838:A:O4'	2.20	0.41
7:G:116:ALA:O	7:G:120:ILE:HG12	2.20	0.41
1:A:378:A:C2	1:A:379:A:C4	3.09	0.41
1:A:434:G:O2'	1:A:479:U:O4	2.38	0.41
5:E:146:ALA:O	5:E:149:GLU:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:G:O4'	1:A:102:G:N3	2.53	0.41
13:M:49:THR:HB	13:M:52:GLU:HG3	2.02	0.41
2:B:76:GLN:HE21	2:B:76:GLN:H	1.68	0.41
1:A:1329:G:OP2	9:I:107:ARG:HG2	2.21	0.41
3:C:113:ALA:HB3	3:C:114:PRO:HD3	2.02	0.41
1:A:486:G:C6	1:A:487:C:C4	3.08	0.41
13:M:16:ASP:HB3	13:M:41:PRO:HB3	2.02	0.41
1:A:1455:C:H2'	1:A:1456:C:C6	2.55	0.41
2:B:213:LEU:O	2:B:217:ARG:HG2	2.20	0.41
1:A:289:G:H2'	1:A:290:U:C6	2.55	0.41
19:S:36:ARG:HH12	19:S:75:ALA:HB3	1.86	0.41
17:Q:24:GLU:HG3	17:Q:39:SER:HB3	2.03	0.41
1:A:77:G:H22	1:A:87:C:H5	1.69	0.41
1:A:923:G:C2	1:A:924:A:C8	3.08	0.41
1:A:821:G:H1	1:A:827:C:N4	2.14	0.41
2:B:19:HIS:CE1	2:B:206:ASP:HB2	2.56	0.41
1:A:269:A:N6	1:A:270:A:C6	2.89	0.41
1:A:298:G:N3	1:A:540:C:H4'	2.36	0.41
11:K:16:SER:HA	11:K:79:SER:O	2.21	0.41
1:A:799:A:N6	1:A:1487:C:H1'	2.36	0.41
14:N:24:CYS:HB3	14:N:27:CYS:HB2	1.11	0.41
1:A:564:U:H2'	1:A:565:G:O4'	2.21	0.41
1:A:788:U:H5"	1:A:789:C:OP2	2.21	0.41
1:A:569:G:N3	1:A:857:C:H4'	2.35	0.41
2:B:236:TYR:O	2:B:239:VAL:HG23	2.20	0.41
7:G:86:GLN:HB2	7:G:148:ASN:ND2	2.35	0.41
13:M:19:LEU:HD13	13:M:19:LEU:HA	1.84	0.41
17:Q:27:PHE:HA	17:Q:28:PRO:HD2	1.80	0.41
1:A:1375:G:H2'	1:A:1376:U:H6	1.85	0.41
2:B:69:LEU:HB3	2:B:162:ILE:HG22	2.03	0.41
4:D:20:TYR:HD1	4:D:26:CYS:O	2.04	0.41
1:A:1198:G:H5"	14:N:5:ALA:HB2	2.03	0.41
1:A:417:U:O4	3:C:127:ARG:NE	2.54	0.41
1:A:19:C:H2'	1:A:20:C:O4'	2.21	0.41
11:K:11:LYS:HA	11:K:11:LYS:HD2	1.90	0.41
1:A:814:G:C6	1:A:815:U:N3	2.89	0.41
1:A:1464:G:H2'	1:A:1465:G:O4'	2.20	0.41
10:J:47:PHE:HD1	14:N:34:TYR:CE2	2.39	0.41
2:B:96:ARG:HH12	2:B:169:LYS:HE3	1.86	0.41
1:A:376:G:C2	1:A:380:G:C6	3.08	0.41
18:R:72:ARG:O	18:R:76:LEU:HD22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:924:A:H2'	1:A:925:G:H8	1.82	0.41
4:D:20:TYR:O	4:D:21:LEU:HD23	2.21	0.41
2:B:16:HIS:HB3	2:B:210:SER:CB	2.52	0.41
1:A:1049:C:C2'	1:A:1050:A:H5'	2.51	0.41
1:A:916:A:C6	1:A:917:G:C5	3.09	0.41
1:A:1053:U:H2'	1:A:1054:C:H6	1.86	0.41
6:F:23:LYS:NZ	6:F:42:GLU:OE2	2.51	0.41
13:M:78:ILE:O	13:M:81:LEU:N	2.53	0.41
19:S:43:GLU:HA	19:S:45:VAL:HG13	2.02	0.40
2:B:118:LEU:HD12	2:B:142:LEU:HB2	2.01	0.40
12:L:36:VAL:HA	12:L:82:VAL:HA	2.03	0.40
3:C:73:PRO:O	3:C:76:VAL:HG22	2.21	0.40
19:S:16:LEU:O	19:S:20:LEU:N	2.40	0.40
1:A:1370:G:C6	1:A:1371:C:N4	2.89	0.40
13:M:108:ARG:O	13:M:111:LYS:O	2.40	0.40
4:D:14:ARG:HD3	4:D:14:ARG:O	2.21	0.40
1:A:1209:A:C3'	1:A:1209:A:C8	3.05	0.40
10:J:45:ARG:NH1	10:J:45:ARG:HB3	2.32	0.40
1:A:859:G:OP2	12:L:12:ARG:NH2	2.54	0.40
12:L:33:ARG:HA	12:L:33:ARG:HD3	1.67	0.40
3:C:188:LEU:HB3	3:C:189:ALA:H	1.70	0.40
8:H:69:ARG:NH1	8:H:75:ARG:O	2.53	0.40
1:A:1151:A:H2'	1:A:1152:A:C8	2.57	0.40
1:A:1327:U:C5	1:A:1360:A:C2	3.09	0.40
18:R:25:THR:CG2	18:R:42:ARG:HH11	2.33	0.40
16:P:75:ARG:O	16:P:78:GLY:N	2.52	0.40
9:I:97:LYS:HB2	9:I:98:PRO:HD3	2.03	0.40
2:B:8:LYS:HB2	2:B:9:GLU:H	1.70	0.40
1:A:935:U:O2'	1:A:937:A:N7	2.42	0.40
15:O:44:LYS:HE3	15:O:44:LYS:HB2	1.90	0.40
9:I:54:ASP:C	9:I:56:LEU:HG	2.40	0.40
1:A:648:G:H1	1:A:725:G:H1	1.69	0.40
1:A:674:G:H2'	1:A:675:G:O4'	2.21	0.40
1:A:326:C:H2'	1:A:327:G:H5'	2.03	0.40
1:A:628:G:C5	1:A:629:C:C5	3.10	0.40
1:A:22:G:H2'	1:A:23:G:C8	2.56	0.40
14:N:18:VAL:O	14:N:20:ALA:N	2.54	0.40
1:A:1339:A:N7	1:A:1340:U:C5	2.89	0.40
1:A:1251:A:C2	1:A:1295:U:O4'	2.73	0.40
1:A:836:G:H22	1:A:847:G:H3'	1.86	0.40
5:E:80:ILE:CD1	5:E:91:LEU:HD23	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:69:LEU:HD12	2:B:70:PHE:N	2.37	0.40
8:H:17:THR:HG22	8:H:63:LEU:HG	2.03	0.40
3:C:68:VAL:HG12	3:C:70:VAL:HG23	2.02	0.40
1:A:104:C:C4	1:A:105:G:C5	3.10	0.40
11:K:121:PRO:HB2	11:K:126:ARG:HG3	2.04	0.40
4:D:68:TYR:CE2	4:D:97:LEU:HB3	2.56	0.40
1:A:830:G:C6	1:A:831:G:N7	2.90	0.40
14:N:36:PHE:O	14:N:36:PHE:CD1	2.74	0.40
19:S:71:LEU:HA	19:S:71:LEU:HD23	1.94	0.40
17:Q:68:ARG:H	17:Q:70:ARG:HH11	1.66	0.40
1:A:1350:C:C2	1:A:1351:G:C8	3.10	0.40
5:E:80:ILE:HG23	8:H:104:ARG:NH2	2.37	0.40
4:D:8:VAL:C	4:D:10:ARG:N	2.71	0.40
1:A:555:U:O2	1:A:896:A:H5'	2.21	0.40
1:A:400:U:C2	1:A:401:U:C5	3.09	0.40
4:D:171:GLY:C	4:D:173:TRP:H	2.25	0.40
1:A:1233:A:O2'	1:A:1234:A:P	2.80	0.40
4:D:92:VAL:O	4:D:96:LEU:HD13	2.21	0.40
1:A:228:G:H2'	1:A:229:C:O4'	2.22	0.40
17:Q:33:GLY:O	17:Q:34:LYS:C	2.59	0.40
1:A:569:G:O3'	17:Q:34:LYS:NZ	2.54	0.40
12:L:110:VAL:H	12:L:122:THR:HG22	1.85	0.40
15:O:8:LYS:O	15:O:11:VAL:N	2.55	0.40
12:L:46:LYS:HG2	12:L:94:PRO:HD3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	233/235 (99%)	168 (72%)	48 (21%)	17 (7%)	1 14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	C	205/207 (99%)	151 (74%)	39 (19%)	15 (7%)	1 14
4	D	206/208 (99%)	165 (80%)	24 (12%)	17 (8%)	1 11
5	E	149/151 (99%)	132 (89%)	14 (9%)	3 (2%)	9 48
6	F	99/101 (98%)	85 (86%)	13 (13%)	1 (1%)	19 63
7	G	153/155 (99%)	122 (80%)	22 (14%)	9 (6%)	2 19
8	H	136/138 (99%)	122 (90%)	12 (9%)	2 (2%)	13 54
9	I	125/127 (98%)	99 (79%)	20 (16%)	6 (5%)	3 25
10	J	97/99 (98%)	74 (76%)	15 (16%)	8 (8%)	1 11
11	K	117/119 (98%)	103 (88%)	12 (10%)	2 (2%)	11 51
12	L	124/126 (98%)	98 (79%)	17 (14%)	9 (7%)	1 14
13	M	119/121 (98%)	84 (71%)	26 (22%)	9 (8%)	1 13
14	N	58/60 (97%)	49 (84%)	3 (5%)	6 (10%)	1 7
15	O	86/88 (98%)	68 (79%)	15 (17%)	3 (4%)	4 35
16	P	82/84 (98%)	70 (85%)	11 (13%)	1 (1%)	16 59
17	Q	98/100 (98%)	87 (89%)	9 (9%)	2 (2%)	9 48
18	R	68/70 (97%)	66 (97%)	1 (2%)	1 (2%)	13 54
19	S	77/79 (98%)	60 (78%)	11 (14%)	6 (8%)	1 12
20	T	97/99 (98%)	74 (76%)	16 (16%)	7 (7%)	1 14
21	U	23/25 (92%)	18 (78%)	4 (17%)	1 (4%)	3 29
All	All	2352/2392 (98%)	1895 (81%)	332 (14%)	125 (5%)	2 22

All (125) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	17	PHE
3	C	15	THR
3	C	82	GLU
3	C	189	ALA
3	C	207	VAL
4	D	13	ARG
4	D	14	ARG
4	D	26	CYS
4	D	27	TYR
4	D	29	PRO
4	D	82	ALA

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Mol	Chain	Res	Type
4	D	83	SER
4	D	89	THR
5	E	72	GLN
5	E	153	LYS
8	H	2	LEU
9	I	118	LYS
12	L	28	LYS
12	L	47	LYS
12	L	91	LYS
13	M	6	GLY
13	M	83	ASP
13	M	113	PRO
14	N	3	ARG
14	N	44	LEU
19	S	6	LYS
19	S	45	VAL
19	S	65	ASN
20	T	75	ASN
2	B	131	PRO
2	B	132	LYS
3	C	47	LEU
3	C	81	GLY
3	C	154	SER
3	C	156	ARG
4	D	5	ILE
4	D	69	GLY
4	D	102	ASP
4	D	171	GLY
5	E	22	GLY
7	G	7	ALA
7	G	67	GLU
7	G	80	VAL
7	G	155	ARG
9	I	119	ALA
10	J	59	SER
10	J	82	ILE
10	J	92	THR
11	K	91	ARG
12	L	29	GLY
13	M	67	GLU
13	M	89	GLY
13	M	91	ARG

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Mol	Chain	Res	Type
14	N	4	LYS
17	Q	74	LEU
19	S	46	GLY
19	S	64	GLU
19	S	80	TYR
20	T	74	LYS
20	T	97	ALA
20	T	100	ILE
2	B	9	GLU
2	B	78	GLN
2	B	105	PHE
2	B	155	LEU
2	B	195	ASP
3	C	36	ASP
3	C	60	ALA
3	C	67	THR
3	C	96	GLY
4	D	9	CYS
4	D	30	LYS
9	I	56	LEU
9	I	94	ALA
10	J	32	ALA
10	J	91	PRO
11	K	89	ALA
13	M	59	TYR
13	M	90	LEU
14	N	16	PHE
14	N	43	CYS
15	O	47	LYS
15	O	86	GLY
16	P	83	GLU
18	R	87	ARG
20	T	50	GLU
2	B	15	VAL
2	B	18	GLY
2	B	227	GLY
3	C	53	ALA
3	C	101	LEU
7	G	116	ALA
9	I	109	VAL
12	L	27	LEU
12	L	30	ALA

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Mol	Chain	Res	Type
12	L	82	VAL
13	M	4	ILE
17	Q	49	GLU
20	T	73	HIS
21	U	25	LYS
2	B	87	ARG
2	B	177	ALA
3	C	4	LYS
4	D	37	PRO
4	D	172	PRO
7	G	82	GLY
10	J	55	LYS
10	J	57	LYS
12	L	115	LYS
15	O	87	ILE
20	T	11	SER
2	B	231	GLU
4	D	55	ALA
7	G	109	ASN
7	G	146	GLU
12	L	48	PRO
6	F	81	ILE
7	G	61	VAL
9	I	24	GLY
2	B	230	VAL
2	B	233	SER
14	N	42	ILE
2	B	130	ARG
8	H	73	ASP
10	J	36	GLY

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	202/203 (100%)	160 (79%)	42 (21%)	1 6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	C	160/161 (99%)	140 (88%)	20 (12%)	6 27
4	D	180/180 (100%)	152 (84%)	28 (16%)	3 18
5	E	115/116 (99%)	95 (83%)	20 (17%)	2 13
6	F	90/90 (100%)	82 (91%)	8 (9%)	12 45
7	G	126/126 (100%)	113 (90%)	13 (10%)	9 37
8	H	119/119 (100%)	103 (87%)	16 (13%)	5 24
9	I	98/98 (100%)	82 (84%)	16 (16%)	3 16
10	J	88/89 (99%)	70 (80%)	18 (20%)	1 7
11	K	90/90 (100%)	80 (89%)	10 (11%)	8 33
12	L	104/105 (99%)	90 (86%)	14 (14%)	5 24
13	M	96/97 (99%)	76 (79%)	20 (21%)	1 6
14	N	49/49 (100%)	42 (86%)	7 (14%)	4 22
15	O	79/79 (100%)	66 (84%)	13 (16%)	3 15
16	P	72/72 (100%)	60 (83%)	12 (17%)	3 14
17	Q	94/95 (99%)	80 (85%)	14 (15%)	4 20
18	R	61/61 (100%)	56 (92%)	5 (8%)	14 50
19	S	69/69 (100%)	59 (86%)	10 (14%)	4 21
20	T	76/76 (100%)	62 (82%)	14 (18%)	2 10
21	U	19/20 (95%)	16 (84%)	3 (16%)	3 17
All	All	1987/1995 (100%)	1684 (85%)	303 (15%)	3 19

All (303) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	8	LYS
2	B	12	GLU
2	B	15	VAL
2	B	17	PHE
2	B	20	GLU
2	B	24	TRP
2	B	27	LYS
2	B	28	PHE
2	B	30	ARG
2	B	35	GLU
2	B	39	ILE

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Mol	Chain	Res	Type
2	B	42	ILE
2	B	45	GLN
2	B	51	LEU
2	B	61	LEU
2	B	67	THR
2	B	71	VAL
2	B	75	LYS
2	B	76	GLN
2	B	78	GLN
2	B	80	ILE
2	B	87	ARG
2	B	97	TRP
2	B	102	LEU
2	B	108	ILE
2	B	113	HIS
2	B	133	LYS
2	B	137	ARG
2	B	144	ARG
2	B	150	SER
2	B	155	LEU
2	B	156	LYS
2	B	168	THR
2	B	169	LYS
2	B	170	GLU
2	B	172	ILE
2	B	185	ILE
2	B	187	LEU
2	B	191	ASP
2	B	196	LEU
2	B	223	ILE
2	B	235	SER
3	C	3	ASN
3	C	14	ILE
3	C	16	ARG
3	C	23	TYR
3	C	36	ASP
3	C	48	TYR
3	C	52	LEU
3	C	63	ASN
3	C	72	LYS
3	C	85	ARG
3	C	94	LEU

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Mol	Chain	Res	Type
3	C	104	GLN
3	C	119	ARG
3	C	166	GLU
3	C	167	TRP
3	C	178	LEU
3	C	188	LEU
3	C	192	THR
3	C	203	PHE
3	C	206	GLU
4	D	5	ILE
4	D	8	VAL
4	D	10	ARG
4	D	19	LEU
4	D	25	ARG
4	D	27	TYR
4	D	30	LYS
4	D	33	MET
4	D	34	GLU
4	D	49	ARG
4	D	58	LEU
4	D	59	ARG
4	D	70	ILE
4	D	76	ARG
4	D	86	LYS
4	D	122	ARG
4	D	127	THR
4	D	135	LEU
4	D	137	SER
4	D	139	ARG
4	D	150	GLU
4	D	151	LYS
4	D	170	VAL
4	D	175	SER
4	D	187	ARG
4	D	194	LEU
4	D	198	VAL
4	D	209	ARG
5	E	12	LEU
5	E	16	THR
5	E	18	ARG
5	E	27	ARG
5	E	31	LEU

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Mol	Chain	Res	Type
5	E	41	VAL
5	E	45	PHE
5	E	64	ARG
5	E	68	GLU
5	E	78	HIS
5	E	79	GLU
5	E	80	ILE
5	E	87	SER
5	E	91	LEU
5	E	100	VAL
5	E	101	ILE
5	E	125	SER
5	E	144	THR
5	E	147	ASP
5	E	153	LYS
6	F	25	ILE
6	F	46	ARG
6	F	54	LYS
6	F	61	LEU
6	F	65	VAL
6	F	75	LEU
6	F	77	ARG
6	F	98	LEU
7	G	11	GLN
7	G	38	LEU
7	G	54	THR
7	G	64	GLN
7	G	72	ARG
7	G	80	VAL
7	G	84	ASN
7	G	94	ARG
7	G	104	LEU
7	G	113	GLU
7	G	114	ARG
7	G	136	LYS
7	G	153	HIS
8	H	21	LYS
8	H	26	VAL
8	H	30	ARG
8	H	50	ARG
8	H	51	VAL
8	H	53	VAL

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Mol	Chain	Res	Type
8	H	56	LYS
8	H	75	ARG
8	H	85	ARG
8	H	92	ARG
8	H	97	VAL
8	H	98	LYS
8	H	99	GLU
8	H	105	ARG
8	H	109	ILE
8	H	133	LEU
9	I	3	GLN
9	I	10	ARG
9	I	23	ASN
9	I	29	ASN
9	I	34	ASN
9	I	44	VAL
9	I	47	LEU
9	I	66	ARG
9	I	75	ASP
9	I	79	LEU
9	I	92	TYR
9	I	102	LEU
9	I	104	ARG
9	I	117	HIS
9	I	125	TYR
9	I	128	ARG
10	J	3	LYS
10	J	4	ILE
10	J	13	HIS
10	J	14	LYS
10	J	17	ASP
10	J	29	ARG
10	J	38	ILE
10	J	45	ARG
10	J	55	LYS
10	J	57	LYS
10	J	70	ARG
10	J	76	ASN
10	J	78	ASN
10	J	79	ARG
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	12	ARG
11	K	29	ILE
11	K	36	ASP
11	K	67	ASP
11	K	84	VAL
11	K	91	ARG
11	K	93	GLN
11	K	96	ARG
11	K	114	VAL
11	K	124	LYS
12	L	18	VAL
12	L	20	LYS
12	L	21	LYS
12	L	33	ARG
12	L	44	THR
12	L	46	LYS
12	L	48	PRO
12	L	52	LEU
12	L	59	ARG
12	L	60	LEU
12	L	73	GLU
12	L	83	VAL
12	L	113	ARG
12	L	114	LYS
13	M	7	VAL
13	M	15	VAL
13	M	19	LEU
13	M	47	ASP
13	M	48	LEU
13	M	64	TRP
13	M	66	LEU
13	M	79	LYS
13	M	82	MET
13	M	86	CYS
13	M	88	ARG
13	M	93	ARG
13	M	101	GLN
13	M	104	ARG
13	M	108	ARG
13	M	115	LYS

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Mol	Chain	Res	Type
13	M	116	THR
13	M	117	VAL
13	M	120	LYS
13	M	121	LYS
14	N	3	ARG
14	N	4	LYS
14	N	6	LEU
14	N	22	THR
14	N	23	ARG
14	N	33	VAL
14	N	57	ARG
15	O	3	ILE
15	O	5	LYS
15	O	10	LYS
15	O	26	GLU
15	O	31	LEU
15	O	32	LEU
15	O	40	SER
15	O	46	HIS
15	O	65	ARG
15	O	66	LEU
15	O	76	GLU
15	O	82	ILE
15	O	88	ARG
16	P	1	MET
16	P	2	VAL
16	P	5	ARG
16	P	19	ILE
16	P	27	LYS
16	P	43	LYS
16	P	45	THR
16	P	53	VAL
16	P	54	GLU
16	P	62	VAL
16	P	69	THR
16	P	76	GLN
17	Q	7	THR
17	Q	14	LYS
17	Q	19	VAL
17	Q	52	LYS
17	Q	53	LEU
17	Q	55	ASP

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Mol	Chain	Res	Type
17	Q	59	ILE
17	Q	61	GLU
17	Q	68	ARG
17	Q	74	LEU
17	Q	76	LEU
17	Q	87	LYS
17	Q	94	ASN
17	Q	100	LYS
18	R	45	SER
18	R	47	THR
18	R	76	LEU
18	R	84	LYS
18	R	88	LYS
19	S	4	SER
19	S	5	LEU
19	S	6	LYS
19	S	11	VAL
19	S	13	ASP
19	S	22	LEU
19	S	31	ILE
19	S	37	ARG
19	S	41	VAL
19	S	79	THR
20	T	10	LEU
20	T	13	LEU
20	T	23	ARG
20	T	24	LEU
20	T	35	THR
20	T	51	GLU
20	T	62	LEU
20	T	72	LEU
20	T	73	HIS
20	T	74	LYS
20	T	80	ARG
20	T	84	LEU
20	T	87	LYS
20	T	104	LEU
21	U	10	ARG
21	U	15	ARG
21	U	24	ARG

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

Mol	Chain	Res	Type
2	B	78	GLN
2	B	95	GLN
4	D	116	GLN
4	D	129	ASN
4	D	161	ASN
11	K	99	GLN
16	P	16	HIS
19	S	65	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1509/1517 (99%)	306 (20%)	33 (2%)
22	X	4/5 (80%)	2 (50%)	0
23	Y	8/11 (72%)	3 (37%)	0
All	All	1521/1533 (99%)	311 (20%)	33 (2%)

All (311) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	7	G
1	A	8	G
1	A	10	G
1	A	33	A
1	A	40	G
1	A	48	C
1	A	49	C
1	A	51	A
1	A	52	A
1	A	74	G
1	A	81	U
1	A	82	U
1	A	83	U
1	A	84	A
1	A	86	U
1	A	92	G
1	A	95	A
1	A	102	G
1	A	110	A
1	A	115	C
1	A	126	C
1	A	151	G

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Mol	Chain	Res	Type
1	A	177	U
1	A	191	G
1	A	193	G
1	A	197	U
1	A	202	A
1	A	204	A
1	A	209	U
1	A	210	U
1	A	211	U
1	A	212	G
1	A	213	C
1	A	222	G
1	A	227	G
1	A	243	G
1	A	247	G
1	A	258	A
1	A	262	G
1	A	263	C
1	A	275	A
1	A	279	C
1	A	285	G
1	A	293	G
1	A	294	A
1	A	297	G
1	A	302	G
1	A	317	A
1	A	324	C
1	A	325	A
1	A	326	C
1	A	328	G
1	A	337	C
1	A	341	C
1	A	347	G
1	A	348	C
1	A	349	A
1	A	350	G
1	A	351	C
1	A	363	U
1	A	368	C
1	A	369	A
1	A	384	G
1	A	386	C

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Mol	Chain	Res	Type
1	A	392	G
1	A	393	A
1	A	394	C
1	A	402	G
1	A	408	A
1	A	409	G
1	A	417	U
1	A	418	C
1	A	419	G
1	A	420	G
1	A	425	U
1	A	426	A
1	A	447	A
1	A	448	A
1	A	455	A
1	A	456	C
1	A	469	G
1	A	470	G
1	A	481	A
1	A	482	U
1	A	483	A
1	A	489	G
1	A	492	C
1	A	493	A
1	A	494	A
1	A	495	C
1	A	498	C
1	A	501	G
1	A	502	C
1	A	505	G
1	A	511	G
1	A	515	U
1	A	516	A
1	A	517	A
1	A	520	C
1	A	531	A
1	A	545	U
1	A	551	G
1	A	555	U
1	A	556	A
1	A	557	A
1	A	560	G

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Mol	Chain	Res	Type
1	A	580	C
1	A	591	A
1	A	614	G
1	A	615	G
1	A	616	A
1	A	634	G
1	A	637	A
1	A	649	A
1	A	650	G
1	A	671	A
1	A	672	G
1	A	705	G
1	A	707	U
1	A	708	G
1	A	715	G
1	A	718	G
1	A	739	G
1	A	743	A
1	A	744	G
1	A	761	A
1	A	769	G
1	A	776	A
1	A	777	U
1	A	778	A
1	A	800	A
1	A	801	C
1	A	802	G
1	A	812	A
1	A	820	G
1	A	823	U
1	A	824	C
1	A	825	U
1	A	826	C
1	A	829	G
1	A	836	G
1	A	837	A
1	A	838	A
1	A	854	G
1	A	863	G
1	A	880	G
1	A	892	A
1	A	894	G

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Mol	Chain	Res	Type
1	A	904	G
1	A	905	G
1	A	909	C
1	A	912	C
1	A	913	A
1	A	915	A
1	A	921	U
1	A	931	G
1	A	936	A
1	A	938	U
1	A	939	U
1	A	941	G
1	A	944	G
1	A	946	A
1	A	947	A
1	A	949	G
1	A	950	C
1	A	952	A
1	A	953	A
1	A	954	G
1	A	955	A
1	A	956	A
1	A	958	C
1	A	962	C
1	A	967	C
1	A	969	U
1	A	970	U
1	A	971	G
1	A	980	G
1	A	984	A
1	A	988	G
1	A	995	A
1	A	998	C
1	A	1005	G
1	A	1009	C
1	A	1012	G
1	A	1013	A
1	A	1014	G
1	A	1015	G
1	A	1016	G
1	A	1017	G
1	A	1018	A

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Mol	Chain	Res	Type
1	A	1022	C
1	A	1036	G
1	A	1037	C
1	A	1038	A
1	A	1044	G
1	A	1051	G
1	A	1061	U
1	A	1075	A
1	A	1077	G
1	A	1078	U
1	A	1079	C
1	A	1084	A
1	A	1091	G
1	A	1100	G
1	A	1105	U
1	A	1106	A
1	A	1107	G
1	A	1108	U
1	A	1109	U
1	A	1110	G
1	A	1112	C
1	A	1113	A
1	A	1115	C
1	A	1116	G
1	A	1117	G
1	A	1118	U
1	A	1119	U
1	A	1120	C
1	A	1121	G
1	A	1122	G
1	A	1123	C
1	A	1124	C
1	A	1125	G
1	A	1126	G
1	A	1129	A
1	A	1137	G
1	A	1142	U
1	A	1143	G
1	A	1153	G
1	A	1154	C
1	A	1156	G
1	A	1163	G

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Mol	Chain	Res	Type
1	A	1169	G
1	A	1178	U
1	A	1179	G
1	A	1181	U
1	A	1183	A
1	A	1184	G
1	A	1193	U
1	A	1194	U
1	A	1196	C
1	A	1200	C
1	A	1209	A
1	A	1210	C
1	A	1220	A
1	A	1229	U
1	A	1230	A
1	A	1231	C
1	A	1232	A
1	A	1233	A
1	A	1234	A
1	A	1235	G
1	A	1239	U
1	A	1244	C
1	A	1260	U
1	A	1262	A
1	A	1267	A
1	A	1268	A
1	A	1269	A
1	A	1271	A
1	A	1279	C
1	A	1282	G
1	A	1284	U
1	A	1287	G
1	A	1299	C
1	A	1302	C
1	A	1304	C
1	A	1313	G
1	A	1317	C
1	A	1318	C
1	A	1320	G
1	A	1328	A
1	A	1329	G
1	A	1334	C

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Mol	Chain	Res	Type
1	A	1345	C
1	A	1346	A
1	A	1347	U
1	A	1353	G
1	A	1358	A
1	A	1375	G
1	A	1377	A
1	A	1381	A
1	A	1383	C
1	A	1385	C
1	A	1394	C
1	A	1402	G
1	A	1426	G
1	A	1447	G
1	A	1463	U
1	A	1465	G
1	A	1470	A
1	A	1472	G
1	A	1475	G
1	A	1477	A
1	A	1481	A
1	A	1482	G
1	A	1484	U
1	A	1485	A
1	A	1495	G
1	A	1497	A
1	A	1507	G
1	A	1508	G
1	A	1510	U
1	A	1511	C
1	A	1519	U
1	A	1522	U
22	X	5	A
22	X	8	A
23	Y	33	U
23	Y	35	G
23	Y	40	C

All (33) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	8	G

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Mol	Chain	Res	Type
1	A	81	U
1	A	109	G
1	A	113	A
1	A	239	A
1	A	262	G
1	A	417	U
1	A	425	U
1	A	469	G
1	A	480	A
1	A	492	C
1	A	493	A
1	A	544	U
1	A	559	G
1	A	671	A
1	A	707	U
1	A	777	U
1	A	891	A
1	A	938	U
1	A	954	G
1	A	970	U
1	A	1013	A
1	A	1037	C
1	A	1050	A
1	A	1109	U
1	A	1128	C
1	A	1183	A
1	A	1207	A
1	A	1230	A
1	A	1233	A
1	A	1317	C
1	A	1477	A
1	A	1507	G

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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%)	-0.18	23 (1%) 76 71	49, 80, 148, 246	0
2	B	235/235 (100%)	-0.09	5 (2%) 67 61	65, 115, 172, 216	0
3	C	207/207 (100%)	-0.26	1 (0%) 91 89	73, 106, 146, 172	0
4	D	208/208 (100%)	-0.27	3 (1%) 78 73	69, 98, 133, 149	0
5	E	151/151 (100%)	-0.42	1 (0%) 89 85	57, 77, 105, 134	0
6	F	101/101 (100%)	-0.29	1 (0%) 84 79	80, 110, 133, 149	0
7	G	155/155 (100%)	-0.16	5 (3%) 51 47	76, 103, 158, 199	0
8	H	138/138 (100%)	-0.54	0 100 100	51, 73, 95, 118	0
9	I	127/127 (100%)	-0.18	0 100 100	66, 115, 149, 166	0
10	J	99/99 (100%)	0.17	5 (5%) 32 28	68, 142, 187, 196	0
11	K	119/119 (100%)	-0.29	1 (0%) 87 83	52, 87, 121, 160	0
12	L	126/126 (100%)	-0.31	3 (2%) 62 57	51, 84, 122, 176	0
13	M	121/121 (100%)	-0.24	5 (4%) 41 36	66, 104, 147, 176	0
14	N	60/60 (100%)	-0.27	0 100 100	78, 99, 124, 133	0
15	O	88/88 (100%)	-0.49	0 100 100	58, 87, 124, 152	0
16	P	84/84 (100%)	-0.35	3 (3%) 46 41	59, 75, 101, 142	0
17	Q	100/100 (100%)	-0.46	0 100 100	56, 78, 110, 127	0
18	R	70/70 (100%)	-0.42	0 100 100	74, 96, 128, 134	0
19	S	79/79 (100%)	-0.19	4 (5%) 32 28	85, 122, 170, 196	0
20	T	99/99 (100%)	-0.46	1 (1%) 84 79	58, 84, 120, 148	0
21	U	25/25 (100%)	-0.26	0 100 100	71, 91, 120, 137	0
22	X	5/5 (100%)	0.47	0 100 100	65, 81, 128, 129	0
23	Y	9/11 (81%)	0.53	1 (11%) 7 7	73, 84, 116, 137	0
All	All	3917/3925 (99%)	-0.24	62 (1%) 74 69	49, 90, 150, 246	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
19	S	82	GLY	7.9
1	A	1518	U	7.0
10	J	33	GLN	5.9
7	G	82	GLY	5.5
1	A	1017	G	5.2
2	B	7	VAL	4.6
6	F	101	ALA	4.3
2	B	15	VAL	4.2
1	A	1009	C	4.2
13	M	119	GLY	4.0
1	A	1010	G	3.7
12	L	28	LYS	3.4
19	S	43	GLU	3.2
1	A	982	G	3.2
7	G	156	TRP	3.2
1	A	614	G	3.2
20	T	106	ALA	3.2
1	A	1519	U	3.1
1	A	1232	A	3.0
16	P	82	GLN	3.0
1	A	1012	G	2.9
19	S	30	LEU	2.9
1	A	981	G	2.9
2	B	128	GLU	2.8
12	L	127	GLU	2.7
4	D	26	CYS	2.6
1	A	1006	C	2.6
1	A	1404	G	2.6
13	M	120	LYS	2.6
7	G	83	ALA	2.6
10	J	90	LEU	2.6
13	M	7	VAL	2.6
10	J	29	ARG	2.6
1	A	1118	U	2.5
4	D	31	CYS	2.5
1	A	1126	G	2.5
1	A	707	U	2.4
3	C	2	GLY	2.4
10	J	89	ASP	2.4
19	S	81	ARG	2.4
4	D	9	CYS	2.4
7	G	81	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
16	P	83	GLU	2.4
1	A	1021	C	2.4
12	L	128	ALA	2.4
1	A	1194	U	2.4
1	A	1016	G	2.4
13	M	118	ALA	2.3
2	B	238	LEU	2.3
1	A	1114	G	2.3
1	A	1112	C	2.3
23	Y	40	C	2.2
16	P	84	ALA	2.2
1	A	985	C	2.1
13	M	121	LYS	2.1
2	B	37	ASN	2.1
1	A	999	U	2.1
11	K	128	ALA	2.1
7	G	84	ASN	2.1
5	E	154	GLY	2.0
10	J	34	VAL	2.0
1	A	1003	G	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.