Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 03:03 PM GMT

PDB ID	:	4B3T
Title	:	Crystal structure of the 30S ribosome in complex with compound 39
Authors	:	Ng, C.L.; Lang, K.; Shcherbakov, D.; Matt, T.; Perez-Fernandez, D.; Patak, R.; Meyer, M.; Duscha, S.; Akbergenov, R.; Boukari, H.; Freihofer, P.; Kudyba, I.; Reddy, M.S.K.; Nandurikar, R.S.; Ramakrishnan, V.; Vasella, A.; Bottger, E.C.
Deposited on	:	2012-07-26
Resolution	:	3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
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:

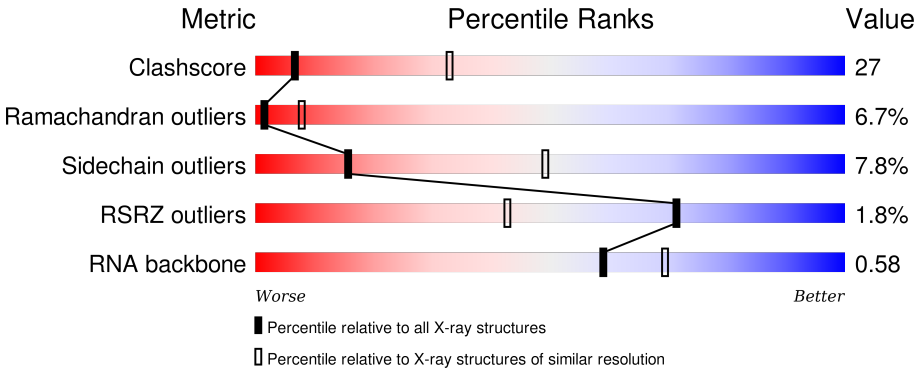
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)
RNA backbone	2183	1036 (3.40-2.60)

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	1521	% 38% 48% 11%
2	B	256	3% 28% 51% 12% 8%
3	C	239	32% 46% 8% 13%
4	D	208	3% 53% 38% 8%
5	E	161	49% 40% 6%

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Mol	Chain	Length	Quality of chain
6	F	101	40% 56%
7	G	155	3% 42% 55%
8	H	138	% 67% 30%
9	I	128	% 34% 53% 12%
10	J	104	13% 22% 55% 16% 5%
11	K	129	3% 39% 49% 8%
12	L	132	2% 47% 38% 10% 5%
13	M	126	6% 29% 53% 15%
14	N	60	32% 55% 12%
15	O	88	% 50% 44% 6%
16	P	88	% 50% 40% 6% 5%
17	Q	104	5% 53% 38% 10%
18	R	88	% 30% 50% 17%
19	S	92	3% 30% 47% 11% 12%
20	T	106	36% 42% 14% 7%
21	V	26	4% 65% 31%
22	W	6	33% 33% 33%
23	Z	16	50% 38% 6% 6%

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	2549	-	-	-	X
24	MG	A	2554	-	-	-	X
24	MG	A	2562	-	-	-	X
24	MG	A	2565	-	-	-	X
24	MG	A	2568	-	-	-	X
24	MG	A	2569	-	-	-	X
24	MG	A	2574	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	MG	A	2576	-	-	-	X
24	MG	A	2578	-	-	-	X
24	MG	A	2582	-	-	-	X
24	MG	A	2584	-	-	-	X
24	MG	A	2585	-	-	-	X
24	MG	A	2598	-	-	-	X
24	MG	A	2599	-	-	-	X
24	MG	A	2601	-	-	-	X
24	MG	A	2605	-	-	-	X
24	MG	A	2609	-	-	-	X
24	MG	A	2610	-	-	-	X
24	MG	A	2612	-	-	-	X
24	MG	A	2617	-	-	-	X
24	MG	A	2623	-	-	-	X
24	MG	A	2632	-	-	-	X
24	MG	A	2637	-	-	-	X
24	MG	A	2640	-	-	-	X
24	MG	A	2647	-	-	-	X
24	MG	A	2649	-	-	-	X
24	MG	A	2651	-	-	-	X
24	MG	A	2659	-	-	-	X
24	MG	A	2662	-	-	-	X
24	MG	A	2665	-	-	-	X
24	MG	A	2689	-	-	-	X
24	MG	A	2693	-	-	-	X
24	MG	A	2695	-	-	-	X
24	MG	A	2702	-	-	-	X
24	MG	A	2704	-	-	-	X
24	MG	A	2705	-	-	-	X
24	MG	A	2706	-	-	-	X
24	MG	A	2710	-	-	-	X
24	MG	A	2717	-	-	-	X
24	MG	A	2718	-	-	-	X
24	MG	A	2723	-	-	-	X
24	MG	A	2729	-	-	-	X
24	MG	A	3813	-	-	-	X
24	MG	A	3923	-	-	-	X
24	MG	C	1207	-	-	-	X
24	MG	G	1156	-	-	-	X
25	K	A	2671	-	-	-	X
25	K	A	2672	-	-	-	X
26	3TS	A	2733	-	-	-	X

2 Entry composition

There are 28 unique types of molecules in this entry. The entry contains 52411 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	1512	32486	14462	6011	10503	1510	0	0	0

- 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
			Total	C	N	O	S			
6	F	101	843	531	155	154	3	0	0	0

- 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	57	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	125	Total	C	N	O	S	0	0	1
			971	611	196	163	1			

- Molecule 13 is a protein called 30S RIBOSOMAL PROTEIN S13.

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

- Molecule 14 is a protein called 30S RIBOSOMAL PROTEIN S14 TYPE Z.

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

- Molecule 15 is a protein called 30S RIBOSOMAL PROTEIN S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	O	88	Total	C	N	O	S	0	0	0
			733	458	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	104	Total	C	N	O	S	0	0	0
			857	547	161	147	2			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	95	GLN	GLU	CONFLICT	UNP Q5SHP7

- Molecule 18 is a protein called 30S RIBOSOMAL PROTEIN S18.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	45	GLY	ALA	CONFLICT	UNP Q5SLQ0

- Molecule 19 is a protein called 30S RIBOSOMAL PROTEIN S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	S	81	Total	C	N	O	S	0	0	1
			648	414	120	112	2			

- Molecule 20 is a protein called 30S RIBOSOMAL PROTEIN S20.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	34	VAL	ILE	CONFLICT	UNP P80380

- Molecule 21 is a protein called 30S RIBOSOMAL PROTEIN THX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	V	25	Total	C	N	O	0	0	1
			209	128	51	30			

- Molecule 22 is a RNA chain called 5'-R(*UP*UP*CP*AP*AP*AP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	W	4	Total	C	N	O	P	0	0	0
			79	37	12	27	3			

- Molecule 23 is a RNA chain called 5'-R(*GP*GP*GP*AP*UP*UP*GP*AP*AP*AP*AP* UP*CP*CP*CP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	Z	15	Total	C	N	O	P	0	0	0
			319	144	60	101	14			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	P	1	Total	Mg	0	0
			1	1		
24	G	1	Total	Mg	0	0
			1	1		

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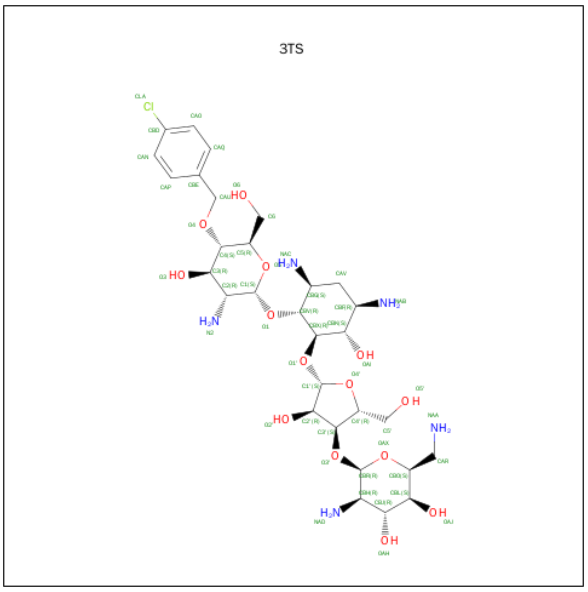
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	Q	1	Total Mg 1 1	0	0
24	D	1	Total Mg 1 1	0	0
24	E	2	Total Mg 2 2	0	0
24	H	1	Total Mg 1 1	0	0
24	C	1	Total Mg 1 1	0	0
24	A	204	Total Mg 204 204	0	0
24	T	2	Total Mg 2 2	0	0
24	N	1	Total Mg 1 1	0	0
24	L	3	Total Mg 3 3	0	0
24	M	1	Total Mg 1 1	0	0

- Molecule 25 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	16	Total K 16 16	0	0
25	E	1	Total K 1 1	0	0

- Molecule 26 is (2S,3S,4R,5R,6R)-2-(AMINOMETHYL)-5-AZANYL-6-[(2R,3S,4R,5S)-5-[(1R,2R,3S,5R,6S)-3,5-BIS(AZANYL)-2-[(2S,3R,4R,5S,6R)-3-AZANYL-5-[(4-CHLOROPHENYL)METHOXY]-6-(HYDROXYMETHYL)-4-OXIDANYL-OXAN-2-YL]OXY-6-OXIDANYL-CYCLOHEXYL]OXY-2-(HYDROXYMETHYL)-4-OXIDANYL-OXOLAN-3-YL]OXY-OXANE-3,4-DIOL (three-letter code: 3TS) (formula: $C_{30}H_{50}ClN_5O_{14}$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
26	A	1	Total	C	Cl	N	O	0	0
			50	30	1	5	14		

- Molecule 27 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 28 is water.

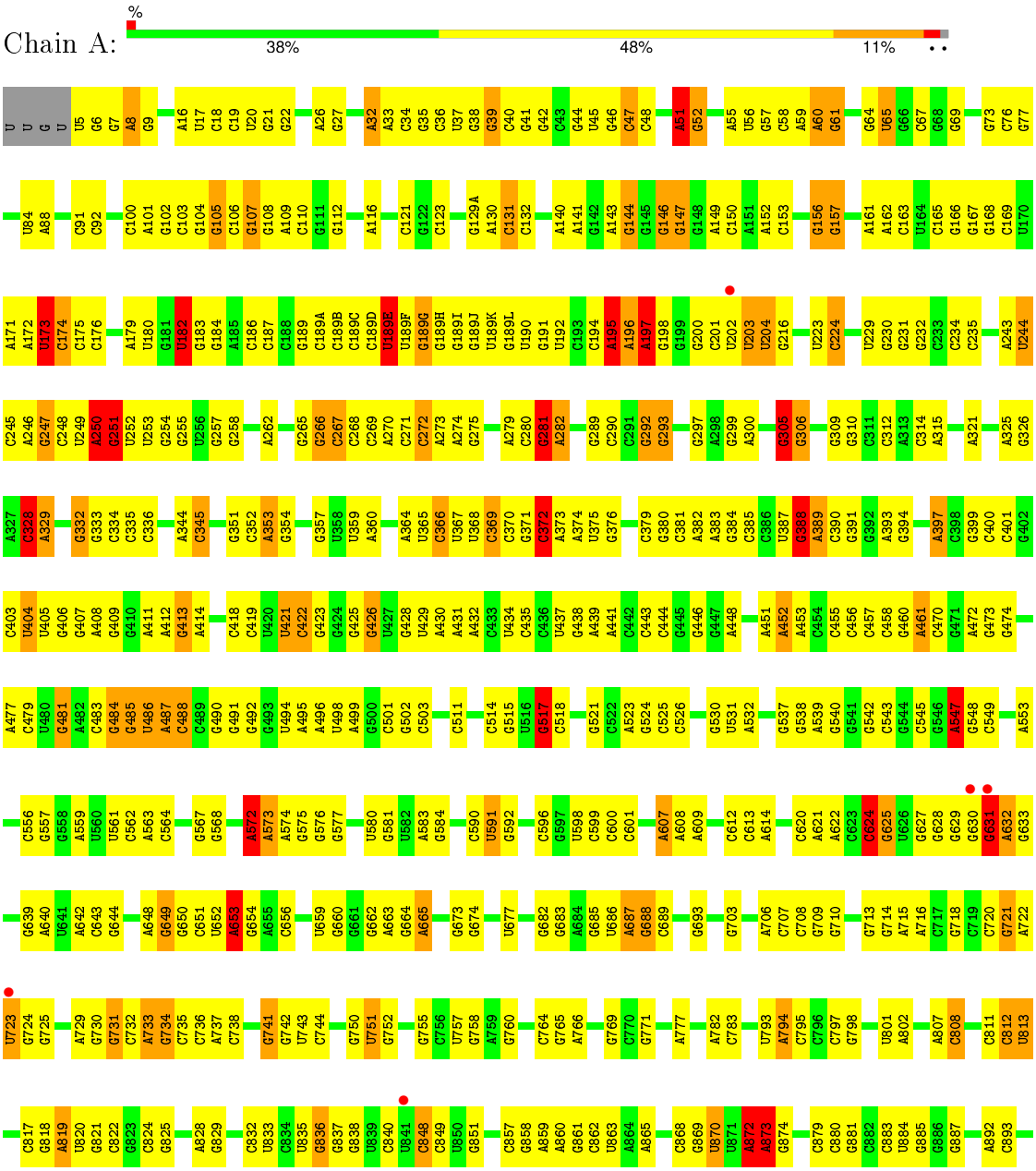
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	A	1	Total	O	0	0
			1	1		

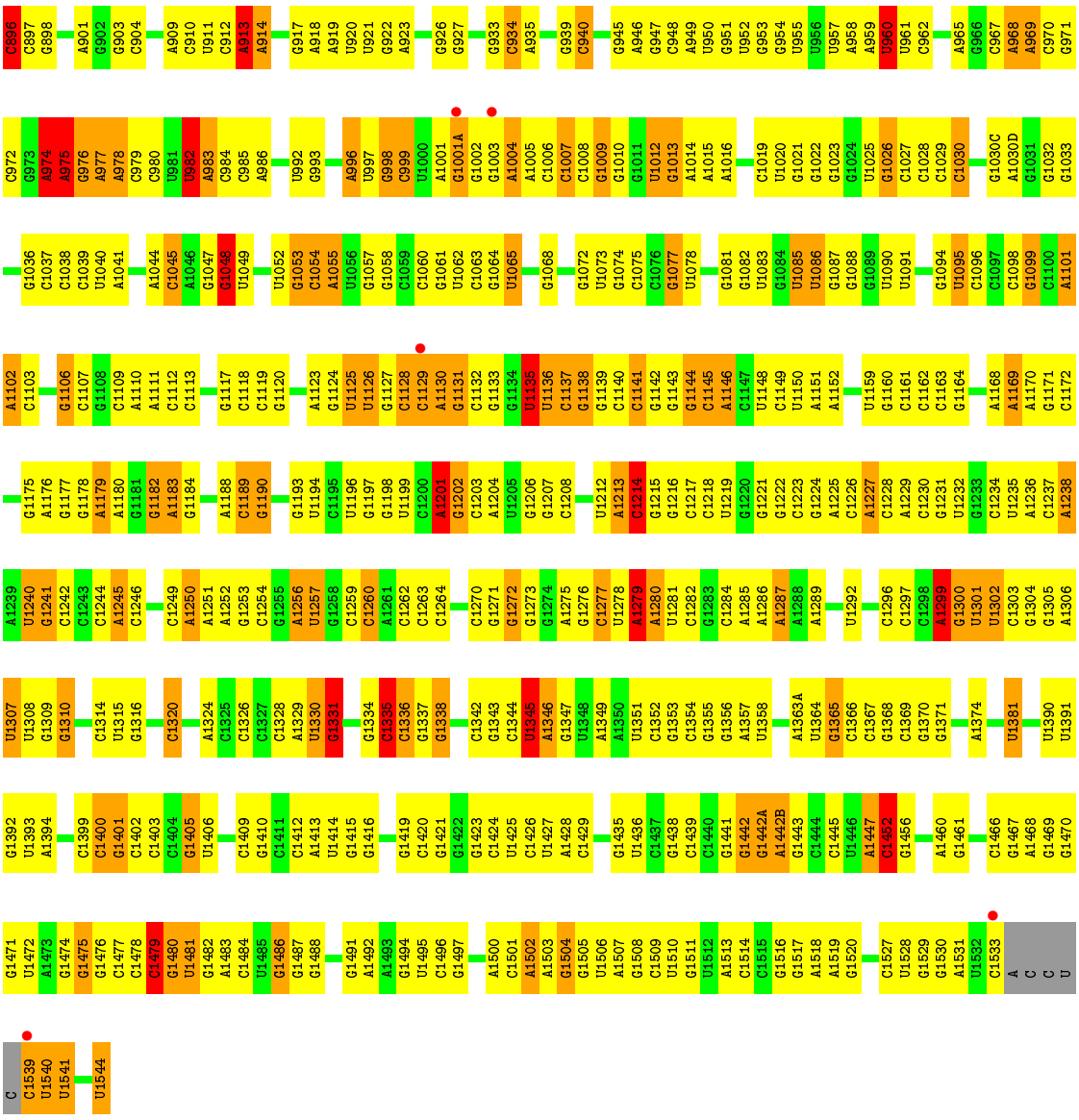
3 Residue-property plots (i)

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

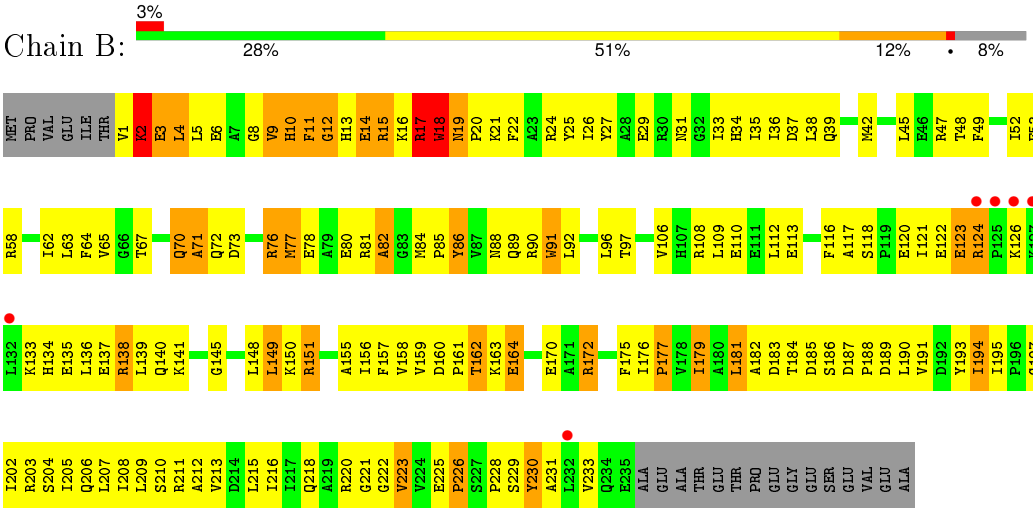
Chain A:





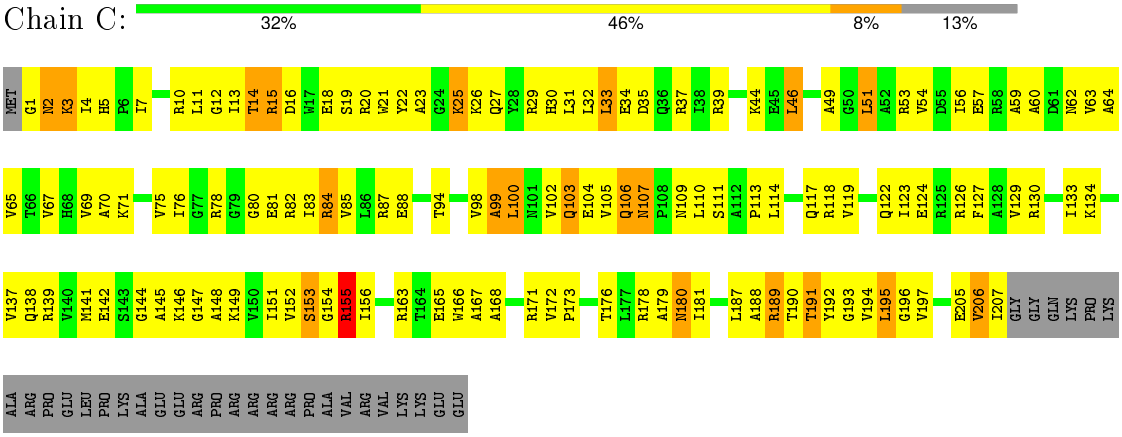
• Molecule 2: 30S RIBOSOMAL PROTEIN S2

Chain B:



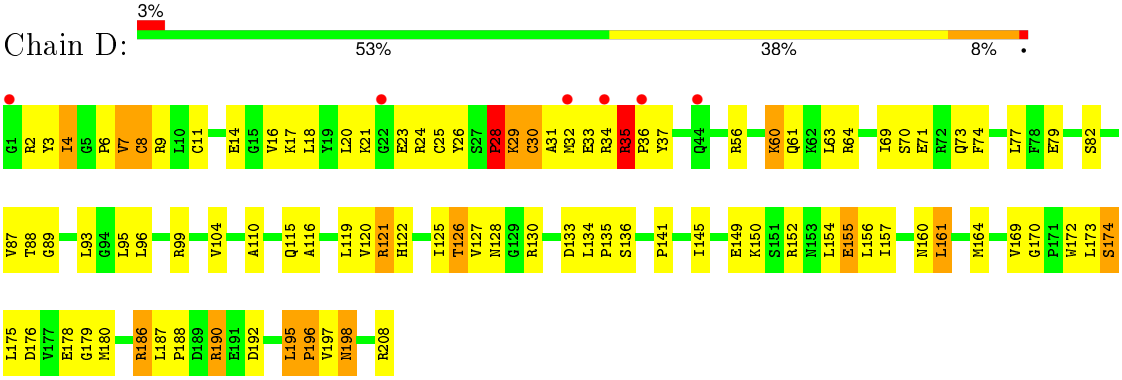
- Molecule 3: 30S RIBOSOMAL PROTEIN S3

Chain C:



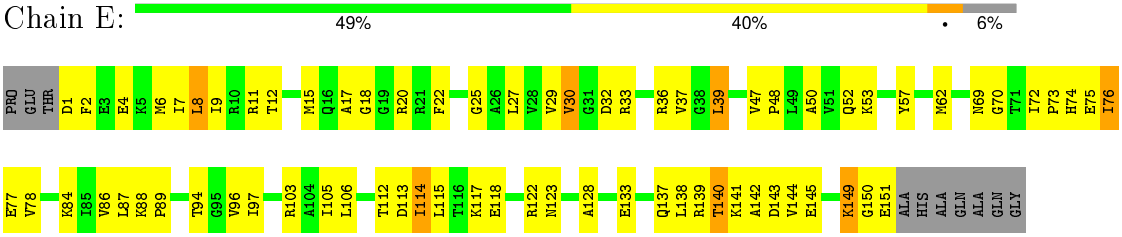
- Molecule 4: 30S RIBOSOMAL PROTEIN S4

Chain D:



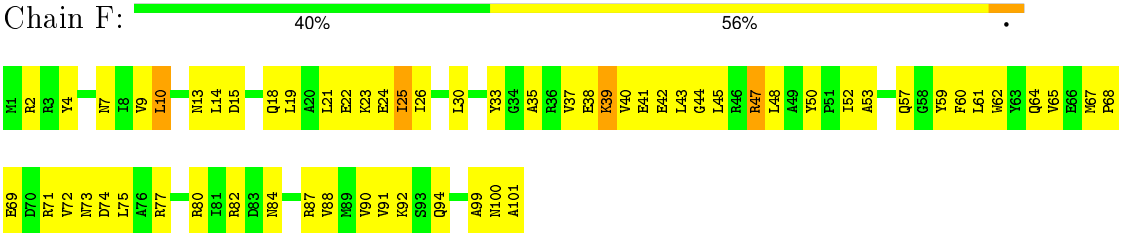
- Molecule 5: 30S RIBOSOMAL PROTEIN S5

Chain E:



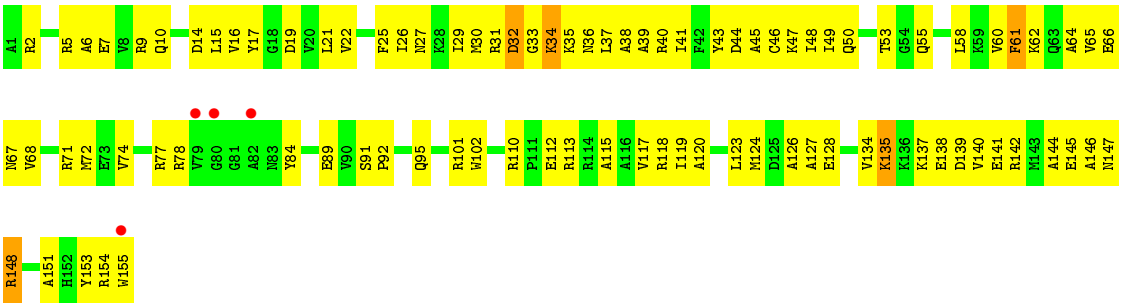
- Molecule 6: 30S RIBOSOMAL PROTEIN S6

Chain F:



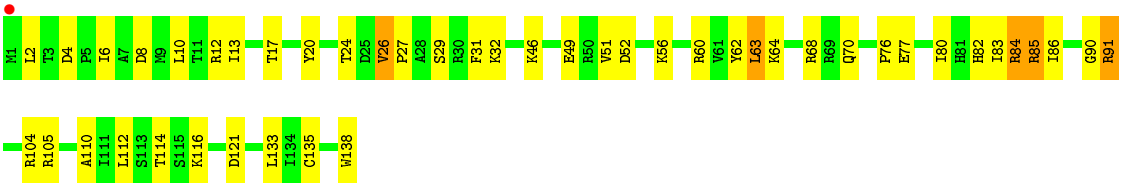
- Molecule 7: 30S RIBOSOMAL PROTEIN S7

Chain G:



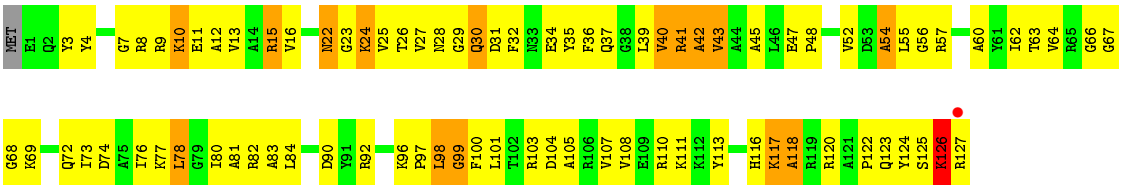
- Molecule 8: 30S RIBOSOMAL PROTEIN S8

Chain H:



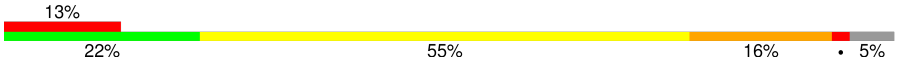
- Molecule 9: 30S RIBOSOMAL PROTEIN S9

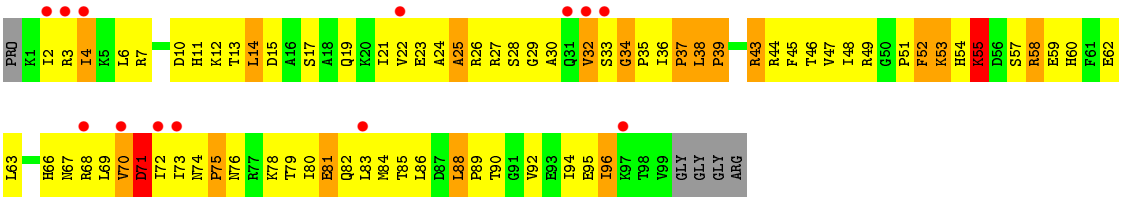
Chain I:



- Molecule 10: 30S RIBOSOMAL PROTEIN S10

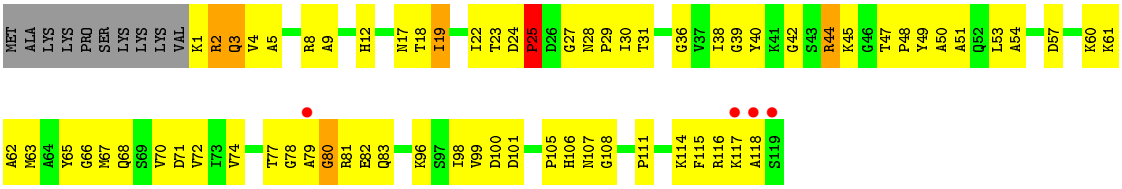
Chain J:





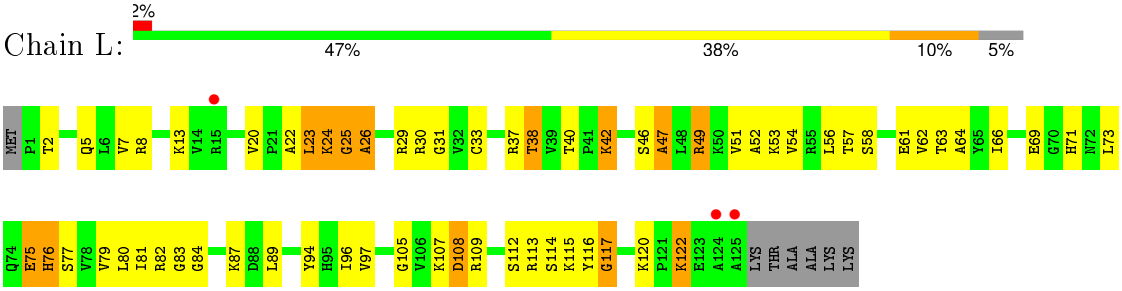
- Molecule 11: 30S RIBOSOMAL PROTEIN S11

Chain K:



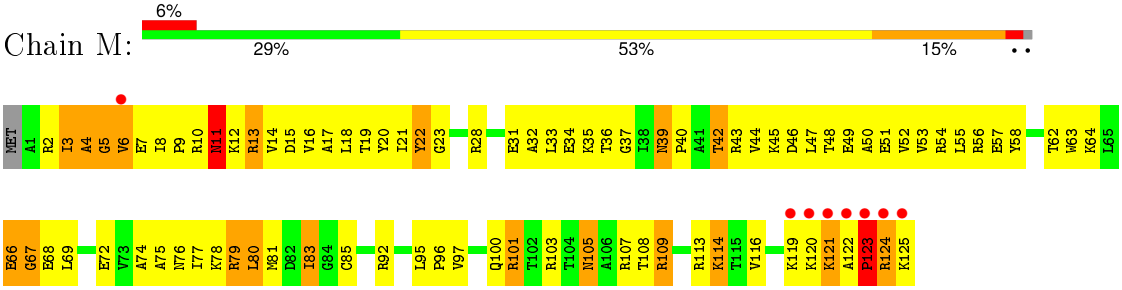
- Molecule 12: 30S RIBOSOMAL PROTEIN S12

Chain L:



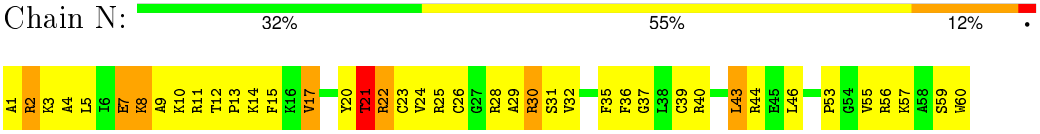
- Molecule 13: 30S RIBOSOMAL PROTEIN S13

Chain M:



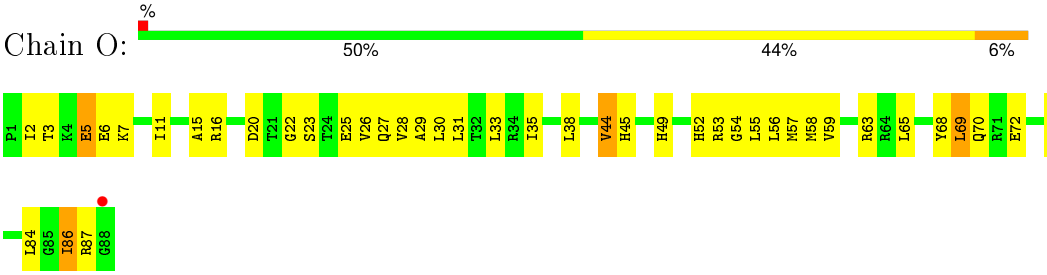
- Molecule 14: 30S RIBOSOMAL PROTEIN S14 TYPE Z

Chain N:



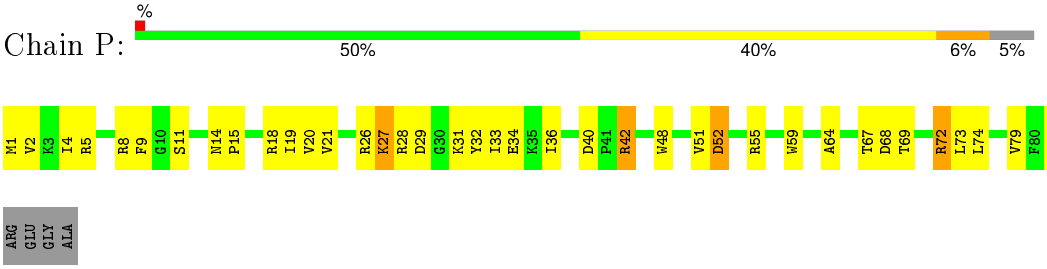
- Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain O:



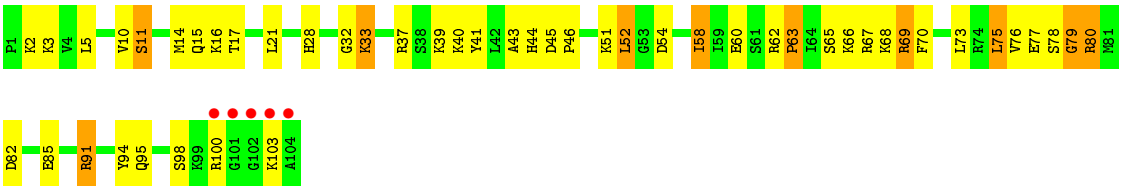
- Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain P:



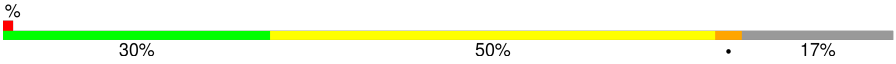
- Molecule 17: 30S RIBOSOMAL PROTEIN S17

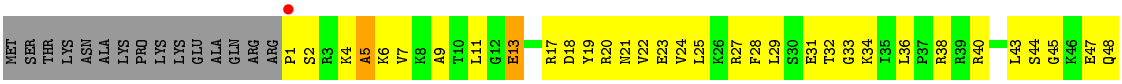
Chain Q:

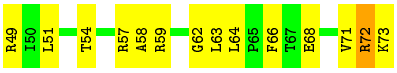


• Molecule 18: 30S RIBOSOMAL PROTEIN S18

Chain R:

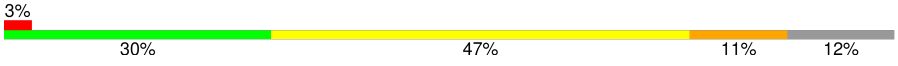


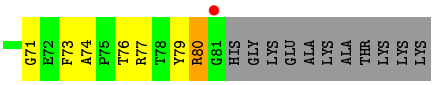




• Molecule 19: 30S RIBOSOMAL PROTEIN S19

Chain S:



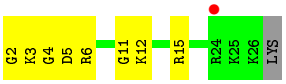


• Molecule 20: 30S RIBOSOMAL PROTEIN S20

Chain T:

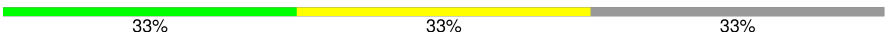
• Molecule 21: 30S RIBOSOMAL PROTEIN THX

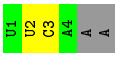
Chain V:



• Molecule 22: 5'-R(*UP*UP*CP*AP*AP*AP)-3'

Chain W:





• Molecule 23: 5'-R(*GP*GP*GP*AP*UP*UP*GP*AP*AP*AP*AP*UP*CP*CP*CP)-3'

Chain Z:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	401.73Å 401.73Å 173.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.00 39.51 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (40.00-3.00) 99.8 (39.51-3.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.35 (at 3.01Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.210 , 0.243 0.213 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	76.5	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 72.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 280162 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	52411	wwPDB-VP
Average B, all atoms (Å^2)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.52% 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: K, MG, ZN, 3TS

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	0.48	7/36362 (0.0%)	0.77	59/56750 (0.1%)
2	B	0.37	0/1936	0.61	0/2611
3	C	0.38	0/1637	0.66	0/2207
4	D	0.38	0/1733	0.60	0/2318
5	E	0.44	0/1163	0.71	0/1566
6	F	0.35	0/856	0.61	0/1154
7	G	0.35	0/1276	0.57	0/1709
8	H	0.43	0/1136	0.70	0/1527
9	I	0.38	0/1029	0.64	0/1378
10	J	0.40	0/808	0.68	0/1087
11	K	0.41	0/900	0.70	1/1213 (0.1%)
12	L	0.45	0/987	0.75	0/1322
13	M	0.36	0/1008	0.66	0/1347
14	N	0.48	0/501	0.73	0/664
15	O	0.37	0/743	0.60	1/988 (0.1%)
16	P	0.46	0/717	0.75	0/965
17	Q	0.41	0/870	0.72	0/1159
18	R	0.33	0/603	0.62	0/799
19	S	0.44	0/662	0.67	0/892
20	T	0.40	0/764	0.70	1/1006 (0.1%)
21	V	0.55	0/213	0.67	0/279
22	W	0.38	0/87	0.74	0/133
23	Z	0.47	0/357	0.68	0/555
All	All	0.45	7/56348 (0.0%)	0.74	62/83629 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	36	35

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1539	C	C2-O2	9.20	1.32	1.24
1	A	1539	C	N1-C2	7.27	1.47	1.40
1	A	1539	C	C2-N3	6.35	1.40	1.35
1	A	1539	C	N3-C4	6.14	1.38	1.33
1	A	1539	C	C4-N4	5.96	1.39	1.33
1	A	182	U	C2-O2	5.49	1.27	1.22
1	A	913	A	C5-C6	-5.15	1.36	1.41

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	281	G	N9-C1'-C2'	13.05	130.96	114.00
1	A	305	G	N9-C1'-C2'	10.59	127.77	114.00
1	A	517	G	C2'-C3'-O3'	10.28	132.12	109.50
1	A	872	A	C2'-C3'-O3'	9.89	131.25	109.50
1	A	366	C	C2'-C3'-O3'	9.56	130.54	109.50
1	A	1345	U	C2'-C3'-O3'	9.34	130.05	109.50
1	A	189(G)	G	C2'-C3'-O3'	9.15	129.63	109.50
1	A	1085	U	C2'-C3'-O3'	9.08	129.48	109.50
1	A	873	A	N9-C1'-C2'	9.07	125.80	114.00
1	A	653	A	C2'-C3'-O3'	8.85	128.97	109.50
1	A	47	C	C2'-C3'-O3'	8.79	128.85	109.50
1	A	1452	C	C2'-C3'-O3'	8.64	128.51	109.50
1	A	572	A	C2'-C3'-O3'	8.59	128.41	109.50
1	A	982	U	N1-C1'-C2'	8.23	124.70	114.00
1	A	631	G	C2'-C3'-O3'	8.14	127.41	109.50
1	A	292	G	C2'-C3'-O3'	7.99	127.08	109.50
1	A	388	G	N9-C1'-C2'	7.90	124.28	114.00
1	A	328	C	N1-C1'-C2'	7.65	123.95	114.00
1	A	1502	A	N9-C1'-C2'	7.47	123.71	114.00
1	A	196	A	C2'-C3'-O3'	7.33	125.62	109.50
1	A	372	C	C2'-C3'-O3'	7.17	125.26	109.50
1	A	771	G	C5'-C4'-C3'	-7.03	104.75	116.00
1	A	173	U	N1-C1'-C2'	6.96	123.05	114.00
1	A	281	G	C5'-C4'-O4'	6.79	117.25	109.10
1	A	1240	U	C2'-C3'-O3'	6.64	124.32	113.70
1	A	1201	A	C2'-C3'-O3'	6.44	124.00	113.70
1	A	1214	C	N1-C1'-C2'	6.40	122.32	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	982	U	C2'-C3'-O3'	6.39	123.93	113.70
1	A	783	C	C5'-C4'-C3'	-6.35	105.84	116.00
1	A	1479	C	C2'-C3'-O3'	6.27	123.73	113.70
1	A	782	A	C5'-C4'-C3'	-6.18	106.11	116.00
1	A	913	A	N9-C1'-C2'	6.16	122.01	114.00
1	A	305	G	C5'-C4'-O4'	6.16	116.49	109.10
1	A	1299	A	N9-C1'-C2'	6.09	121.92	114.00
1	A	870	U	C5'-C4'-C3'	-5.94	106.49	116.00
1	A	896	C	C5'-C4'-C3'	-5.94	106.50	116.00
1	A	189(E)	U	C5'-C4'-C3'	5.83	125.34	116.00
1	A	547	A	N9-C1'-C2'	5.78	121.51	114.00
1	A	1335	C	C5'-C4'-C3'	-5.72	106.84	116.00
1	A	387	U	C5'-C4'-C3'	-5.65	106.96	116.00
1	A	173	U	C5'-C4'-O4'	5.63	115.85	109.10
1	A	47	C	C4'-C3'-O3'	5.59	124.17	113.00
1	A	960	U	N1-C1'-C2'	5.54	121.20	114.00
1	A	624	C	C2'-C3'-O3'	5.52	122.54	113.70
1	A	1279	A	N9-C1'-C2'	5.52	121.17	114.00
1	A	974	A	N9-C1'-C2'	5.41	121.04	114.00
1	A	107	G	C5'-C4'-C3'	-5.39	107.38	116.00
1	A	822	C	C5'-C4'-C3'	-5.37	107.42	116.00
1	A	1135	U	C2'-C3'-O3'	5.31	122.20	113.70
1	A	173	U	O4'-C1'-N1	5.31	112.45	108.20
20	T	6	LEU	N-CA-C	-5.30	96.68	111.00
1	A	1135	U	N1-C1'-C2'	5.28	120.86	114.00
1	A	1048	G	C2'-C3'-O3'	5.26	122.12	113.70
1	A	1544	U	C2'-C3'-O3'	-5.25	97.94	109.50
1	A	189(G)	G	C4'-C3'-O3'	5.18	123.36	113.00
1	A	729	A	C5'-C4'-C3'	-5.14	107.78	116.00
1	A	1085	U	C4'-C3'-O3'	5.10	123.19	113.00
15	O	44	VAL	N-CA-C	-5.09	97.26	111.00
1	A	1077	G	C5'-C4'-C3'	-5.08	107.87	116.00
1	A	1381	U	C5'-C4'-C3'	-5.08	107.88	116.00
11	K	27	GLY	N-CA-C	5.06	125.75	113.10
1	A	631	G	C4'-C3'-O3'	5.01	123.03	113.00

All (36) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	47	C	C3'
1	A	173	U	C4',C3',C1'
1	A	189(E)	U	C4'

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Mol	Chain	Res	Type	Atom
1	A	189(G)	G	C3'
1	A	196	A	C3'
1	A	281	G	C4',C3',C1'
1	A	292	G	C3'
1	A	305	G	C4',C3',C1'
1	A	366	C	C3'
1	A	388	G	C4'
1	A	422	C	C4'
1	A	517	G	C3'
1	A	547	A	C4',C3',C1'
1	A	631	G	C3'
1	A	872	A	C3'
1	A	873	A	C4',C3',C1'
1	A	913	A	C4'
1	A	982	U	C4',C3'
1	A	1048	G	C3'
1	A	1085	U	C3'
1	A	1135	U	C4',C3'
1	A	1345	U	C3'
1	A	1479	C	C4',C3'

All (35) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1048	G	Sidechain
1	A	112	G	Sidechain
1	A	1279	A	Sidechain
1	A	1289	A	Sidechain
1	A	1299	A	Sidechain
1	A	1307	U	Sidechain
1	A	1331	G	Sidechain
1	A	1405	G	Sidechain
1	A	1445	C	Sidechain
1	A	182	U	Sidechain
1	A	195	A	Sidechain
1	A	197	A	Sidechain
1	A	250	A	Sidechain
1	A	251	G	Sidechain
1	A	281	G	Sidechain
1	A	290	C	Sidechain
1	A	297	G	Sidechain
1	A	305	G	Sidechain

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Mol	Chain	Res	Type	Group
1	A	368	U	Sidechain
1	A	37	U	Sidechain
1	A	380	G	Sidechain
1	A	404	U	Sidechain
1	A	51	A	Sidechain
1	A	573	A	Sidechain
1	A	624	C	Sidechain
1	A	741	G	Sidechain
1	A	760	G	Sidechain
1	A	808	C	Sidechain
1	A	879	C	Sidechain
1	A	883	C	Sidechain
1	A	887	G	Sidechain
1	A	898	G	Sidechain
1	A	940	C	Sidechain
1	A	960	U	Sidechain
1	A	975	A	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32486	0	16402	923	0
2	B	1901	0	1954	211	0
3	C	1613	0	1680	163	0
4	D	1703	0	1766	124	0
5	E	1147	0	1210	75	0
6	F	843	0	857	77	0
7	G	1257	0	1299	98	0
8	H	1116	0	1177	50	0
9	I	1011	0	1046	92	0
10	J	795	0	843	116	0
11	K	885	0	907	77	0
12	L	971	0	1059	74	0
13	M	997	0	1075	110	0
14	N	492	0	533	59	0
15	O	733	0	768	50	0
16	P	701	0	720	48	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	Q	857	0	932	53	0
18	R	597	0	670	65	0
19	S	648	0	675	81	0
20	T	762	0	862	59	0
21	V	209	0	221	17	0
22	W	79	0	44	3	0
23	Z	319	0	164	7	0
24	A	204	0	0	0	0
24	C	1	0	0	0	0
24	D	1	0	0	0	0
24	E	2	0	0	0	0
24	G	1	0	0	0	0
24	H	1	0	0	0	0
24	L	3	0	0	0	0
24	M	1	0	0	0	0
24	N	1	0	0	0	0
24	P	1	0	0	0	0
24	Q	1	0	0	0	0
24	T	2	0	0	0	0
25	A	16	0	0	0	0
25	E	1	0	0	0	0
26	A	50	0	50	6	0
27	D	1	0	0	0	0
27	N	1	0	0	0	0
28	A	1	0	0	0	0
All	All	52411	0	36914	2416	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 27.

All (2416) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:425:G:H2'	1:A:426:G:H5"	1.22	1.17
1:A:1329:A:H2'	1:A:1330:U:H5"	1.18	1.13
1:A:243:A:H4'	1:A:244:U:H5'	1.19	1.13
4:D:17:LYS:NZ	4:D:30:CYS:HB3	1.64	1.12
3:C:190:THR:HG22	3:C:191:THR:H	1.09	1.12
1:A:872:A:H1'	1:A:873:A:H5'	1.16	1.11
1:A:1008:C:H2'	1:A:1009:G:H5"	1.26	1.10
1:A:975:A:H5"	1:A:976:G:H5'	1.31	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:86:ILE:HG22	15:O:87:ARG:H	1.10	1.09
1:A:1271:G:H2'	1:A:1272:G:H5"	1.31	1.09
1:A:872:A:C1'	1:A:873:A:H5'	1.82	1.09
1:A:972:C:H4'	10:J:55:LYS:HG2	1.35	1.09
1:A:1012:U:H3'	1:A:1013:G:H5"	1.30	1.08
1:A:1029:C:H2'	1:A:1030:C:H5"	1.36	1.08
1:A:1098:C:H2'	1:A:1099:G:H5"	1.07	1.07
1:A:1054:C:O2'	1:A:1055:A:H5'	1.56	1.06
1:A:1098:C:C2'	1:A:1099:G:H5"	1.83	1.06
3:C:107:ASN:HD22	3:C:110:LEU:HG	1.20	1.06
19:S:27:LYS:HG2	19:S:28:ARG:H	1.15	1.06
1:A:223:U:H2'	1:A:224:C:H5"	1.37	1.05
1:A:1330:U:H6	1:A:1330:U:H5'	1.22	1.05
2:B:126:LYS:HA	2:B:129:GLN:HB3	1.38	1.05
10:J:43:ARG:HH11	10:J:43:ARG:HB3	1.19	1.04
1:A:1421:G:H1	1:A:1479:C:H42	1.04	1.04
10:J:36:ILE:HB	10:J:69:LEU:HB2	1.33	1.03
1:A:1329:A:C2'	1:A:1330:U:H5"	1.89	1.02
10:J:88:LEU:H	10:J:89:PRO:HD2	1.20	1.02
7:G:78:ARG:HH11	7:G:78:ARG:HB3	1.22	1.01
1:A:648:A:H2'	1:A:649:G:H5"	1.38	1.01
17:Q:91:ARG:HB3	17:Q:91:ARG:HH11	1.24	1.01
1:A:1276:G:H2'	1:A:1277:C:H5"	1.41	1.00
1:A:1188:A:H2'	1:A:1189:C:H5"	1.43	1.00
1:A:1047:G:H2'	1:A:1048:G:H5"	1.39	0.99
6:F:25:ILE:HD12	6:F:25:ILE:H	1.24	0.98
1:A:1086:U:H3	1:A:1099:G:H22	1.02	0.98
1:A:1223:C:H5'	1:A:1224:G:H5"	1.45	0.98
9:I:15:ARG:HB2	9:I:63:THR:HB	1.44	0.97
1:A:104:G:H2'	1:A:105:G:H5"	1.42	0.97
1:A:1223:C:C5'	1:A:1224:G:H5"	1.93	0.96
1:A:1244:C:H2'	1:A:1245:A:H5"	1.47	0.96
2:B:78:GLU:HB3	2:B:213:VAL:HG21	1.44	0.96
11:K:44:ARG:O	11:K:47:THR:HG22	1.65	0.96
1:A:1244:C:C2'	1:A:1245:A:H5"	1.95	0.96
3:C:49:ALA:HB1	3:C:69:VAL:HG11	1.48	0.95
10:J:43:ARG:NH1	10:J:43:ARG:HB3	1.81	0.95
1:A:1271:G:C2'	1:A:1272:G:H5"	1.97	0.95
2:B:1:VAL:HG21	2:B:215:LEU:HD23	1.46	0.94
7:G:78:ARG:NH1	7:G:78:ARG:HB3	1.82	0.94
1:A:1101:A:H4'	1:A:1102:A:H5'	1.48	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:2:ASN:HD22	3:C:2:ASN:H	1.14	0.93
19:S:4:LEU:O	19:S:5:LYS:HB2	1.65	0.93
1:A:1309:G:H3'	1:A:1310:G:H5"	1.47	0.93
1:A:425:G:C2'	1:A:426:G:H5"	1.98	0.92
3:C:190:THR:HG22	3:C:191:THR:N	1.83	0.92
1:A:591:U:H5'	1:A:591:U:H6	1.33	0.92
13:M:48:THR:HG22	13:M:50:ALA:H	1.34	0.92
5:E:47:VAL:HB	5:E:48:PRO:HD3	1.52	0.91
1:A:64:G:H4'	1:A:65:U:H5'	1.51	0.91
1:A:1502:A:H2	1:A:1505:G:H1	1.18	0.91
1:A:371:G:O2'	1:A:372:C:H5'	1.71	0.91
1:A:939:G:H5"	7:G:101:ARG:NH2	1.87	0.90
2:B:134:HIS:HA	2:B:137:GLU:HG2	1.53	0.90
4:D:195:LEU:H	4:D:195:LEU:HD23	1.36	0.90
1:A:1047:G:C2'	1:A:1048:G:H5"	2.01	0.89
1:A:1029:C:C2'	1:A:1030:C:H5"	2.02	0.89
1:A:1442(A):G:H5"	1:A:1442(B):A:H5'	1.54	0.89
1:A:38:G:H22	1:A:397:A:H5'	1.36	0.89
4:D:17:LYS:HZ3	4:D:30:CYS:HB3	1.30	0.89
16:P:51:VAL:O	16:P:52:ASP:HB3	1.73	0.89
1:A:1182:G:H4'	1:A:1183:A:H5'	1.54	0.89
5:E:76:ILE:CD1	5:E:87:LEU:HB2	2.03	0.89
1:A:1188:A:C2'	1:A:1189:C:H5"	2.01	0.89
3:C:25:LYS:NZ	3:C:25:LYS:H	1.71	0.88
1:A:272:C:H5'	1:A:272:C:H6	1.39	0.88
1:A:1421:G:H1	1:A:1479:C:N4	1.72	0.88
16:P:42:ARG:HH11	16:P:42:ARG:HG2	1.37	0.88
3:C:190:THR:CG2	3:C:191:THR:H	1.87	0.88
1:A:1213:A:O2'	1:A:1214:C:H5"	1.74	0.88
1:A:1231:G:O3'	9:I:125:SER:HB3	1.75	0.87
1:A:648:A:C2'	1:A:649:G:H5"	2.03	0.87
1:A:1008:C:C2'	1:A:1009:G:H5"	2.02	0.86
3:C:63:VAL:HB	3:C:98:VAL:HG23	1.57	0.86
1:A:1048:G:H8	1:A:1048:G:H5'	1.38	0.86
11:K:77:THR:HA	11:K:81:ARG:HH21	1.39	0.86
1:A:223:U:C2'	1:A:224:C:H5"	2.05	0.85
3:C:189:ARG:HB3	3:C:189:ARG:HH11	1.41	0.85
1:A:1391:U:H2'	1:A:1392:G:C8	2.12	0.85
1:A:1329:A:H2'	1:A:1330:U:C5'	2.04	0.84
3:C:109:ASN:ND2	3:C:139:ARG:HB3	1.91	0.84
11:K:38:ILE:HG22	11:K:39:GLY:H	1.41	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:872:A:H1'	1:A:873:A:C5'	2.06	0.84
1:A:1276:G:C2'	1:A:1277:C:H5"	2.07	0.84
13:M:39:ASN:O	13:M:42:THR:HG23	1.78	0.84
1:A:487:A:H8	1:A:487:A:H5'	1.42	0.84
2:B:71:ALA:HB2	2:B:205:ILE:HD13	1.58	0.84
20:T:83:GLN:O	20:T:86:GLU:HB2	1.78	0.84
15:O:86:ILE:HG22	15:O:87:ARG:N	1.91	0.83
4:D:17:LYS:HZ2	4:D:30:CYS:HB3	1.39	0.83
3:C:25:LYS:H	3:C:25:LYS:HZ3	1.26	0.83
1:A:483:C:H3'	1:A:484:G:H5"	1.58	0.83
10:J:6:LEU:HB2	10:J:68:ARG:HB2	1.59	0.83
1:A:60:A:H4'	1:A:61:G:H5'	1.59	0.83
2:B:194:ILE:HD12	2:B:194:ILE:H	1.44	0.83
17:Q:91:ARG:NH1	17:Q:91:ARG:HB3	1.91	0.83
1:A:1012:U:C3'	1:A:1013:G:H5"	2.09	0.83
1:A:1334:G:H5'	1:A:1335:C:OP1	1.77	0.83
4:D:33:GLU:HG3	4:D:34:ARG:HH11	1.42	0.82
1:A:1330:U:C6	1:A:1330:U:H5'	2.12	0.82
14:N:26:CYS:SG	14:N:28:ARG:HB2	2.20	0.82
3:C:107:ASN:ND2	3:C:110:LEU:HG	1.92	0.82
10:J:44:ARG:HG2	10:J:44:ARG:HH11	1.43	0.82
3:C:13:ILE:HG22	3:C:14:THR:H	1.45	0.82
1:A:404:U:H2'	1:A:405:U:H6	1.44	0.81
12:L:37:ARG:HH12	12:L:53:LYS:HE2	1.46	0.81
3:C:12:GLY:HA3	14:N:56:ARG:CZ	2.10	0.81
1:A:250:A:H4'	1:A:251:G:O5'	1.80	0.81
1:A:580:U:H2'	1:A:581:G:O4'	1.80	0.81
3:C:33:LEU:HG	14:N:24:VAL:HG21	1.61	0.81
1:A:1004:A:H8	1:A:1036:G:H1	1.28	0.81
1:A:1164:G:H1	1:A:1172:C:H42	1.29	0.81
2:B:118:SER:O	2:B:121:ILE:HG13	1.81	0.81
3:C:109:ASN:O	3:C:110:LEU:HD23	1.81	0.81
10:J:37:PRO:HA	10:J:68:ARG:HH11	1.46	0.81
4:D:25:CYS:HA	4:D:30:CYS:HB2	1.62	0.81
1:A:1309:G:C3'	1:A:1310:G:H5"	2.11	0.81
8:H:82:HIS:NE2	8:H:84:ARG:HB2	1.96	0.80
2:B:108:ARG:NH1	2:B:112:LEU:HG	1.96	0.80
11:K:12:HIS:HB3	11:K:19:ILE:CD1	2.09	0.80
1:A:1260:C:OP2	1:A:1284:C:H4'	1.82	0.80
12:L:71:HIS:HD2	12:L:73:LEU:H	1.28	0.80
1:A:189(D):C:H2'	1:A:189(E):U:H1'	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:24:LYS:C	12:L:26:ALA:H	1.85	0.80
10:J:88:LEU:H	10:J:89:PRO:CD	1.95	0.80
1:A:1256:A:H61	1:A:1278:U:H3	1.26	0.80
1:A:939:G:H5"	7:G:101:ARG:HH22	1.46	0.80
12:L:29:ARG:HD3	12:L:58:SER:HB3	1.64	0.79
1:A:1125:U:H3	10:J:3:ARG:HH21	1.30	0.79
1:A:664:G:H22	1:A:741:G:H1	1.29	0.79
3:C:118:ARG:HG2	3:C:139:ARG:NH2	1.97	0.79
12:L:22:ALA:O	12:L:23:LEU:O	2.01	0.79
1:A:1326:C:H5'	21:V:12:LYS:NZ	1.96	0.79
9:I:69:LYS:O	9:I:73:ILE:HG13	1.83	0.79
15:O:38:LEU:HD12	15:O:55:LEU:HB2	1.65	0.79
3:C:25:LYS:HB3	3:C:25:LYS:HZ2	1.48	0.79
12:L:37:ARG:HG2	12:L:38:THR:H	1.46	0.79
1:A:751:U:H1'	15:O:22:GLY:O	1.82	0.79
1:A:1245:A:H5'	1:A:1245:A:H8	1.46	0.78
1:A:1502:A:H2	1:A:1505:G:N1	1.82	0.78
13:M:66:GLU:HG3	13:M:67:GLY:H	1.49	0.78
3:C:103:GLN:HE21	3:C:104:GLU:H	1.31	0.78
21:V:6:ARG:HG2	21:V:15:ARG:NH1	1.99	0.78
4:D:28:PRO:O	4:D:29:LYS:HG3	1.84	0.78
1:A:1060:C:C5	3:C:1:GLY:HA3	2.19	0.78
16:P:15:PRO:HD2	16:P:42:ARG:HD2	1.66	0.78
6:F:48:LEU:HG	6:F:57:GLN:HA	1.66	0.78
6:F:15:ASP:H	6:F:18:GLN:NE2	1.81	0.78
11:K:44:ARG:HB3	11:K:44:ARG:NH1	1.98	0.78
1:A:1188:A:C3'	1:A:1189:C:H5"	2.14	0.77
3:C:2:ASN:ND2	3:C:2:ASN:H	1.81	0.77
11:K:100:ASP:HB2	18:R:73:LYS:HD2	1.66	0.77
3:C:14:THR:O	3:C:15:ARG:HB2	1.84	0.77
21:V:6:ARG:NE	21:V:15:ARG:HH12	1.83	0.77
6:F:10:LEU:CD1	6:F:59:TYR:HB3	2.13	0.77
2:B:6:GLU:HB3	2:B:10:HIS:HE1	1.49	0.77
4:D:150:LYS:H	4:D:150:LYS:HD2	1.48	0.77
7:G:53:THR:HG22	7:G:55:GLN:H	1.48	0.77
2:B:76:ARG:HA	2:B:86:TYR:CE2	2.20	0.77
1:A:613:C:O2'	1:A:614:A:H5'	1.84	0.77
1:A:720:C:H3'	1:A:721:G:H5"	1.66	0.77
19:S:27:LYS:HG2	19:S:28:ARG:N	1.96	0.77
7:G:36:ASN:ND2	9:I:40:VAL:HG23	2.00	0.77
1:A:371:G:C2'	1:A:372:C:H5'	2.16	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:V:6:ARG:HE	21:V:15:ARG:HH12	1.33	0.76
4:D:34:ARG:O	4:D:35:ARG:HB2	1.85	0.76
4:D:35:ARG:H	4:D:36:PRO:CD	1.98	0.76
11:K:81:ARG:CZ	18:R:73:LYS:HE2	2.15	0.76
4:D:178:GLU:HG3	4:D:179:GLY:H	1.49	0.76
1:A:1126:U:H2'	1:A:1126:U:O2	1.85	0.76
1:A:1098:C:H2'	1:A:1099:G:C5'	2.03	0.76
1:A:946:A:H2'	1:A:947:G:C8	2.21	0.76
1:A:1330:U:H2'	1:A:1331:G:H5'	1.66	0.76
1:A:1007:C:H2'	1:A:1008:C:C6	2.20	0.76
10:J:32:VAL:HG22	10:J:72:ILE:HG23	1.66	0.76
13:M:49:GLU:O	13:M:53:VAL:HG23	1.86	0.76
10:J:4:ILE:H	10:J:4:ILE:HD13	1.50	0.76
12:L:56:LEU:HD21	12:L:62:VAL:HG22	1.68	0.76
1:A:1435:G:H2'	1:A:1436:U:C6	2.20	0.75
1:A:280:C:H4'	1:A:281:G:OP1	1.85	0.75
4:D:186:ARG:HH22	4:D:187:LEU:HD12	1.50	0.75
1:A:1189:C:H6	1:A:1189:C:H5'	1.51	0.75
2:B:230:TYR:HD1	2:B:233:VAL:HG21	1.51	0.75
13:M:121:LYS:HG3	13:M:122:ALA:H	1.48	0.75
15:O:3:THR:HB	15:O:5:GLU:OE2	1.86	0.75
2:B:6:GLU:HB3	2:B:10:HIS:CE1	2.22	0.75
4:D:2:ARG:NH2	4:D:73:GLN:HE21	1.82	0.75
19:S:27:LYS:CG	19:S:28:ARG:H	1.96	0.75
4:D:33:GLU:HG3	4:D:34:ARG:NH1	2.02	0.75
1:A:104:G:C2'	1:A:105:G:H5"	2.16	0.75
1:A:1223:C:H5"	1:A:1224:G:H5"	1.69	0.74
19:S:44:VAL:HA	19:S:61:ILE:HD12	1.69	0.74
8:H:84:ARG:HG3	8:H:84:ARG:HH11	1.51	0.74
1:A:293:G:H5'	1:A:609:A:H61	1.52	0.74
1:A:835:U:OP2	18:R:49:ARG:NH2	2.20	0.74
2:B:15:ARG:NH1	2:B:17:ARG:HG2	2.01	0.74
13:M:9:PRO:HB2	13:M:17:ALA:HB1	1.69	0.74
20:T:46:LEU:HB2	20:T:93:ILE:CG2	2.17	0.74
3:C:12:GLY:HA3	14:N:56:ARG:NH2	2.02	0.74
1:A:146:G:H2'	1:A:147:G:H5"	1.68	0.74
1:A:149:A:H2'	1:A:150:C:C6	2.23	0.74
7:G:120:ALA:O	7:G:124:MET:HG3	1.88	0.74
13:M:3:ILE:HG22	13:M:4:ALA:N	2.03	0.74
1:A:1480:G:HO2'	1:A:1481:U:H6	1.35	0.74
11:K:38:ILE:HG22	11:K:39:GLY:N	2.00	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:U:H2'	1:A:57:G:H8	1.53	0.74
3:C:2:ASN:ND2	3:C:2:ASN:N	2.33	0.74
2:B:172:ARG:NH2	8:H:68:ARG:HH22	1.86	0.74
7:G:112:GLU:HG2	7:G:118:ARG:HG2	1.68	0.74
1:A:837:G:H1	1:A:849:C:H42	1.34	0.74
1:A:1474:G:C2'	1:A:1475:G:H5"	2.18	0.74
1:A:404:U:H2'	1:A:405:U:C6	2.22	0.73
10:J:59:GLU:OE1	14:N:44:ARG:NH1	2.21	0.73
17:Q:66:LYS:O	17:Q:67:ARG:HG2	1.88	0.73
1:A:751:U:H5'	1:A:752:G:OP1	1.88	0.73
1:A:1412:C:H2'	1:A:1413:A:C8	2.23	0.73
1:A:624:C:H4'	1:A:625:G:OP2	1.89	0.73
1:A:147:G:H8	1:A:147:G:H5'	1.53	0.73
4:D:173:LEU:O	4:D:174:SER:HB3	1.88	0.73
1:A:818:G:O2'	1:A:819:A:H5"	1.88	0.73
9:I:92:ARG:HB3	9:I:92:ARG:NH1	2.04	0.73
14:N:25:ARG:NE	14:N:46:LEU:HD21	2.04	0.73
3:C:26:LYS:HB2	3:C:27:GLN:HE21	1.53	0.73
13:M:3:ILE:HG22	13:M:4:ALA:H	1.53	0.73
19:S:32:THR:HG22	19:S:34:SER:H	1.52	0.73
2:B:78:GLU:OE2	2:B:210:SER:HA	1.88	0.73
1:A:1343:G:H2'	1:A:1344:C:C6	2.24	0.73
1:A:1474:G:H2'	1:A:1475:G:H5"	1.71	0.72
11:K:12:HIS:HB3	11:K:19:ILE:HD13	1.68	0.72
1:A:1065:U:C5	1:A:1190:G:H1'	2.23	0.72
1:A:998:G:H3'	1:A:999:C:H5"	1.68	0.72
6:F:101:ALA:CB	18:R:13:GLU:HG3	2.20	0.72
1:A:948:C:OP1	13:M:108:THR:HG22	1.89	0.72
1:A:718:G:H5'	11:K:107:ASN:HB2	1.71	0.72
1:A:1148:U:H2'	1:A:1149:C:O4'	1.89	0.72
20:T:3:LEU:O	20:T:6:LEU:HD13	1.88	0.72
1:A:1244:C:H2'	1:A:1245:A:C5'	2.18	0.72
1:A:1057:G:H5"	3:C:153:SER:HB2	1.72	0.72
10:J:4:ILE:N	10:J:4:ILE:HD13	2.05	0.72
13:M:64:LYS:HE3	13:M:68:GLU:HG2	1.71	0.72
13:M:121:LYS:CG	13:M:122:ALA:H	2.02	0.72
12:L:33:CYS:HB2	12:L:75:GLU:O	1.90	0.72
12:L:71:HIS:CD2	12:L:73:LEU:H	2.07	0.72
2:B:17:ARG:NH1	2:B:18:TRP:HA	2.04	0.72
2:B:76:ARG:HA	2:B:86:TYR:HE2	1.54	0.71
17:Q:58:ILE:HG23	17:Q:70:PHE:CD2	2.25	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1222:G:OP1	19:S:76:THR:HG21	1.90	0.71
1:A:1030(C):G:H2'	1:A:1030(D):A:C8	2.24	0.71
1:A:1442(A):G:C5'	1:A:1442(B):A:H5'	2.20	0.71
2:B:86:TYR:O	2:B:145:GLY:HA3	1.91	0.71
1:A:146:G:C2'	1:A:147:G:H5"	2.20	0.71
1:A:1189:C:P	10:J:49:ARG:HH22	2.13	0.71
13:M:14:VAL:HG23	13:M:42:THR:O	1.91	0.71
1:A:344:A:H5"	1:A:345:C:H5	1.54	0.71
9:I:98:LEU:HB2	9:I:100:PHE:CE1	2.26	0.71
19:S:14:LEU:HA	19:S:17:LYS:HB3	1.71	0.71
19:S:61:ILE:HD13	19:S:62:THR:N	2.06	0.71
1:A:499:A:H61	1:A:547:A:H5"	1.54	0.71
1:A:872:A:C2'	1:A:873:A:H5'	2.21	0.71
16:P:11:SER:HB2	16:P:14:ASN:HB3	1.73	0.71
2:B:92:LEU:HD23	2:B:92:LEU:N	2.04	0.71
11:K:47:THR:HG23	11:K:50:ALA:H	1.56	0.70
11:K:30:ILE:HG22	11:K:31:THR:HG23	1.73	0.70
1:A:21:G:H2'	1:A:22:G:C8	2.27	0.70
13:M:83:ILE:HD12	19:S:64:ASN:ND2	2.06	0.70
1:A:1216:G:H5"	14:N:4:ALA:CB	2.21	0.70
7:G:148:ARG:HD2	11:K:49:TYR:CE1	2.26	0.70
13:M:58:TYR:O	13:M:62:THR:HG22	1.91	0.70
1:A:1123:A:H4'	10:J:35:PRO:HD2	1.73	0.70
5:E:77:GLU:HG2	5:E:86:VAL:HG22	1.74	0.70
13:M:51:GLU:HG2	13:M:54:ARG:HH21	1.57	0.70
10:J:2:ILE:HD11	10:J:75:PRO:HA	1.73	0.70
11:K:9:ALA:HB2	11:K:70:VAL:HG11	1.73	0.70
1:A:460:G:H2'	1:A:461:A:H5"	1.74	0.70
1:A:1150:U:H4'	10:J:39:PRO:HG3	1.72	0.70
1:A:730:G:H5'	1:A:731:G:OP2	1.90	0.70
1:A:486:U:C2'	1:A:487:A:H5"	2.22	0.70
4:D:186:ARG:CZ	4:D:187:LEU:H	2.05	0.70
1:A:1486:G:H2'	1:A:1487:G:O4'	1.92	0.70
1:A:1326:C:H5'	21:V:12:LYS:HZ2	1.54	0.70
9:I:16:VAL:HG22	9:I:62:ILE:HD12	1.72	0.70
1:A:1005:A:H5"	1:A:1006:C:H5	1.57	0.70
18:R:31:GLU:H	18:R:31:GLU:CD	1.94	0.70
12:L:24:LYS:O	12:L:26:ALA:N	2.24	0.70
1:A:1125:U:H5"	1:A:1126:U:N3	2.07	0.70
1:A:1193:G:O2'	1:A:1194:U:H5'	1.92	0.70
12:L:79:VAL:HG22	12:L:80:LEU:H	1.57	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:6:LYS:O	19:S:6:LYS:HG2	1.91	0.70
2:B:126:LYS:HA	2:B:129:GLN:CB	2.18	0.70
7:G:34:LYS:HD3	7:G:37:LEU:HD23	1.74	0.69
2:B:194:ILE:HD12	2:B:194:ILE:N	2.06	0.69
1:A:1250:A:O3'	9:I:66:GLY:HA2	1.92	0.69
2:B:81:ARG:HB3	2:B:81:ARG:HH11	1.57	0.69
3:C:179:ALA:O	3:C:180:ASN:HB3	1.91	0.69
10:J:14:LEU:HD13	10:J:14:LEU:O	1.92	0.69
12:L:79:VAL:HG22	12:L:80:LEU:N	2.07	0.69
1:A:881:G:P	12:L:8:ARG:HH22	2.15	0.69
5:E:74:HIS:HE1	5:E:139:ARG:H	1.37	0.69
7:G:77:ARG:HD2	7:G:155:TRP:HZ3	1.56	0.69
9:I:117:LYS:HG3	9:I:120:ARG:HB3	1.75	0.69
17:Q:51:LYS:O	17:Q:54:ASP:HB2	1.92	0.69
2:B:13:HIS:NE2	2:B:200:ASP:HB3	2.07	0.69
1:A:673:G:H2'	1:A:674:G:C8	2.28	0.69
1:A:408:A:H5'	4:D:115:GLN:HE21	1.58	0.69
1:A:1504:G:OP2	1:A:1507:A:H4'	1.92	0.69
1:A:1163:C:H2'	1:A:1164:G:H8	1.57	0.69
1:A:460:G:H3'	1:A:461:A:C5'	2.23	0.69
9:I:117:LYS:O	9:I:118:ALA:HB3	1.93	0.69
18:R:32:THR:HA	18:R:68:GLU:HB2	1.75	0.69
19:S:63:GLU:O	19:S:66:VAL:HG23	1.93	0.69
1:A:1129:C:O2'	1:A:1131:G:H5"	1.93	0.69
1:A:1305:G:N2	1:A:1331:G:H1'	2.06	0.69
13:M:48:THR:HG22	13:M:50:ALA:N	2.05	0.69
3:C:18:GLU:HG2	3:C:53:ARG:HE	1.57	0.69
1:A:1223:C:H5'	1:A:1224:G:C5'	2.22	0.69
3:C:103:GLN:HE21	3:C:104:GLU:N	1.89	0.69
2:B:65:VAL:HG12	2:B:164:GLU:HG2	1.75	0.69
1:A:56:U:H2'	1:A:57:G:C8	2.28	0.68
1:A:254:G:O2'	1:A:255:G:H5'	1.93	0.68
2:B:138:ARG:HA	2:B:141:LYS:HG2	1.74	0.68
5:E:106:LEU:HD13	5:E:114:ILE:HG21	1.75	0.68
13:M:3:ILE:HG23	13:M:56:ARG:HA	1.76	0.68
13:M:16:VAL:O	13:M:19:THR:HB	1.93	0.68
1:A:172:A:O2'	1:A:173:U:H5'	1.93	0.68
1:A:1048:G:C8	1:A:1048:G:H5'	2.26	0.68
3:C:122:GLN:O	3:C:127:PHE:HB2	1.93	0.68
2:B:207:LEU:HD22	2:B:208:ILE:HD13	1.75	0.68
11:K:44:ARG:HB3	11:K:44:ARG:HH11	1.54	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1152:A:OP2	10:J:66:HIS:ND1	2.26	0.68
6:F:80:ARG:NH1	6:F:88:VAL:HB	2.09	0.68
16:P:26:ARG:HD2	16:P:31:LYS:O	1.94	0.68
2:B:1:VAL:HG21	2:B:215:LEU:CD2	2.23	0.68
1:A:1231:G:H4'	9:I:125:SER:CB	2.24	0.68
9:I:26:THR:HG23	9:I:29:GLY:O	1.94	0.68
10:J:11:HIS:O	10:J:15:ASP:HB2	1.94	0.68
16:P:42:ARG:NH1	16:P:42:ARG:HG2	2.08	0.67
10:J:47:VAL:O	10:J:58:ARG:HA	1.94	0.67
14:N:22:ARG:NH1	14:N:29:ALA:HB2	2.09	0.67
2:B:172:ARG:HH22	8:H:68:ARG:HH22	1.40	0.67
17:Q:52:LEU:HD12	17:Q:52:LEU:H	1.59	0.67
18:R:23:GLU:CD	18:R:23:GLU:H	1.97	0.67
1:A:1352:C:H2'	1:A:1353:G:C8	2.30	0.67
5:E:76:ILE:HD12	5:E:87:LEU:HB2	1.77	0.67
13:M:10:ARG:CG	13:M:11:ASN:N	2.57	0.67
2:B:17:ARG:HH12	2:B:185:ASP:HA	1.58	0.67
1:A:1353:G:H2'	1:A:1354:C:H6	1.58	0.67
3:C:129:VAL:O	3:C:133:ILE:HG12	1.94	0.67
4:D:88:THR:O	4:D:88:THR:HG22	1.94	0.67
14:N:43:LEU:O	14:N:43:LEU:HD12	1.93	0.67
2:B:19:ASN:HD22	2:B:19:ASN:C	1.97	0.67
17:Q:67:ARG:HG3	17:Q:67:ARG:O	1.93	0.67
1:A:1075:C:H5'	2:B:97:THR:HG21	1.77	0.67
1:A:1054:C:H3'	1:A:1054:C:O2	1.94	0.67
19:S:15:LEU:O	19:S:19:LEU:HG	1.95	0.67
16:P:81:ARG:HB2	16:P:81:ARG:HH11	1.60	0.67
19:S:17:LYS:O	19:S:21:LEU:HG	1.95	0.67
4:D:2:ARG:NH1	4:D:69:ILE:HA	2.09	0.67
3:C:84:ARG:HH11	3:C:88:GLU:HB2	1.59	0.67
20:T:66:HIS:O	20:T:67:LYS:HG3	1.95	0.67
7:G:113:ARG:HG2	7:G:113:ARG:HH11	1.58	0.67
3:C:173:PRO:O	3:C:176:THR:HG22	1.95	0.66
3:C:18:GLU:O	3:C:39:ARG:NH2	2.28	0.66
7:G:14:ASP:HB3	7:G:19:ASP:H	1.60	0.66
11:K:38:ILE:HD13	11:K:53:LEU:HB3	1.77	0.66
3:C:57:GLU:OE2	10:J:90:THR:HG21	1.94	0.66
19:S:19:LEU:HA	19:S:22:ASN:HD22	1.59	0.66
1:A:1132:C:H2'	1:A:1133:G:H8	1.60	0.66
10:J:21:ILE:HA	10:J:83:LEU:HD21	1.77	0.66
19:S:19:LEU:HD12	19:S:20:GLU:N	2.11	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:134:HIS:HA	2:B:137:GLU:CG	2.26	0.66
4:D:141:PRO:HG2	4:D:186:ARG:HH21	1.61	0.66
15:O:15:ALA:HB1	15:O:20:ASP:HB3	1.78	0.66
10:J:19:GLN:HG2	10:J:22:VAL:HG11	1.76	0.66
2:B:9:VAL:HG13	2:B:203:ARG:HG2	1.78	0.66
7:G:49:ILE:HG23	7:G:124:MET:HE3	1.78	0.66
10:J:14:LEU:CD2	10:J:92:VAL:HG13	2.26	0.66
1:A:975:A:H5"	1:A:976:G:C5'	2.18	0.66
1:A:1292:U:P	7:G:40:ARG:HH22	2.19	0.66
2:B:157:PHE:HD1	2:B:179:ILE:HB	1.61	0.66
8:H:82:HIS:HD2	8:H:83:ILE:N	1.94	0.66
15:O:5:GLU:CD	15:O:5:GLU:H	1.97	0.66
7:G:71:ARG:O	7:G:72:MET:HG2	1.96	0.66
2:B:209:LEU:O	2:B:213:VAL:HG23	1.96	0.66
13:M:10:ARG:HG3	13:M:11:ASN:H	1.59	0.66
1:A:1054:C:N3	23:Z:34:G:O4'	2.29	0.65
1:A:224:C:C5'	1:A:224:C:H6	2.10	0.65
7:G:47:LYS:O	7:G:50:GLN:HB3	1.95	0.65
10:J:78:LYS:HA	10:J:81:GLU:OE2	1.96	0.65
7:G:58:LEU:O	7:G:62:LYS:HG2	1.95	0.65
1:A:750:G:N3	15:O:22:GLY:HA3	2.11	0.65
1:A:262:A:H5'	20:T:67:LYS:HD3	1.78	0.65
2:B:160:ASP:OD2	2:B:163:LYS:HB2	1.96	0.65
4:D:161:LEU:HD13	4:D:180:MET:HG2	1.77	0.65
13:M:101:ARG:HH11	13:M:101:ARG:HB2	1.61	0.65
9:I:24:LYS:HB3	9:I:24:LYS:NZ	2.12	0.65
19:S:41:PRO:HG2	19:S:42:GLU:OE2	1.96	0.65
1:A:271:C:O2'	1:A:272:C:H5"	1.97	0.65
1:A:1307:U:H5'	13:M:108:THR:HG21	1.78	0.65
1:A:271:C:H2'	1:A:272:C:H5'	1.77	0.65
1:A:1038:C:H2'	1:A:1039:C:H6	1.62	0.65
10:J:3:ARG:HA	10:J:71:ASP:OD1	1.96	0.65
8:H:63:LEU:H	8:H:63:LEU:HD22	1.60	0.65
11:K:38:ILE:HD13	11:K:53:LEU:CB	2.26	0.65
13:M:53:VAL:O	13:M:57:GLU:HG2	1.96	0.65
1:A:1342:C:O2'	1:A:1343:G:H5'	1.96	0.65
26:A:2733:3TS:H1	26:A:2733:3TS:O1'	1.97	0.65
4:D:77:LEU:HD22	4:D:95:LEU:HB3	1.79	0.65
1:A:195:A:H4'	20:T:61:LYS:HE2	1.79	0.65
1:A:1381:U:H2'	1:A:1381:U:O2	1.97	0.65
9:I:7:GLY:HA2	9:I:78:LEU:HD13	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:83:ILE:C	13:M:85:CYS:H	1.99	0.65
19:S:12:ASP:O	19:S:16:GLU:HG2	1.97	0.65
13:M:83:ILE:HG22	19:S:73:PHE:HE2	1.61	0.65
3:C:189:ARG:CB	3:C:189:ARG:HH11	2.09	0.65
3:C:171:ARG:HH11	3:C:171:ARG:HB3	1.62	0.65
20:T:22:LYS:O	20:T:26:ILE:HG13	1.97	0.65
1:A:975:A:H4'	1:A:976:G:O5'	1.97	0.65
1:A:486:U:H2'	1:A:487:A:C5'	2.27	0.65
2:B:172:ARG:HH11	2:B:172:ARG:HG3	1.61	0.65
1:A:1286:A:C8	1:A:1287:A:H4'	2.31	0.65
2:B:53:GLU:HB2	2:B:215:LEU:HD11	1.78	0.64
7:G:17:TYR:CE2	7:G:58:LEU:HB2	2.32	0.64
2:B:67:THR:HG21	2:B:90:ARG:NH1	2.11	0.64
6:F:47:ARG:H	6:F:47:ARG:HD2	1.61	0.64
3:C:109:ASN:HD21	3:C:139:ARG:HB3	1.62	0.64
9:I:110:ARG:HG2	9:I:111:LYS:N	2.11	0.64
7:G:71:ARG:HG2	7:G:141:GLU:OE2	1.96	0.64
1:A:630:G:H2'	1:A:631:G:C8	2.33	0.64
19:S:62:THR:HG23	19:S:65:MET:HE3	1.78	0.64
6:F:22:GLU:O	6:F:26:ILE:HG12	1.97	0.64
4:D:178:GLU:HG3	4:D:179:GLY:N	2.11	0.64
1:A:1129:C:H1'	1:A:1132:C:H5	1.62	0.64
7:G:41:ILE:HD12	7:G:115:ALA:HB3	1.80	0.64
11:K:66:GLY:O	11:K:68:GLN:HG3	1.97	0.64
10:J:19:GLN:O	10:J:22:VAL:HG12	1.97	0.64
1:A:620:C:N1	4:D:134:LEU:HD13	2.13	0.64
1:A:1106:G:H5'	1:A:1107:C:OP2	1.97	0.64
1:A:369:C:H2'	1:A:369:C:O2	1.98	0.64
4:D:104:VAL:HG21	4:D:125:ILE:HD13	1.80	0.64
15:O:38:LEU:CD1	15:O:55:LEU:HB2	2.28	0.64
1:A:1425:U:H2'	1:A:1426:C:H6	1.62	0.64
17:Q:43:ALA:HB2	17:Q:58:ILE:HD11	1.78	0.64
1:A:1301:U:H3'	1:A:1302:U:H5'	1.79	0.64
6:F:94:GLN:HE21	18:R:17:ARG:HH11	1.45	0.64
1:A:203:U:H4'	1:A:204:U:OP1	1.97	0.64
9:I:125:SER:O	9:I:127:ARG:N	2.31	0.64
1:A:1125:U:H5"	1:A:1126:U:C4	2.33	0.64
5:E:70:GLY:HA3	5:E:112:THR:HG22	1.80	0.64
6:F:94:GLN:NE2	18:R:17:ARG:HD3	2.12	0.64
7:G:74:VAL:HG13	7:G:144:ALA:HA	1.78	0.64
1:A:1256:A:O3'	1:A:1257:U:H4'	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:30:LEU:HB3	6:F:35:ALA:HB3	1.78	0.64
1:A:1216:G:H5"	14:N:4:ALA:HB2	1.80	0.63
3:C:100:LEU:HD13	3:C:100:LEU:O	1.95	0.63
10:J:44:ARG:HG2	10:J:44:ARG:NH1	2.13	0.63
1:A:1135:U:H3	1:A:1138:G:H1	1.46	0.63
4:D:145:ILE:N	4:D:145:ILE:HD12	2.12	0.63
18:R:7:VAL:O	18:R:11:LEU:HD23	1.97	0.63
1:A:722:A:H4'	1:A:723:U:C4	2.34	0.63
15:O:2:ILE:HD12	15:O:2:ILE:N	2.13	0.63
1:A:1301:U:H3'	1:A:1302:U:C5'	2.28	0.63
20:T:58:LYS:O	20:T:61:LYS:HB2	1.98	0.63
1:A:1026:G:N3	1:A:1026:G:H2'	2.13	0.63
4:D:34:ARG:N	4:D:34:ARG:HD2	2.13	0.63
19:S:41:PRO:O	19:S:44:VAL:HG23	1.97	0.63
1:A:590:C:C2'	1:A:591:U:H5"	2.27	0.63
1:A:1442(A):G:C4'	1:A:1442(B):A:H5'	2.28	0.63
1:A:1152:A:H4'	10:J:11:HIS:HD2	1.64	0.63
12:L:24:LYS:C	12:L:26:ALA:N	2.51	0.63
6:F:15:ASP:H	6:F:18:GLN:HE21	1.47	0.63
1:A:157:G:H8	1:A:157:G:H5'	1.63	0.63
16:P:34:GLU:OE2	16:P:55:ARG:HD3	1.98	0.63
1:A:1022:G:H2'	1:A:1023:G:H8	1.64	0.63
1:A:1330:U:C2'	1:A:1331:G:H5'	2.27	0.63
10:J:88:LEU:N	10:J:89:PRO:HD2	2.02	0.63
6:F:67:MET:HB2	6:F:68:PRO:CD	2.29	0.63
4:D:176:ASP:OD1	4:D:178:GLU:HG3	1.98	0.63
1:A:1353:G:H2'	1:A:1354:C:C6	2.33	0.63
1:A:1356:G:H2'	1:A:1357:A:C8	2.34	0.63
1:A:957:U:H3	1:A:960:U:H5"	1.62	0.63
1:A:243:A:H4'	1:A:244:U:C5'	2.12	0.63
1:A:1271:G:H2'	1:A:1272:G:C5'	2.17	0.63
3:C:103:GLN:NE2	3:C:104:GLU:H	1.97	0.63
11:K:1:LYS:N	11:K:1:LYS:HD2	2.14	0.63
9:I:64:VAL:HG21	9:I:72:GLN:HB3	1.81	0.63
3:C:153:SER:OG	3:C:154:GLY:N	2.32	0.63
5:E:97:ILE:N	5:E:97:ILE:HD12	2.14	0.63
1:A:271:C:C2'	1:A:272:C:H5"	2.29	0.62
6:F:10:LEU:HD12	6:F:59:TYR:HB3	1.81	0.62
19:S:15:LEU:O	19:S:18:VAL:HG12	1.99	0.62
1:A:1047:G:H2'	1:A:1048:G:C5'	2.23	0.62
11:K:100:ASP:OD2	18:R:73:LYS:HD2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:155:ALA:HB1	2:B:179:ILE:HD11	1.81	0.62
13:M:96:PRO:HB2	13:M:100:GLN:OE1	1.99	0.62
20:T:82:ARG:HG3	20:T:97:LEU:HD13	1.81	0.62
1:A:765:G:H1	1:A:812:C:H2'	1.64	0.62
12:L:2:THR:OG1	12:L:5:GLN:HG3	1.99	0.62
1:A:1198:G:H2'	1:A:1199:U:C6	2.35	0.62
13:M:34:GLU:C	13:M:36:THR:H	2.02	0.62
1:A:1144:G:H21	1:A:1146:A:H62	1.45	0.62
2:B:12:GLY:HA2	2:B:35:ILE:HA	1.80	0.62
20:T:50:ARG:NE	20:T:95:GLY:HA3	2.13	0.62
4:D:7:VAL:C	4:D:9:ARG:H	2.03	0.62
3:C:194:VAL:O	3:C:195:LEU:HD22	1.99	0.62
1:A:996:A:H5'	1:A:996:A:H8	1.64	0.62
14:N:13:PRO:O	14:N:14:LYS:HB3	1.99	0.62
4:D:82:SER:HA	4:D:88:THR:CG2	2.30	0.62
9:I:9:ARG:HD3	9:I:104:ASP:HB3	1.81	0.62
4:D:29:LYS:C	4:D:31:ALA:H	2.00	0.62
1:A:1014:A:C2	1:A:1219:U:H1'	2.34	0.62
1:A:539:A:H2'	1:A:540:G:C8	2.35	0.62
8:H:60:ARG:HG3	8:H:60:ARG:HH11	1.65	0.62
4:D:35:ARG:H	4:D:36:PRO:HD3	1.63	0.62
1:A:1314:C:C5	19:S:5:LYS:HD3	2.34	0.62
1:A:64:G:C4'	1:A:65:U:H5'	2.28	0.62
10:J:4:ILE:HG22	10:J:96:ILE:HG23	1.80	0.62
4:D:2:ARG:NH2	4:D:73:GLN:NE2	2.48	0.62
19:S:32:THR:HG22	19:S:34:SER:N	2.15	0.62
1:A:1301:U:O2'	1:A:1302:U:H5"	2.00	0.62
2:B:91:TRP:CZ2	2:B:96:LEU:HD13	2.35	0.62
10:J:80:ILE:O	10:J:84:MET:HB2	1.99	0.62
2:B:126:LYS:O	2:B:130:VAL:HG23	2.00	0.62
2:B:133:LYS:O	2:B:133:LYS:HD3	2.00	0.62
1:A:1229:A:H2'	1:A:1230:C:H6	1.64	0.62
11:K:67:MET:HE3	11:K:70:VAL:HG22	1.82	0.62
14:N:8:LYS:HD3	14:N:8:LYS:C	2.21	0.62
4:D:2:ARG:HH21	4:D:73:GLN:HE21	1.48	0.62
4:D:82:SER:HA	4:D:88:THR:HG21	1.80	0.62
1:A:451:A:H61	1:A:481:G:H5'	1.65	0.62
1:A:1189:C:OP1	10:J:49:ARG:NH2	2.20	0.61
1:A:370:C:O2'	1:A:371:G:H5'	2.00	0.61
4:D:150:LYS:N	4:D:150:LYS:HD2	2.14	0.61
12:L:107:LYS:O	12:L:108:ASP:HB2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:48:PRO:O	5:E:52:GLN:HG2	2.00	0.61
2:B:71:ALA:HB2	2:B:205:ILE:CD1	2.29	0.61
6:F:67:MET:HE1	6:F:72:VAL:HA	1.81	0.61
20:T:60:ALA:HA	20:T:66:HIS:H	1.65	0.61
20:T:29:LEU:HD12	20:T:55:LEU:HD12	1.80	0.61
6:F:99:ALA:C	6:F:101:ALA:H	2.03	0.61
1:A:335:C:O2'	1:A:336:C:H5'	2.00	0.61
12:L:83:GLY:HA2	12:L:94:TYR:HA	1.81	0.61
1:A:156:G:H2'	1:A:157:G:H5"	1.81	0.61
20:T:43:GLU:H	20:T:92:LEU:HD12	1.65	0.61
17:Q:44:HIS:CD2	17:Q:46:PRO:HG3	2.34	0.61
3:C:138:GLN:HA	3:C:138:GLN:HE21	1.65	0.61
1:A:953:G:H1'	13:M:124:ARG:HA	1.82	0.61
1:A:999:C:H4'	1:A:999:C:OP2	2.00	0.61
2:B:120:GLU:HA	2:B:123:GLU:CG	2.31	0.61
3:C:98:VAL:HG22	3:C:99:ALA:O	2.00	0.61
1:A:487:A:H5'	1:A:487:A:C8	2.31	0.61
1:A:1163:C:H2'	1:A:1164:G:C8	2.36	0.61
1:A:1060:C:C4	3:C:1:GLY:HA3	2.35	0.61
4:D:2:ARG:HH21	4:D:73:GLN:HG3	1.65	0.61
10:J:46:THR:OG1	10:J:60:HIS:CD2	2.53	0.61
1:A:1510:U:H2'	1:A:1511:G:C8	2.36	0.61
1:A:1178:G:N2	1:A:1180:A:H3'	2.15	0.61
1:A:271:C:H2'	1:A:272:C:C5'	2.30	0.61
3:C:63:VAL:HG12	3:C:65:VAL:HG23	1.82	0.61
1:A:1306:A:O2'	13:M:108:THR:HG21	2.01	0.61
1:A:1140:C:H2'	1:A:1140:C:O2	1.99	0.61
12:L:82:ARG:HG3	12:L:82:ARG:HH11	1.66	0.61
1:A:499:A:H61	1:A:547:A:C5'	2.13	0.61
1:A:1425:U:H2'	1:A:1426:C:C6	2.35	0.61
16:P:81:ARG:HG3	16:P:83:GLU:OE1	2.00	0.61
12:L:20:VAL:HG23	12:L:20:VAL:O	2.00	0.61
1:A:1427:U:H2'	1:A:1428:A:C8	2.36	0.61
1:A:1420:C:H2'	1:A:1421:G:H8	1.66	0.61
14:N:8:LYS:HE2	14:N:21:THR:O	2.01	0.61
3:C:124:GLU:HG2	3:C:189:ARG:O	2.00	0.61
10:J:37:PRO:HA	10:J:68:ARG:NH1	2.16	0.61
10:J:37:PRO:O	10:J:38:LEU:HB2	2.00	0.61
2:B:77:MET:HG3	2:B:229:SER:HB3	1.82	0.61
1:A:948:C:O2'	1:A:949:A:H5'	2.01	0.61
1:A:709:G:O2'	1:A:710:G:H5'	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:87:ARG:HE	15:O:87:ARG:N	1.99	0.60
1:A:1420:C:H2'	1:A:1421:G:C8	2.36	0.60
13:M:39:ASN:HD22	13:M:40:PRO:CD	2.13	0.60
4:D:186:ARG:HH22	4:D:187:LEU:CD1	2.14	0.60
6:F:7:ASN:HD21	18:R:19:TYR:HE1	1.49	0.60
15:O:69:LEU:HD13	15:O:77:TYR:HA	1.82	0.60
21:V:6:ARG:HG2	21:V:15:ARG:HH12	1.66	0.60
16:P:28:ARG:HG2	16:P:29:ASP:OD1	2.01	0.60
3:C:13:ILE:O	3:C:15:ARG:N	2.34	0.60
6:F:2:ARG:CD	6:F:69:GLU:HG2	2.31	0.60
13:M:95:LEU:HB3	13:M:96:PRO:HD2	1.83	0.60
3:C:171:ARG:HH12	3:C:173:PRO:HG3	1.66	0.60
1:A:1405:G:O2'	1:A:1406:U:H5'	2.01	0.60
1:A:693:G:C6	1:A:1539:C:H1'	2.35	0.60
1:A:591:U:H6	1:A:591:U:C5'	2.12	0.60
1:A:165:C:H2'	1:A:166:G:H8	1.64	0.60
14:N:30:ARG:HG3	14:N:30:ARG:HH11	1.66	0.60
10:J:6:LEU:CD2	10:J:94:ILE:HG12	2.31	0.60
16:P:26:ARG:CD	16:P:31:LYS:O	2.50	0.60
17:Q:3:LYS:HE3	17:Q:5:LEU:HD21	1.84	0.60
1:A:620:C:H2'	1:A:621:A:O4'	2.02	0.60
2:B:225:GLU:H	2:B:225:GLU:CD	2.05	0.60
1:A:439:A:H2'	1:A:441:A:H5'	1.83	0.60
17:Q:77:GLU:OE1	17:Q:80:ARG:HD2	2.01	0.60
1:A:1222:G:P	19:S:76:THR:HG21	2.41	0.60
13:M:83:ILE:HD12	19:S:64:ASN:HD22	1.65	0.60
3:C:99:ALA:O	3:C:100:LEU:HB2	2.01	0.60
1:A:689:C:P	11:K:36:GLY:HA3	2.41	0.60
2:B:230:TYR:CD1	2:B:233:VAL:HG21	2.36	0.60
13:M:121:LYS:HG3	13:M:122:ALA:N	2.16	0.60
5:E:117:LYS:HD3	5:E:118:GLU:N	2.16	0.60
7:G:119:ILE:N	7:G:119:ILE:HD12	2.17	0.60
1:A:591:U:C6	1:A:591:U:H5'	2.24	0.60
1:A:998:G:H2'	1:A:999:C:C4'	2.32	0.60
2:B:81:ARG:NH1	2:B:81:ARG:HB3	2.16	0.60
3:C:113:PRO:O	3:C:117:GLN:HG3	2.01	0.60
1:A:677:U:H3	1:A:713:G:H22	1.48	0.60
1:A:968:A:O5'	1:A:968:A:H8	1.85	0.60
1:A:1392:G:N2	1:A:1502:A:H8	1.99	0.60
2:B:21:LYS:HD2	2:B:187:ASP:OD2	2.02	0.60
2:B:108:ARG:NH2	2:B:112:LEU:HD21	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:969:A:H61	13:M:125:LYS:HB2	1.66	0.60
1:A:1474:G:H2'	1:A:1475:G:C5'	2.32	0.60
1:A:1300:G:O2'	1:A:1301:U:H5"	2.00	0.60
4:D:7:VAL:HG13	4:D:20:LEU:HD12	1.84	0.60
2:B:72:GLN:HE21	2:B:89:GLN:HA	1.67	0.60
1:A:590:C:H2'	1:A:591:U:H5"	1.83	0.59
1:A:1213:A:C2'	1:A:1214:C:H5"	2.32	0.59
2:B:11:PHE:HB3	2:B:38:LEU:HD21	1.83	0.59
7:G:53:THR:HG22	7:G:55:GLN:N	2.17	0.59
1:A:998:G:C3'	1:A:999:C:H5"	2.32	0.59
1:A:8:A:H5'	5:E:97:ILE:HG22	1.84	0.59
2:B:216:ILE:O	2:B:220:ARG:HG3	2.02	0.59
16:P:36:ILE:O	16:P:51:VAL:O	2.20	0.59
12:L:66:ILE:HD13	12:L:73:LEU:HD12	1.82	0.59
12:L:23:LEU:O	12:L:25:GLY:N	2.35	0.59
2:B:21:LYS:HD3	2:B:189:ASP:OD2	2.02	0.59
18:R:18:ASP:OD2	18:R:21:ASN:HB2	2.02	0.59
1:A:820:U:H4'	1:A:821:G:OP1	2.00	0.59
20:T:89:GLY:O	20:T:90:ALA:HB3	2.02	0.59
2:B:63:LEU:HD23	2:B:64:PHE:N	2.17	0.59
1:A:953:G:H5'	1:A:965:A:H61	1.68	0.59
15:O:3:THR:OG1	15:O:6:GLU:HB2	2.02	0.59
11:K:57:ASP:OD1	11:K:61:LYS:HE3	2.01	0.59
1:A:477:A:O2'	1:A:479:C:H5'	2.03	0.59
3:C:25:LYS:HZ2	3:C:25:LYS:CB	2.15	0.59
2:B:70:GLN:HG3	2:B:200:ASP:OD1	2.02	0.59
5:E:114:ILE:HD13	5:E:115:LEU:N	2.17	0.59
2:B:12:GLY:CA	2:B:35:ILE:HA	2.33	0.59
1:A:1132:C:H2'	1:A:1133:G:C8	2.37	0.59
9:I:7:GLY:HA2	9:I:78:LEU:HB3	1.84	0.59
1:A:35:G:H2'	1:A:36:C:C6	2.37	0.59
1:A:51:A:H4'	1:A:52:G:O5'	2.03	0.59
13:M:72:GLU:O	13:M:75:ALA:HB3	2.03	0.59
4:D:31:ALA:C	4:D:33:GLU:H	2.04	0.59
3:C:49:ALA:HB1	3:C:69:VAL:CG1	2.30	0.59
1:A:179:A:H2'	1:A:180:U:C6	2.37	0.59
16:P:9:PHE:CD2	16:P:18:ARG:HG3	2.38	0.59
4:D:21:LYS:HB2	4:D:25:CYS:SG	2.42	0.59
9:I:68:GLY:O	9:I:72:GLN:HG3	2.02	0.59
19:S:40:VAL:HB	19:S:41:PRO:HD2	1.85	0.59
3:C:138:GLN:HA	3:C:138:GLN:NE2	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:46:THR:HG1	10:J:60:HIS:CD2	2.20	0.59
22:W:2:U:H2'	22:W:3:C:H6	1.68	0.59
1:A:1117:G:H5"	9:I:103:ARG:NH2	2.18	0.59
3:C:190:THR:HG21	3:C:192:TYR:CZ	2.38	0.58
19:S:40:VAL:HG22	19:S:43:MET:CE	2.33	0.58
2:B:212:ALA:O	2:B:216:ILE:HG12	2.03	0.58
1:A:967:C:H4'	9:I:127:ARG:HG3	1.84	0.58
1:A:1135:U:O2	1:A:1135:U:H2'	2.02	0.58
1:A:896:C:H5'	1:A:897:C:OP2	2.02	0.58
3:C:76:ILE:HA	3:C:83:ILE:HB	1.84	0.58
19:S:13:HIS:O	19:S:17:LYS:HE3	2.03	0.58
3:C:5:HIS:HD2	3:C:7:ILE:H	1.51	0.58
18:R:59:ARG:HB3	18:R:66:PHE:CE1	2.39	0.58
18:R:40:ARG:NH1	18:R:40:ARG:HB3	2.18	0.58
19:S:22:ASN:C	19:S:24:LYS:H	2.05	0.58
1:A:881:G:OP1	12:L:8:ARG:NH2	2.36	0.58
1:A:67:C:O2'	1:A:171:A:H1'	2.03	0.58
23:Z:41:C:H2'	23:Z:42:C:C6	2.38	0.58
4:D:149:GLU:HG3	4:D:152:ARG:NH1	2.17	0.58
11:K:105:PRO:C	11:K:107:ASN:H	2.05	0.58
1:A:1022:G:H2'	1:A:1023:G:C8	2.39	0.58
1:A:824:C:H2'	1:A:825:G:H8	1.68	0.58
11:K:99:VAL:HG22	18:R:71:VAL:HA	1.86	0.58
2:B:157:PHE:CD1	2:B:179:ILE:HB	2.39	0.58
12:L:71:HIS:HD2	12:L:73:LEU:N	2.00	0.58
2:B:183:ASP:CG	2:B:184:THR:H	2.06	0.58
1:A:452:A:H4'	16:P:72:ARG:NE	2.19	0.58
20:T:46:LEU:O	20:T:50:ARG:HD2	2.03	0.58
12:L:64:ALA:HB1	12:L:96:ILE:HG13	1.85	0.58
7:G:71:ARG:HH12	7:G:137:LYS:NZ	2.01	0.58
5:E:8:LEU:CD1	5:E:27:LEU:HB2	2.33	0.58
1:A:1277:C:H5'	1:A:1277:C:H6	1.67	0.58
1:A:403:C:O2'	1:A:404:U:H5'	2.04	0.58
18:R:38:ARG:HH11	18:R:44:SER:HA	1.68	0.58
10:J:4:ILE:CG2	10:J:96:ILE:HG23	2.32	0.58
18:R:21:ASN:O	18:R:25:LEU:HG	2.03	0.58
1:A:794:A:H2'	1:A:795:C:C6	2.39	0.58
1:A:1487:G:O2'	1:A:1488:G:H5'	2.04	0.58
1:A:1005:A:H5"	1:A:1006:C:C5	2.39	0.58
10:J:22:VAL:O	10:J:26:ARG:HG3	2.03	0.58
3:C:81:GLU:O	3:C:85:VAL:HG23	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:662:G:H2'	1:A:663:A:C8	2.39	0.58
3:C:54:VAL:HG12	3:C:54:VAL:O	2.03	0.58
2:B:24:ARG:HG3	2:B:25:TYR:CD1	2.39	0.58
11:K:17:ASN:ND2	11:K:45:LYS:HD2	2.18	0.58
1:A:1001:A:N3	1:A:1001(A):G:H5'	2.19	0.58
2:B:31:ASN:O	2:B:33:ILE:HG12	2.03	0.58
1:A:384:G:H2'	1:A:385:C:C6	2.39	0.58
1:A:1391:U:H2'	1:A:1392:G:H8	1.64	0.58
20:T:50:ARG:HG2	20:T:50:ARG:NH1	2.19	0.58
10:J:19:GLN:HG2	10:J:22:VAL:CG1	2.33	0.58
12:L:13:LYS:HE2	12:L:13:LYS:HA	1.86	0.58
14:N:32:VAL:HA	14:N:39:CYS:HA	1.85	0.57
9:I:92:ARG:HB3	9:I:92:ARG:HH11	1.68	0.57
3:C:176:THR:HG23	3:C:179:ALA:HB2	1.86	0.57
1:A:743:U:H2'	1:A:744:C:C6	2.39	0.57
1:A:353:A:H8	1:A:353:A:H5'	1.69	0.57
1:A:1314:C:H5	19:S:5:LYS:HD3	1.69	0.57
9:I:8:ARG:HG3	9:I:13:VAL:HG13	1.86	0.57
1:A:920:U:H2'	1:A:921:U:C6	2.39	0.57
1:A:1245:A:O2'	1:A:1246:C:H5'	2.03	0.57
6:F:2:ARG:NE	6:F:69:GLU:HG2	2.19	0.57
1:A:946:A:H2'	1:A:947:G:H8	1.70	0.57
2:B:13:HIS:HB2	2:B:198:ASN:OD1	2.05	0.57
1:A:1263:C:H2'	1:A:1264:C:C6	2.39	0.57
1:A:26:A:H2'	1:A:27:G:H5'	1.86	0.57
1:A:486:U:H2'	1:A:487:A:H5"	1.85	0.57
2:B:63:LEU:HD12	2:B:149:LEU:HD11	1.87	0.57
15:O:25:GLU:HG3	15:O:80:LEU:HG	1.86	0.57
8:H:84:ARG:HG3	8:H:84:ARG:NH1	2.20	0.57
10:J:2:ILE:HD12	10:J:2:ILE:N	2.19	0.57
21:V:6:ARG:HE	21:V:15:ARG:NH1	2.01	0.57
1:A:147:G:C8	1:A:147:G:H5'	2.38	0.57
1:A:837:G:H1	1:A:849:C:N4	2.02	0.57
3:C:154:GLY:O	3:C:155:ARG:HB2	2.03	0.57
12:L:79:VAL:HG21	12:L:96:ILE:HG23	1.85	0.57
2:B:81:ARG:O	2:B:82:ALA:HB2	2.04	0.57
1:A:1299:A:C8	1:A:1301:U:H1'	2.39	0.57
3:C:57:GLU:H	3:C:64:ALA:HB3	1.69	0.57
2:B:120:GLU:HA	2:B:123:GLU:HG2	1.86	0.57
7:G:119:ILE:HD12	7:G:119:ILE:H	1.69	0.57
1:A:1001(A):G:C2'	1:A:1002:G:H5'	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1346:A:C6	7:G:9:ARG:NH1	2.72	0.57
10:J:82:GLN:O	10:J:86:LEU:HD22	2.04	0.57
1:A:1364:U:O2'	1:A:1365:G:H5"	2.04	0.57
8:H:29:SER:OG	8:H:32:LYS:HG3	2.03	0.57
4:D:198:ASN:C	4:D:198:ASN:HD22	2.08	0.57
1:A:1330:U:C5'	1:A:1330:U:H6	2.08	0.57
13:M:22:TYR:HB3	13:M:66:GLU:HA	1.87	0.57
10:J:30:ALA:C	10:J:32:VAL:H	2.08	0.57
1:A:1296:C:H4'	1:A:1302:U:C4	2.40	0.57
9:I:9:ARG:CD	9:I:104:ASP:HB3	2.35	0.57
13:M:119:LYS:HG2	13:M:120:LYS:N	2.20	0.57
6:F:74:ASP:CG	6:F:77:ARG:HH21	2.08	0.57
1:A:1480:G:O2'	1:A:1481:U:H6	1.87	0.57
1:A:649:G:H5'	1:A:649:G:H8	1.68	0.57
2:B:135:GLU:O	2:B:139:LEU:HG	2.03	0.57
4:D:149:GLU:CD	4:D:149:GLU:H	2.08	0.57
1:A:44:G:C2	1:A:45:U:H1'	2.40	0.57
12:L:122:LYS:HD2	12:L:122:LYS:C	2.24	0.57
1:A:314:C:O2'	1:A:315:A:H5'	2.05	0.57
2:B:134:HIS:CA	2:B:137:GLU:HG2	2.32	0.57
5:E:47:VAL:HB	5:E:48:PRO:CD	2.30	0.57
12:L:37:ARG:NH1	12:L:53:LYS:HE2	2.18	0.57
7:G:144:ALA:O	7:G:146:ALA:N	2.35	0.57
15:O:16:ARG:HD3	15:O:25:GLU:OE1	2.04	0.57
1:A:269:C:H2'	1:A:270:A:C8	2.40	0.57
5:E:72:ILE:HG22	5:E:74:HIS:H	1.70	0.57
1:A:797:C:O2'	1:A:798:G:H5'	2.04	0.57
5:E:140:THR:HG22	5:E:142:ALA:N	2.20	0.57
13:M:39:ASN:HD22	13:M:40:PRO:HD2	1.70	0.57
1:A:1259:C:H5'	1:A:1260:C:OP1	2.05	0.57
13:M:121:LYS:CG	13:M:122:ALA:N	2.68	0.57
2:B:172:ARG:HH22	8:H:68:ARG:NH2	2.03	0.57
1:A:1012:U:H3'	1:A:1013:G:C5'	2.20	0.56
19:S:15:LEU:C	19:S:17:LYS:H	2.08	0.56
19:S:16:GLU:HA	19:S:19:LEU:HD11	1.86	0.56
1:A:721:G:OP1	1:A:721:G:H8	1.88	0.56
1:A:57:G:H2'	1:A:58:C:C6	2.39	0.56
1:A:1151:A:HO2'	1:A:1152:A:H8	1.51	0.56
5:E:15:MET:SD	5:E:20:ARG:HB3	2.44	0.56
13:M:8:ILE:HG22	13:M:8:ILE:O	2.04	0.56
13:M:48:THR:HB	13:M:51:GLU:HG3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1442(A):G:H5"	1:A:1442(B):A:C5'	2.33	0.56
13:M:95:LEU:O	13:M:109:ARG:NH1	2.38	0.56
1:A:1349:A:P	9:I:117:LYS:HE2	2.45	0.56
3:C:57:GLU:HB2	3:C:64:ALA:HB2	1.86	0.56
3:C:194:VAL:HG12	3:C:195:LEU:N	2.20	0.56
17:Q:2:LYS:HD3	17:Q:60:GLU:O	2.05	0.56
1:A:1394:A:C5	1:A:1501:C:H4'	2.40	0.56
1:A:1216:G:O2'	1:A:1217:C:H5'	2.04	0.56
14:N:11:ARG:C	14:N:13:PRO:HD3	2.26	0.56
11:K:81:ARG:NE	18:R:73:LYS:HE2	2.21	0.56
2:B:6:GLU:CB	2:B:10:HIS:HE1	2.18	0.56
1:A:1249:C:H2'	1:A:1250:A:H5"	1.86	0.56
14:N:43:LEU:C	14:N:43:LEU:HD12	2.25	0.56
17:Q:39:LYS:HG2	17:Q:41:TYR:CE1	2.41	0.56
10:J:48:ILE:HD12	10:J:48:ILE:H	1.70	0.56
1:A:411:A:H2'	1:A:412:A:H5"	1.87	0.56
7:G:84:TYR:HD2	7:G:153:TYR:HE2	1.53	0.56
1:A:1276:G:C3'	1:A:1277:C:H5"	2.35	0.56
9:I:111:LYS:HG3	9:I:117:LYS:HA	1.87	0.56
10:J:79:THR:HG22	10:J:83:LEU:HD12	1.87	0.56
1:A:1245:A:H5'	1:A:1245:A:C8	2.34	0.56
1:A:1442(A):G:H4'	1:A:1442(B):A:H5'	1.87	0.56
11:K:38:ILE:CG2	11:K:39:GLY:H	2.18	0.56
1:A:486:U:O2'	1:A:487:A:H5"	2.05	0.56
9:I:42:ALA:N	9:I:73:ILE:HD13	2.20	0.56
2:B:172:ARG:NH1	2:B:172:ARG:HG3	2.21	0.56
13:M:12:LYS:O	13:M:44:VAL:HG23	2.06	0.56
1:A:812:C:O2'	1:A:813:U:P	2.63	0.56
4:D:30:CYS:SG	4:D:30:CYS:O	2.64	0.56
1:A:872:A:C3'	1:A:873:A:H5'	2.36	0.56
15:O:86:ILE:CG2	15:O:87:ARG:H	1.94	0.56
6:F:10:LEU:HD12	6:F:10:LEU:H	1.70	0.56
2:B:22:PHE:CD2	2:B:184:THR:HA	2.40	0.56
16:P:81:ARG:HB2	16:P:81:ARG:NH1	2.21	0.56
6:F:94:GLN:HE21	18:R:17:ARG:HD3	1.70	0.56
1:A:812:C:O2'	1:A:813:U:OP1	2.24	0.56
1:A:1232:U:OP1	9:I:123:GLN:HG2	2.05	0.56
2:B:175:PHE:HD2	8:H:70:GLN:HB3	1.71	0.56
1:A:1244:C:O2'	1:A:1245:A:H5"	2.05	0.56
13:M:33:LEU:HD13	13:M:40:PRO:HA	1.88	0.56
10:J:13:THR:C	10:J:15:ASP:H	2.08	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:G:C2'	1:A:157:G:H5"	2.35	0.56
1:A:501:C:H2'	1:A:502:G:H8	1.71	0.56
1:A:245:C:O2'	1:A:246:A:H5'	2.05	0.56
1:A:1366:C:H2'	1:A:1367:C:C6	2.41	0.56
2:B:215:LEU:HD13	2:B:215:LEU:O	2.06	0.56
4:D:195:LEU:H	4:D:195:LEU:CD2	2.16	0.56
13:M:13:ARG:HB2	13:M:16:VAL:HG12	1.88	0.56
16:P:28:ARG:HH11	16:P:28:ARG:HG2	1.71	0.56
6:F:40:VAL:HG22	6:F:41:GLU:N	2.20	0.56
1:A:243:A:C4'	1:A:244:U:H5'	2.12	0.56
10:J:4:ILE:HA	10:J:95:GLU:O	2.06	0.56
6:F:99:ALA:C	6:F:101:ALA:N	2.60	0.56
3:C:18:GLU:CG	3:C:53:ARG:HE	2.18	0.56
13:M:10:ARG:CG	13:M:11:ASN:H	2.16	0.56
1:A:1540:U:OP1	1:A:1540:U:H3'	2.06	0.56
16:P:20:VAL:CG1	16:P:32:TYR:HB2	2.36	0.56
1:A:1164:G:H1	1:A:1172:C:N4	1.99	0.55
1:A:1229:A:H2'	1:A:1230:C:C6	2.41	0.55
6:F:101:ALA:HB1	18:R:13:GLU:HG3	1.87	0.55
9:I:117:LYS:O	9:I:118:ALA:CB	2.54	0.55
7:G:15:LEU:HD22	7:G:15:LEU:N	2.22	0.55
17:Q:39:LYS:HE3	17:Q:41:TYR:CZ	2.40	0.55
1:A:1095:U:H2'	1:A:1096:C:C6	2.40	0.55
1:A:409:G:OP1	4:D:23:GLU:HB3	2.06	0.55
6:F:91:VAL:HG11	18:R:57:ARG:NH1	2.22	0.55
1:A:1007:C:H2'	1:A:1008:C:H6	1.65	0.55
1:A:1053:G:C4'	1:A:1054:C:H5'	2.37	0.55
11:K:44:ARG:HH11	11:K:44:ARG:CB	2.19	0.55
21:V:6:ARG:CG	21:V:15:ARG:HH12	2.19	0.55
9:I:92:ARG:HH11	9:I:92:ARG:CB	2.20	0.55
11:K:78:GLY:O	11:K:80:GLY:N	2.38	0.55
1:A:1228:C:OP1	13:M:114:LYS:HE3	2.07	0.55
11:K:12:HIS:HB3	11:K:19:ILE:HD11	1.86	0.55
18:R:38:ARG:NH1	18:R:44:SER:HA	2.20	0.55
12:L:56:LEU:CD2	12:L:62:VAL:HG22	2.33	0.55
1:A:146:G:C3'	1:A:147:G:H5"	2.36	0.55
11:K:67:MET:CE	11:K:70:VAL:HG22	2.36	0.55
8:H:63:LEU:HD22	8:H:63:LEU:N	2.20	0.55
3:C:130:ARG:O	3:C:134:LYS:HG3	2.06	0.55
8:H:8:ASP:O	8:H:12:ARG:HG3	2.06	0.55
1:A:1330:U:OP1	13:M:22:TYR:O	2.23	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:977:A:O2'	1:A:978:A:C5'	2.54	0.55
2:B:48:THR:O	2:B:52:ILE:HG12	2.07	0.55
2:B:11:PHE:HD1	2:B:12:GLY:N	2.04	0.55
2:B:6:GLU:C	2:B:8:GLY:H	2.08	0.55
8:H:68:ARG:HH11	8:H:68:ARG:HG2	1.72	0.55
12:L:75:GLU:O	12:L:77:SER:N	2.40	0.55
5:E:114:ILE:HD13	5:E:115:LEU:H	1.72	0.55
26:A:2733:3TS:OAI	26:A:2733:3TS:H1'	2.06	0.55
1:A:413:G:O2'	1:A:428:G:N2	2.40	0.55
1:A:860:A:H2'	1:A:861:G:O4'	2.07	0.55
19:S:40:VAL:HG22	19:S:43:MET:HE2	1.88	0.55
1:A:1392:G:H21	1:A:1502:A:H8	1.54	0.55
4:D:195:LEU:HD23	4:D:195:LEU:N	2.13	0.55
1:A:553:A:H5"	12:L:20:VAL:HG21	1.88	0.55
1:A:421:U:H4'	1:A:422:C:OP2	2.06	0.55
1:A:131:C:H2'	1:A:132:C:C6	2.42	0.55
1:A:224:C:H5'	1:A:224:C:H6	1.72	0.55
3:C:69:VAL:HG12	3:C:70:ALA:N	2.22	0.55
1:A:591:U:O2'	1:A:592:G:H5'	2.07	0.55
1:A:173:U:H2'	1:A:197:A:C5	2.42	0.55
2:B:91:TRP:HZ2	2:B:96:LEU:HD13	1.70	0.55
1:A:1062:U:H2'	1:A:1063:C:C6	2.42	0.55
15:O:26:VAL:O	15:O:30:LEU:HD13	2.07	0.55
1:A:1136:U:H5"	1:A:1137:C:OP1	2.07	0.55
1:A:271:C:C2'	1:A:272:C:C5'	2.84	0.55
1:A:272:C:C6	1:A:272:C:H5'	2.30	0.55
12:L:23:LEU:C	12:L:25:GLY:N	2.59	0.55
12:L:23:LEU:C	12:L:25:GLY:H	2.10	0.55
2:B:76:ARG:NH2	2:B:86:TYR:OH	2.38	0.55
3:C:84:ARG:NH1	3:C:88:GLU:HB2	2.22	0.55
1:A:1141:C:O2'	1:A:1142:G:H5'	2.07	0.55
15:O:16:ARG:HG3	15:O:16:ARG:HH11	1.72	0.55
1:A:1168:A:O2'	1:A:1169:A:C8	2.58	0.55
4:D:99:ARG:HH12	4:D:136:SER:HB3	1.72	0.55
1:A:100:C:H2'	1:A:101:A:C8	2.42	0.55
1:A:1392:G:O2'	1:A:1502:A:H5"	2.06	0.55
1:A:1004:A:H8	1:A:1036:G:N1	2.02	0.55
1:A:1125:U:H3	10:J:3:ARG:NH2	2.03	0.55
13:M:4:ALA:O	13:M:5:GLY:C	2.45	0.55
1:A:1074:G:O3'	2:B:97:THR:CG2	2.55	0.55
20:T:60:ALA:O	20:T:66:HIS:ND1	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1491:G:H2'	26:A:2733:3TS:HAUA	1.88	0.55
5:E:117:LYS:HD3	5:E:118:GLU:H	1.72	0.55
17:Q:69:ARG:HD2	17:Q:69:ARG:N	2.22	0.55
7:G:44:ASP:O	7:G:48:ILE:HG13	2.07	0.55
1:A:972:C:H4'	10:J:55:LYS:CG	2.23	0.55
1:A:972:C:OP1	10:J:55:LYS:HE2	2.07	0.55
1:A:967:C:C4'	9:I:127:ARG:HG3	2.37	0.55
10:J:67:ASN:O	10:J:68:ARG:HD3	2.06	0.55
1:A:818:G:H3'	1:A:819:A:C5'	2.37	0.55
2:B:65:VAL:CG1	2:B:164:GLU:HG2	2.36	0.55
3:C:138:GLN:HE21	3:C:138:GLN:CA	2.19	0.55
7:G:67:ASN:ND2	7:G:127:ALA:HA	2.22	0.55
6:F:33:TYR:HA	6:F:71:ARG:NH2	2.22	0.55
5:E:9:ILE:HG13	5:E:9:ILE:O	2.06	0.55
6:F:38:GLU:O	6:F:39:LYS:HB3	2.05	0.55
2:B:106:VAL:O	2:B:110:GLU:HG3	2.07	0.55
6:F:45:LEU:N	6:F:45:LEU:HD22	2.22	0.55
1:A:1053:G:C3'	1:A:1054:C:H5'	2.36	0.54
1:A:448:A:C4	1:A:487:A:C2	2.95	0.54
1:A:1038:C:H2'	1:A:1039:C:C6	2.42	0.54
6:F:22:GLU:OE1	6:F:22:GLU:HA	2.06	0.54
2:B:10:HIS:HB3	2:B:204:SER:OG	2.07	0.54
2:B:200:ASP:O	2:B:201:ALA:HB3	2.07	0.54
1:A:530:G:O6	22:W:3:C:H1'	2.07	0.54
19:S:41:PRO:C	19:S:43:MET:H	2.11	0.54
10:J:37:PRO:O	10:J:67:ASN:O	2.25	0.54
10:J:58:ARG:HG2	10:J:58:ARG:HH11	1.73	0.54
1:A:255:G:H1'	17:Q:15:GLN:NE2	2.22	0.54
13:M:64:LYS:CE	13:M:68:GLU:HG2	2.37	0.54
6:F:94:GLN:HB3	18:R:17:ARG:HH11	1.71	0.54
1:A:446:G:H1	1:A:488:C:H42	1.56	0.54
1:A:1475:G:H2'	1:A:1476:G:O4'	2.06	0.54
1:A:1252:A:H61	1:A:1285:A:H61	1.55	0.54
7:G:27:ASN:O	7:G:30:MET:HB3	2.08	0.54
15:O:53:ARG:O	15:O:57:MET:HG3	2.06	0.54
5:E:75:GLU:HG3	5:E:89:PRO:HD3	1.89	0.54
3:C:65:VAL:O	3:C:65:VAL:HG12	2.07	0.54
1:A:1326:C:H5'	21:V:12:LYS:HZ1	1.71	0.54
10:J:23:GLU:C	10:J:25:ALA:H	2.11	0.54
1:A:1251:A:H4'	9:I:11:GLU:OE2	2.08	0.54
4:D:3:TYR:O	4:D:4:ILE:HB	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:31:ARG:O	7:G:33:GLY:N	2.41	0.54
8:H:20:TYR:CE1	8:H:76:PRO:HG2	2.42	0.54
1:A:426:G:H8	1:A:426:G:H5'	1.73	0.54
2:B:126:LYS:HE3	2:B:129:GLN:HE22	1.72	0.54
1:A:1188:A:C3'	1:A:1189:C:C5'	2.84	0.54
15:O:87:ARG:NE	15:O:87:ARG:HA	2.22	0.54
19:S:61:ILE:HD13	19:S:61:ILE:C	2.27	0.54
20:T:84:LEU:C	20:T:86:GLU:H	2.11	0.54
1:A:403:C:O3'	4:D:121:ARG:HD2	2.07	0.54
4:D:150:LYS:CD	4:D:150:LYS:H	2.17	0.54
1:A:954:G:H2'	1:A:955:U:C6	2.43	0.54
1:A:268:C:O2'	1:A:269:C:H5'	2.08	0.54
14:N:8:LYS:HD3	14:N:9:ALA:N	2.22	0.54
1:A:612:C:O2'	1:A:613:C:H5'	2.08	0.54
20:T:50:ARG:HG2	20:T:50:ARG:HH11	1.72	0.54
3:C:180:ASN:C	3:C:181:ILE:HD12	2.27	0.54
1:A:1301:U:C3'	1:A:1302:U:C5'	2.85	0.54
6:F:47:ARG:N	6:F:47:ARG:HD2	2.23	0.54
18:R:4:LYS:O	18:R:5:ALA:HB3	2.06	0.54
8:H:82:HIS:CD2	8:H:83:ILE:N	2.75	0.54
20:T:87:ALA:O	20:T:88:ALA:HB3	2.08	0.54
4:D:56:ARG:HH11	4:D:56:ARG:HG3	1.73	0.54
5:E:76:ILE:HD12	5:E:76:ILE:N	2.23	0.54
13:M:13:ARG:NH1	13:M:15:ASP:OD2	2.41	0.54
4:D:157:ILE:O	4:D:161:LEU:HB2	2.08	0.54
7:G:145:GLU:C	7:G:147:ASN:H	2.09	0.54
1:A:1251:A:O2'	1:A:1370:G:H5'	2.07	0.54
5:E:8:LEU:HD13	5:E:27:LEU:HB2	1.89	0.54
16:P:20:VAL:HG13	16:P:32:TYR:HB2	1.90	0.54
1:A:1077:G:H5'	1:A:1078:U:OP1	2.07	0.54
1:A:682:G:O2'	1:A:683:G:H5'	2.08	0.54
12:L:37:ARG:HH22	12:L:53:LYS:CE	2.20	0.54
2:B:15:ARG:HH11	2:B:17:ARG:HG2	1.73	0.54
1:A:1286:A:H8	1:A:1287:A:H4'	1.72	0.54
1:A:439:A:C2'	1:A:441:A:H5'	2.37	0.54
5:E:33:ARG:HH11	5:E:33:ARG:HG2	1.72	0.54
1:A:486:U:H2'	1:A:487:A:H5'	1.89	0.53
1:A:262:A:C5'	20:T:67:LYS:HD3	2.37	0.53
13:M:101:ARG:NH1	13:M:101:ARG:HB2	2.23	0.53
4:D:149:GLU:HG3	4:D:152:ARG:CZ	2.38	0.53
18:R:58:ALA:HB3	18:R:64:LEU:HD12	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1030:C:H6	1:A:1030:C:H5'	1.73	0.53
11:K:74:VAL:HG12	18:R:73:LYS:HZ3	1.73	0.53
10:J:29:GLY:HA2	10:J:76:ASN:ND2	2.22	0.53
5:E:94:THR:HG22	5:E:97:ILE:CD1	2.38	0.53
1:A:353:A:H5'	1:A:353:A:C8	2.43	0.53
23:Z:31:A:H2'	23:Z:32:U:O4'	2.08	0.53
6:F:60:PHE:C	6:F:61:LEU:HD12	2.29	0.53
1:A:1315:U:H2'	1:A:1316:G:O4'	2.08	0.53
3:C:106:GLN:NE2	3:C:106:GLN:H	2.07	0.53
3:C:109:ASN:HD22	3:C:139:ARG:HB3	1.72	0.53
1:A:1047:G:H5"	14:N:3:LYS:HD2	1.89	0.53
6:F:25:ILE:CD1	6:F:25:ILE:H	2.02	0.53
13:M:14:VAL:HG21	13:M:47:LEU:HD21	1.89	0.53
9:I:45:ALA:HB1	9:I:76:ILE:CG2	2.38	0.53
6:F:15:ASP:N	6:F:18:GLN:HE21	2.05	0.53
13:M:36:THR:O	13:M:36:THR:HG22	2.08	0.53
11:K:17:ASN:HD22	11:K:45:LYS:CE	2.21	0.53
2:B:16:LYS:HD2	2:B:29:GLU:OE2	2.09	0.53
2:B:47:ARG:NH1	2:B:193:TYR:CD1	2.75	0.53
19:S:29:LEU:HD23	19:S:47:THR:HG22	1.89	0.53
1:A:1218:C:H2'	1:A:1219:U:C6	2.43	0.53
11:K:17:ASN:ND2	11:K:45:LYS:HB3	2.23	0.53
1:A:1001:A:N3	1:A:1001:A:H2'	2.24	0.53
1:A:1447:A:O2'	1:A:1452:C:OP2	2.26	0.53
1:A:1014:A:H2	1:A:1219:U:O2	1.90	0.53
11:K:100:ASP:CB	18:R:73:LYS:HD2	2.38	0.53
1:A:1112:C:H5'	1:A:1113:C:OP1	2.08	0.53
1:A:254:G:OP1	17:Q:66:LYS:O	2.26	0.53
4:D:208:ARG:HH11	4:D:208:ARG:HG2	1.74	0.53
19:S:4:LEU:O	19:S:4:LEU:HD23	2.08	0.53
2:B:191:VAL:HB	2:B:194:ILE:HG13	1.89	0.53
13:M:123:PRO:C	13:M:125:LYS:H	2.12	0.53
1:A:460:G:O6	1:A:470:C:H5"	2.09	0.53
5:E:139:ARG:NH1	8:H:77:GLU:OE2	2.39	0.53
1:A:523:A:C2	12:L:87:LYS:HB3	2.44	0.53
10:J:36:ILE:HB	10:J:69:LEU:CB	2.22	0.53
1:A:390:C:H2'	1:A:391:G:C8	2.43	0.53
1:A:166:G:O2'	1:A:167:G:H5'	2.08	0.53
5:E:7:ILE:HB	5:E:27:LEU:HB3	1.91	0.53
5:E:29:VAL:HG11	5:E:105:ILE:HA	1.91	0.53
1:A:1118:C:H1'	1:A:1179:A:C4	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189(J):G:O2'	1:A:189(K):U:H5'	2.09	0.53
1:A:1245:A:H2'	1:A:1246:C:O4'	2.09	0.53
19:S:32:THR:HG22	19:S:33:TRP:N	2.23	0.53
7:G:14:ASP:OD1	7:G:43:TYR:OH	2.25	0.53
1:A:542:G:OP2	4:D:9:ARG:NH2	2.42	0.53
2:B:175:PHE:CD2	8:H:70:GLN:HB3	2.44	0.53
1:A:526:C:OP2	1:A:913:A:H4'	2.09	0.53
7:G:64:ALA:CB	7:G:123:LEU:HD23	2.38	0.53
10:J:7:ARG:HB3	10:J:7:ARG:NH1	2.23	0.53
13:M:83:ILE:HG21	19:S:65:MET:HB3	1.90	0.53
6:F:21:LEU:O	6:F:24:GLU:HB3	2.08	0.53
1:A:818:G:C2'	1:A:819:A:H5"	2.38	0.53
1:A:460:G:C6	1:A:470:C:H5"	2.43	0.53
1:A:1129:C:H1'	1:A:1132:C:C5	2.42	0.53
1:A:1296:C:H4'	1:A:1302:U:C5	2.44	0.53
7:G:144:ALA:C	7:G:146:ALA:H	2.12	0.53
1:A:1263:C:H2'	1:A:1264:C:H6	1.74	0.53
17:Q:10:VAL:O	17:Q:11:SER:HB2	2.09	0.53
11:K:3:GLN:HA	11:K:65:TYR:O	2.08	0.53
10:J:43:ARG:O	10:J:62:GLU:HA	2.09	0.53
1:A:1479:C:H2'	1:A:1480:G:H5'	1.90	0.53
1:A:1014:A:H2'	1:A:1015:A:C8	2.44	0.53
14:N:2:ARG:NH1	14:N:5:LEU:HD11	2.24	0.53
5:E:76:ILE:H	5:E:76:ILE:HD12	1.74	0.53
9:I:62:ILE:HG21	9:I:76:ILE:HG13	1.91	0.53
1:A:1149:C:H2'	1:A:1150:U:C6	2.44	0.53
1:A:1250:A:H4'	9:I:67:GLY:N	2.24	0.53
1:A:1369:C:H2'	1:A:1370:G:C8	2.44	0.53
2:B:85:PRO:HB3	2:B:148:LEU:HB2	1.91	0.53
18:R:28:PHE:O	18:R:36:LEU:HG	2.09	0.53
1:A:1481:U:H2'	1:A:1482:G:O4'	2.09	0.52
1:A:1278:U:H5"	1:A:1279:A:O4'	2.09	0.52
1:A:818:G:C3'	1:A:819:A:C5'	2.86	0.52
5:E:77:GLU:OE1	5:E:84:LYS:HE2	2.10	0.52
9:I:117:LYS:CG	9:I:120:ARG:HB3	2.39	0.52
16:P:72:ARG:HG3	16:P:73:LEU:N	2.22	0.52
1:A:17:U:H2'	1:A:18:C:C6	2.44	0.52
15:O:87:ARG:NE	15:O:87:ARG:CA	2.72	0.52
1:A:706:A:H4'	11:K:19:ILE:HD11	1.90	0.52
10:J:19:GLN:C	10:J:22:VAL:HG12	2.29	0.52
1:A:1371:G:OP2	9:I:10:LYS:O	2.27	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:96:LEU:N	2:B:96:LEU:HD12	2.24	0.52
17:Q:39:LYS:HE3	17:Q:41:TYR:OH	2.08	0.52
16:P:74:LEU:HD22	16:P:79:VAL:HG21	1.91	0.52
23:Z:34:G:H2'	23:Z:35:A:C8	2.43	0.52
1:A:486:U:C2'	1:A:487:A:C5'	2.86	0.52
12:L:37:ARG:HH22	12:L:53:LYS:HE2	1.74	0.52
1:A:1230:C:H1'	13:M:125:LYS:HA	1.90	0.52
2:B:17:ARG:O	2:B:18:TRP:O	2.27	0.52
3:C:179:ALA:O	3:C:180:ASN:CB	2.57	0.52
5:E:88:LYS:HB3	5:E:115:LEU:HB2	1.91	0.52
7:G:74:VAL:CG1	7:G:144:ALA:HA	2.40	0.52
3:C:187:LEU:HG	3:C:188:ALA:H	1.73	0.52
10:J:46:THR:HG23	10:J:60:HIS:CD2	2.44	0.52
4:D:63:LEU:HD12	4:D:74:PHE:CZ	2.43	0.52
1:A:1468:A:H2'	1:A:1469:G:O4'	2.09	0.52
1:A:1256:A:O3'	1:A:1257:U:C4'	2.57	0.52
20:T:38:GLN:HG2	20:T:84:LEU:HD13	1.91	0.52
7:G:49:ILE:HA	7:G:124:MET:CE	2.39	0.52
1:A:818:G:H3'	1:A:819:A:H5'	1.91	0.52
4:D:104:VAL:CG2	4:D:125:ILE:HD13	2.39	0.52
11:K:63:MET:C	11:K:65:TYR:H	2.13	0.52
20:T:49:MET:HE3	20:T:81:VAL:HG11	1.91	0.52
12:L:109:ARG:HH11	12:L:109:ARG:HG2	1.73	0.52
20:T:41:LYS:O	20:T:45:ALA:HB2	2.10	0.52
1:A:737:A:H1'	6:F:73:ASN:OD1	2.08	0.52
10:J:73:ILE:O	10:J:74:ASN:HB3	2.09	0.52
10:J:74:ASN:O	10:J:76:ASN:N	2.40	0.52
1:A:818:G:C3'	1:A:819:A:H5"	2.39	0.52
18:R:72:ARG:HH11	18:R:72:ARG:HG2	1.75	0.52
7:G:68:VAL:HG12	7:G:68:VAL:O	2.09	0.52
3:C:25:LYS:NZ	3:C:25:LYS:N	2.52	0.52
7:G:14:ASP:OD1	7:G:15:LEU:N	2.42	0.52
9:I:78:LEU:HD22	9:I:82:ARG:HD2	1.91	0.52
11:K:17:ASN:OD1	11:K:18:THR:N	2.42	0.52
2:B:194:ILE:H	2:B:194:ILE:CD1	2.20	0.52
1:A:1064:G:H21	1:A:1190:G:H2'	1.75	0.52
4:D:161:LEU:HD13	4:D:180:MET:CG	2.40	0.52
9:I:7:GLY:HA2	9:I:78:LEU:CD1	2.39	0.52
12:L:113:ARG:NH2	12:L:120:LYS:HB2	2.24	0.52
1:A:757:U:H2'	1:A:758:G:O4'	2.09	0.52
18:R:22:VAL:CG1	18:R:63:LEU:HB3	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1256:A:N1	1:A:1278:U:O2	2.43	0.52
2:B:191:VAL:CG1	2:B:194:ILE:HG13	2.39	0.52
2:B:45:LEU:HD22	2:B:49:PHE:CE1	2.45	0.52
3:C:26:LYS:HB2	3:C:27:GLN:NE2	2.22	0.52
6:F:19:LEU:HD11	6:F:23:LYS:HE3	1.92	0.52
7:G:25:PHE:CE2	7:G:29:ILE:HD11	2.45	0.52
1:A:1124:G:HO2'	1:A:1145:C:N4	2.09	0.51
1:A:1189:C:P	10:J:49:ARG:NH2	2.83	0.51
9:I:126:LYS:HB2	13:M:125:LYS:NZ	2.26	0.51
1:A:632:A:C2'	1:A:633:G:H5'	2.40	0.51
11:K:17:ASN:HD21	11:K:45:LYS:HD2	1.74	0.51
1:A:101:A:O2'	1:A:102:G:H5'	2.10	0.51
1:A:1508:G:O2'	1:A:1509:C:H5'	2.10	0.51
17:Q:75:LEU:HD23	17:Q:76:VAL:N	2.25	0.51
3:C:30:HIS:C	3:C:32:LEU:H	2.13	0.51
3:C:33:LEU:CG	14:N:24:VAL:HG21	2.36	0.51
20:T:50:ARG:HH11	20:T:50:ARG:CG	2.23	0.51
2:B:172:ARG:HH21	2:B:190:LEU:HA	1.75	0.51
1:A:723:U:O2	1:A:723:U:H2'	2.10	0.51
9:I:9:ARG:O	9:I:11:GLU:N	2.43	0.51
10:J:80:ILE:O	10:J:80:ILE:HG22	2.11	0.51
8:H:80:ILE:HG22	8:H:80:ILE:O	2.09	0.51
19:S:76:THR:HG22	19:S:77:ARG:HG3	1.91	0.51
2:B:181:LEU:HD23	2:B:195:ILE:O	2.09	0.51
9:I:45:ALA:HB2	9:I:73:ILE:HG23	1.92	0.51
2:B:172:ARG:NH2	8:H:68:ARG:NH2	2.55	0.51
1:A:269:C:H2'	1:A:270:A:H8	1.76	0.51
6:F:23:LYS:NZ	6:F:42:GLU:OE2	2.39	0.51
1:A:514:C:O2'	1:A:515:G:H5'	2.09	0.51
1:A:248:C:O2'	1:A:249:U:H5'	2.10	0.51
17:Q:62:ARG:HG2	17:Q:63:PRO:HD2	1.92	0.51
20:T:20:LYS:O	20:T:24:SER:HB2	2.11	0.51
19:S:50:VAL:O	19:S:56:HIS:HA	2.11	0.51
4:D:11:CYS:SG	4:D:18:LEU:HB2	2.51	0.51
2:B:206:GLN:NE2	2:B:210:SER:HB3	2.25	0.51
2:B:112:LEU:HD11	2:B:135:GLU:OE1	2.11	0.51
6:F:44:GLY:O	6:F:59:TYR:HA	2.10	0.51
1:A:344:A:H5"	1:A:345:C:C5	2.41	0.51
26:A:2733:3TS:CLA	12:L:40:THR:HG21	2.47	0.51
1:A:629:G:O2'	1:A:630:G:H5'	2.10	0.51
1:A:157:G:C8	1:A:157:G:H5'	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:109:ARG:HH12	12:L:112:SER:H	1.56	0.51
1:A:627:G:O2'	1:A:628:G:H5'	2.10	0.51
4:D:35:ARG:HD2	4:D:37:TYR:OH	2.10	0.51
1:A:1124:G:N7	1:A:1145:C:H2'	2.26	0.51
1:A:1004:A:N3	1:A:1004:A:H5"	2.25	0.51
1:A:1262:C:H2'	1:A:1263:C:C6	2.45	0.51
1:A:983:A:H5'	1:A:984:C:OP1	2.09	0.51
1:A:325:A:OP1	20:T:63:SER:HB3	2.10	0.51
1:A:174:C:H5'	1:A:174:C:H6	1.75	0.51
1:A:1054:C:C3'	1:A:1054:C:O2	2.59	0.51
9:I:126:LYS:H	9:I:126:LYS:CD	2.23	0.51
9:I:126:LYS:N	9:I:126:LYS:HD2	2.25	0.51
12:L:79:VAL:CG2	12:L:80:LEU:H	2.24	0.51
3:C:173:PRO:HB2	3:C:176:THR:HG22	1.93	0.51
3:C:57:GLU:CD	10:J:90:THR:HG21	2.30	0.51
9:I:7:GLY:CA	9:I:78:LEU:HB3	2.40	0.51
6:F:38:GLU:HB2	6:F:64:GLN:O	2.11	0.51
7:G:22:VAL:HG12	7:G:26:ILE:HD11	1.93	0.51
1:A:1039:C:H2'	1:A:1040:U:C6	2.46	0.51
2:B:233:VAL:O	2:B:233:VAL:HG12	2.11	0.51
9:I:98:LEU:CB	9:I:100:PHE:CE1	2.94	0.51
10:J:14:LEU:HD23	10:J:92:VAL:HG13	1.93	0.51
1:A:1140:C:H2'	1:A:1141:C:H5"	1.93	0.51
6:F:37:VAL:HA	6:F:65:VAL:HG12	1.91	0.51
12:L:105:GLY:HA3	12:L:117:GLY:O	2.11	0.51
4:D:130:ARG:HH11	4:D:130:ARG:HG3	1.75	0.51
13:M:77:ILE:O	13:M:80:LEU:HD23	2.11	0.51
6:F:22:GLU:OE1	6:F:82:ARG:HD3	2.10	0.51
5:E:73:PRO:O	5:E:74:HIS:HB3	2.11	0.51
1:A:501:C:H2'	1:A:502:G:C8	2.46	0.51
5:E:6:MET:SD	5:E:9:ILE:HG23	2.51	0.51
1:A:418:C:O2'	1:A:419:C:H5'	2.11	0.51
1:A:152:A:H2'	1:A:153:C:H5'	1.92	0.51
1:A:1206:G:O2'	1:A:1207:G:H5'	2.11	0.51
2:B:62:ILE:HG12	2:B:155:ALA:HB3	1.92	0.51
1:A:1326:C:C5'	21:V:12:LYS:HZ2	2.22	0.51
1:A:1190:G:OP1	3:C:3:LYS:HA	2.10	0.51
4:D:30:CYS:C	4:D:32:MET:H	2.14	0.51
1:A:976:G:C8	1:A:1358:U:C2	2.99	0.51
1:A:1231:G:H4'	9:I:125:SER:HB3	1.93	0.51
2:B:14:GLU:HG2	2:B:183:ASP:OD2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:502:G:P	12:L:114:SER:HG	2.34	0.51
3:C:181:ILE:HD12	3:C:181:ILE:N	2.25	0.50
1:A:1001(A):G:H2'	1:A:1002:G:H5'	1.93	0.50
7:G:91:SER:O	7:G:95:GLN:HG3	2.10	0.50
12:L:46:SER:O	12:L:47:ALA:HB2	2.11	0.50
1:A:1064:G:H4'	1:A:1065:U:OP1	2.11	0.50
1:A:173:U:H6	1:A:198:G:HO2'	1.58	0.50
2:B:207:LEU:HD23	2:B:207:LEU:C	2.30	0.50
7:G:16:VAL:HG12	7:G:16:VAL:O	2.09	0.50
17:Q:77:GLU:CD	17:Q:80:ARG:HD2	2.31	0.50
16:P:20:VAL:HG11	16:P:32:TYR:CB	2.41	0.50
3:C:13:ILE:HG22	3:C:14:THR:N	2.22	0.50
1:A:945:G:C2	1:A:946:A:C8	2.98	0.50
2:B:17:ARG:HH12	2:B:185:ASP:CA	2.24	0.50
1:A:407:G:H2'	1:A:408:A:H8	1.77	0.50
10:J:25:ALA:C	10:J:27:ARG:H	2.14	0.50
17:Q:78:SER:O	17:Q:79:GLY:O	2.29	0.50
1:A:140:A:O2'	1:A:141:A:H5'	2.10	0.50
1:A:1161:C:H2'	1:A:1162:C:H6	1.76	0.50
1:A:556:C:O2'	1:A:557:G:H5'	2.11	0.50
1:A:1402:C:O2	1:A:1500:A:N1	2.45	0.50
4:D:31:ALA:C	4:D:33:GLU:N	2.65	0.50
1:A:1272:G:H8	1:A:1272:G:H5'	1.76	0.50
1:A:1102:A:H2'	1:A:1103:C:C6	2.45	0.50
1:A:404:U:O2'	1:A:405:U:H5'	2.11	0.50
2:B:11:PHE:CD1	2:B:12:GLY:N	2.79	0.50
2:B:86:TYR:CE1	2:B:145:GLY:HA2	2.46	0.50
1:A:262:A:H5'	20:T:67:LYS:CD	2.40	0.50
6:F:33:TYR:CD2	6:F:75:LEU:HD23	2.46	0.50
15:O:54:GLY:O	15:O:58:MET:HG3	2.12	0.50
12:L:76:HIS:ND1	12:L:76:HIS:N	2.60	0.50
2:B:126:LYS:HE3	2:B:129:GLN:NE2	2.26	0.50
1:A:1254:C:OP1	10:J:43:ARG:HD2	2.11	0.50
1:A:1277:C:H2'	1:A:1278:U:H5'	1.94	0.50
1:A:952:U:H2'	1:A:953:G:H8	1.77	0.50
3:C:83:ILE:O	3:C:83:ILE:HG12	2.11	0.50
1:A:162:A:H2'	1:A:163:C:O4'	2.11	0.50
20:T:52:ALA:O	20:T:56:ILE:HG13	2.11	0.50
11:K:23:THR:HG22	11:K:29:PRO:HA	1.92	0.50
10:J:6:LEU:HD23	10:J:94:ILE:HG12	1.93	0.50
14:N:28:ARG:HB3	14:N:39:CYS:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:V:6:ARG:CD	21:V:15:ARG:HH12	2.24	0.50
2:B:86:TYR:N	2:B:86:TYR:CD1	2.80	0.50
7:G:36:ASN:HD21	9:I:40:VAL:H	1.60	0.50
1:A:58:C:H1'	1:A:388:G:N7	2.26	0.50
10:J:13:THR:C	10:J:15:ASP:N	2.65	0.50
16:P:59:TRP:HB3	16:P:64:ALA:HB2	1.94	0.50
1:A:1176:A:H2'	1:A:1177:G:O4'	2.11	0.50
11:K:22:ILE:HD12	11:K:62:ALA:HB2	1.93	0.50
13:M:22:TYR:CB	13:M:66:GLU:HA	2.42	0.50
1:A:1098:C:C3'	1:A:1099:G:H5"	2.40	0.50
1:A:192:U:H1'	20:T:96:GLY:HA2	1.94	0.50
1:A:1314:C:OP2	19:S:5:LYS:HD2	2.12	0.50
1:A:738:C:H5"	6:F:69:GLU:HB3	1.93	0.50
1:A:1057:G:H5"	3:C:153:SER:CB	2.39	0.50
13:M:10:ARG:HG2	13:M:11:ASN:N	2.26	0.50
10:J:86:LEU:N	10:J:86:LEU:HD12	2.26	0.50
1:A:983:A:H2	1:A:984:C:C6	2.30	0.50
1:A:393:A:O2'	1:A:394:G:H5'	2.12	0.50
1:A:1203:C:OP1	14:N:1:ALA:HB3	2.12	0.50
2:B:131:ARG:HB3	2:B:131:ARG:HH11	1.76	0.50
1:A:1334:G:C5'	1:A:1335:C:OP1	2.55	0.50
2:B:73:ASP:O	2:B:76:ARG:HB3	2.12	0.50
13:M:3:ILE:CG2	13:M:4:ALA:H	2.16	0.50
7:G:144:ALA:O	7:G:145:GLU:HB3	2.11	0.50
5:E:39:LEU:HD11	5:E:128:ALA:HB1	1.93	0.50
5:E:140:THR:HB	5:E:143:ASP:OD2	2.11	0.50
15:O:23:SER:HB2	15:O:26:VAL:HG23	1.94	0.50
5:E:33:ARG:NH1	5:E:33:ARG:HG2	2.27	0.50
1:A:961:U:C2'	1:A:962:C:H5'	2.42	0.50
1:A:1144:G:N2	1:A:1146:A:H62	2.09	0.49
2:B:112:LEU:O	2:B:136:LEU:HD11	2.12	0.49
20:T:46:LEU:HD12	20:T:93:ILE:HG22	1.93	0.49
1:A:460:G:C3'	1:A:461:A:C5'	2.90	0.49
2:B:70:GLN:O	2:B:202:ILE:HD13	2.12	0.49
22:W:2:U:H2'	22:W:3:C:C6	2.46	0.49
17:Q:65:SER:OG	17:Q:68:LYS:CB	2.60	0.49
1:A:1201:A:H4'	1:A:1202:G:O5'	2.12	0.49
4:D:35:ARG:N	4:D:36:PRO:CD	2.69	0.49
1:A:1213:A:C3'	1:A:1214:C:H5"	2.42	0.49
18:R:73:LYS:HG2	18:R:73:LYS:OXT	2.12	0.49
1:A:741:G:O2'	1:A:742:G:H5'	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:C:H2'	1:A:166:G:C8	2.45	0.49
3:C:114:LEU:HD23	3:C:117:GLN:NE2	2.27	0.49
1:A:431:A:O2'	1:A:432:A:H5'	2.12	0.49
5:E:1:ASP:CG	5:E:2:PHE:H	2.15	0.49
1:A:189(B):C:H2'	1:A:189(C):C:C6	2.47	0.49
12:L:49:ARG:HB3	12:L:89:LEU:HD11	1.94	0.49
1:A:1400:C:H6	1:A:1400:C:O5'	1.95	0.49
13:M:66:GLU:HG3	13:M:67:GLY:N	2.23	0.49
3:C:118:ARG:HG2	3:C:139:ARG:HH21	1.77	0.49
12:L:79:VAL:HG21	12:L:96:ILE:CG2	2.41	0.49
18:R:22:VAL:HG12	18:R:63:LEU:HB3	1.94	0.49
3:C:166:TRP:O	3:C:167:ALA:HB3	2.12	0.49
1:A:632:A:O2'	1:A:633:G:H5'	2.13	0.49
1:A:1138:G:C8	1:A:1140:C:H1'	2.47	0.49
9:I:9:ARG:O	9:I:10:LYS:C	2.50	0.49
1:A:390:C:H2'	1:A:391:G:H8	1.77	0.49
1:A:743:U:H2'	1:A:744:C:H6	1.76	0.49
17:Q:65:SER:OG	17:Q:68:LYS:HB3	2.12	0.49
9:I:25:VAL:HG13	9:I:60:ALA:HB3	1.95	0.49
1:A:229:U:H5"	16:P:33:ILE:HD13	1.94	0.49
1:A:1495:U:H2'	1:A:1496:C:H6	1.76	0.49
1:A:1052:U:H2'	1:A:1055:A:OP2	2.12	0.49
1:A:485:G:C2'	1:A:486:U:OP2	2.60	0.49
3:C:103:GLN:CA	3:C:103:GLN:HE21	2.24	0.49
2:B:231:ALA:C	2:B:233:VAL:H	2.15	0.49
13:M:2:ARG:HE	13:M:6:VAL:HA	1.77	0.49
1:A:631:G:H2'	1:A:632:A:C8	2.48	0.49
2:B:63:LEU:HB3	2:B:156:ILE:HD13	1.94	0.49
4:D:99:ARG:NH1	4:D:136:SER:HA	2.28	0.49
1:A:979:C:H2'	1:A:980:C:H5'	1.94	0.49
1:A:1072:G:H2'	1:A:1073:U:C6	2.46	0.49
1:A:650:G:O2'	1:A:651:C:H5'	2.12	0.49
1:A:1119:C:O2'	1:A:1120:G:H5'	2.12	0.49
19:S:62:THR:OG1	19:S:65:MET:HG2	2.11	0.49
14:N:4:ALA:O	14:N:7:GLU:HG2	2.11	0.49
16:P:42:ARG:NH1	16:P:42:ARG:CG	2.75	0.49
7:G:124:MET:O	7:G:128:GLU:HG2	2.12	0.49
1:A:720:C:H2'	1:A:721:G:C8	2.48	0.49
4:D:164:MET:HE2	4:D:175:LEU:HD22	1.93	0.49
9:I:116:HIS:CD2	9:I:122:PRO:HA	2.48	0.49
13:M:119:LYS:HG2	13:M:120:LYS:H	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:13:PRO:O	14:N:14:LYS:CB	2.60	0.49
13:M:119:LYS:C	13:M:120:LYS:HD2	2.33	0.49
17:Q:17:THR:HG23	17:Q:68:LYS:HE3	1.94	0.49
1:A:431:A:C2'	1:A:432:A:H5'	2.42	0.49
1:A:600:C:O2'	1:A:601:C:H5'	2.13	0.49
1:A:305:G:H4'	1:A:306:G:OP2	2.12	0.49
1:A:733:A:H4'	1:A:734:G:OP2	2.12	0.49
3:C:31:LEU:O	3:C:35:ASP:HB2	2.13	0.49
1:A:976:G:N7	1:A:1358:U:C2	2.81	0.49
6:F:61:LEU:N	6:F:61:LEU:HD12	2.27	0.49
5:E:11:ARG:HD3	5:E:22:PHE:CD1	2.47	0.49
1:A:1029:C:C3'	1:A:1030:C:H5"	2.42	0.49
1:A:223:U:C3'	1:A:224:C:H5"	2.42	0.49
1:A:1188:A:H3'	1:A:1189:C:C5'	2.43	0.49
1:A:1309:G:H3'	1:A:1310:G:C5'	2.32	0.49
1:A:397:A:N3	1:A:397:A:H3'	2.27	0.49
1:A:1343:G:OP1	9:I:124:TYR:HE1	1.95	0.49
1:A:1128:C:H2'	1:A:1129:C:H5"	1.93	0.49
1:A:1286:A:H3'	1:A:1286:A:C8	2.48	0.49
1:A:51:A:H4'	1:A:52:G:C5'	2.43	0.49
5:E:4:GLU:HG2	5:E:30:VAL:HG13	1.95	0.49
5:E:53:LYS:O	5:E:57:TYR:HD1	1.95	0.49
2:B:26:ILE:HD12	2:B:34:HIS:HB3	1.95	0.49
1:A:653:A:OP1	8:H:56:LYS:NZ	2.41	0.49
10:J:17:SER:OG	10:J:89:PRO:HG3	2.13	0.49
12:L:37:ARG:HH12	12:L:53:LYS:CE	2.20	0.49
2:B:108:ARG:HH22	2:B:112:LEU:HD21	1.75	0.49
1:A:1125:U:H5"	1:A:1126:U:H3	1.78	0.49
1:A:1225:A:H2'	1:A:1226:C:C5	2.48	0.49
2:B:162:THR:HG22	2:B:186:SER:HB3	1.94	0.49
17:Q:2:LYS:HB3	17:Q:60:GLU:HB3	1.94	0.49
1:A:189(I):G:O2'	1:A:189(J):G:H5'	2.11	0.49
21:V:2:GLY:C	21:V:4:GLY:H	2.14	0.49
3:C:178:ARG:O	3:C:178:ARG:CG	2.61	0.49
1:A:332:G:O2'	1:A:333:G:H5'	2.12	0.49
1:A:521:G:OP1	12:L:69:GLU:O	2.30	0.49
1:A:918:A:H2'	1:A:919:A:C8	2.47	0.49
9:I:4:TYR:O	9:I:83:ALA:HA	2.12	0.49
1:A:1221:G:H4'	19:S:52:ASN:O	2.13	0.49
1:A:1479:C:H2'	1:A:1480:G:C5'	2.42	0.49
15:O:38:LEU:HD12	15:O:55:LEU:HD13	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:163:LYS:C	2:B:163:LYS:HD3	2.33	0.49
13:M:34:GLU:O	13:M:36:THR:N	2.46	0.49
1:A:1232:U:H5"	9:I:123:GLN:O	2.13	0.49
1:A:913:A:H2'	1:A:914:A:C1'	2.43	0.49
11:K:24:ASP:OD2	11:K:28:ASN:HB2	2.13	0.49
1:A:1061:G:H1'	10:J:54:HIS:CE1	2.48	0.49
3:C:34:GLU:O	3:C:37:ARG:N	2.45	0.49
17:Q:94:TYR:N	17:Q:94:TYR:CD1	2.80	0.49
1:A:977:A:N6	1:A:1224:G:O5'	2.46	0.48
3:C:109:ASN:C	3:C:110:LEU:HD23	2.34	0.48
18:R:32:THR:C	18:R:34:LYS:H	2.16	0.48
7:G:138:GLU:O	7:G:142:ARG:HG3	2.13	0.48
1:A:1207:G:H2'	1:A:1208:C:H6	1.77	0.48
1:A:162:A:H2'	1:A:163:C:C4'	2.43	0.48
1:A:472:A:H2'	1:A:473:G:O4'	2.13	0.48
19:S:14:LEU:O	19:S:18:VAL:N	2.46	0.48
16:P:20:VAL:CG1	16:P:32:TYR:CB	2.91	0.48
1:A:19:C:H2'	1:A:20:U:H6	1.78	0.48
13:M:83:ILE:N	13:M:83:ILE:HD13	2.28	0.48
1:A:1256:A:H3'	3:C:26:LYS:HE2	1.94	0.48
14:N:10:LYS:C	14:N:12:THR:H	2.15	0.48
1:A:1335:C:H4'	1:A:1336:C:O5'	2.12	0.48
1:A:1040:U:H2'	1:A:1041:A:C8	2.48	0.48
12:L:51:VAL:CG1	12:L:52:ALA:N	2.76	0.48
9:I:126:LYS:O	13:M:125:LYS:NZ	2.45	0.48
7:G:134:VAL:O	7:G:138:GLU:HG3	2.12	0.48
15:O:70:GLN:HG3	15:O:77:TYR:CD2	2.48	0.48
1:A:1540:U:O2'	1:A:1541:U:H5'	2.13	0.48
1:A:434:U:H2'	1:A:435:C:C6	2.48	0.48
1:A:376:G:OP2	16:P:67:THR:HG21	2.13	0.48
15:O:52:HIS:CE1	15:O:56:LEU:HD13	2.48	0.48
4:D:190:ARG:O	4:D:190:ARG:HD3	2.13	0.48
4:D:29:LYS:C	4:D:31:ALA:N	2.67	0.48
3:C:29:ARG:O	3:C:32:LEU:HB3	2.14	0.48
3:C:46:LEU:HD12	3:C:46:LEU:N	2.27	0.48
11:K:74:VAL:CG1	18:R:73:LYS:HZ3	2.25	0.48
13:M:39:ASN:HB3	13:M:42:THR:CG2	2.43	0.48
10:J:4:ILE:N	10:J:4:ILE:CD1	2.73	0.48
2:B:15:ARG:HH12	2:B:17:ARG:HG2	1.77	0.48
1:A:149:A:H2'	1:A:150:C:H6	1.77	0.48
2:B:19:ASN:ND2	2:B:21:LYS:H	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:538:G:O2'	1:A:539:A:H5'	2.13	0.48
7:G:84:TYR:HD2	7:G:153:TYR:CE2	2.31	0.48
1:A:131:C:H2'	1:A:132:C:H6	1.77	0.48
1:A:913:A:O5'	1:A:913:A:H1'	2.14	0.48
1:A:1416:G:H1	1:A:1484:C:H42	1.60	0.48
4:D:33:GLU:O	4:D:34:ARG:HB2	2.13	0.48
13:M:83:ILE:C	13:M:85:CYS:N	2.66	0.48
14:N:35:PHE:O	14:N:35:PHE:CD1	2.67	0.48
1:A:590:C:C3'	1:A:591:U:H5"	2.43	0.48
16:P:19:ILE:HG22	16:P:36:ILE:CG1	2.44	0.48
12:L:79:VAL:CG2	12:L:80:LEU:N	2.75	0.48
1:A:1300:G:HO2'	1:A:1301:U:H6	1.57	0.48
1:A:1368:G:O2'	1:A:1369:C:H5'	2.12	0.48
7:G:27:ASN:OD1	7:G:35:LYS:NZ	2.47	0.48
17:Q:94:TYR:HD1	17:Q:94:TYR:N	2.11	0.48
3:C:119:VAL:HB	3:C:197:VAL:HG11	1.96	0.48
9:I:74:ASP:O	9:I:77:LYS:HB3	2.13	0.48
1:A:1170:A:H2'	1:A:1171:G:O4'	2.13	0.48
1:A:1090:U:H2'	1:A:1091:U:H6	1.76	0.48
2:B:55:LEU:HD13	2:B:55:LEU:O	2.13	0.48
7:G:110:ARG:HB3	7:G:112:GLU:OE2	2.13	0.48
20:T:3:LEU:HD23	20:T:3:LEU:N	2.29	0.48
1:A:1057:G:H2'	1:A:1058:G:O4'	2.14	0.48
7:G:77:ARG:HD2	7:G:155:TRP:CZ3	2.42	0.48
9:I:29:GLY:O	9:I:30:GLN:O	2.31	0.48
8:H:91:ARG:O	8:H:91:ARG:HG3	2.14	0.48
1:A:1393:U:O4'	1:A:1502:A:H5'	2.14	0.48
6:F:26:ILE:O	6:F:30:LEU:HG	2.14	0.48
10:J:29:GLY:HA2	10:J:76:ASN:CG	2.34	0.48
10:J:30:ALA:H	10:J:76:ASN:HD21	1.61	0.48
7:G:41:ILE:HD12	7:G:115:ALA:CB	2.43	0.48
1:A:166:G:H2'	1:A:167:G:H8	1.78	0.48
16:P:20:VAL:HG11	16:P:32:TYR:HB3	1.96	0.48
1:A:1320:C:C2	19:S:71:GLY:HA3	2.49	0.48
1:A:1466:C:H2'	1:A:1467:G:O4'	2.14	0.48
2:B:213:VAL:O	2:B:216:ILE:HB	2.13	0.48
4:D:195:LEU:CD2	4:D:195:LEU:N	2.77	0.48
10:J:30:ALA:C	10:J:32:VAL:N	2.67	0.48
20:T:50:ARG:HE	20:T:95:GLY:HA3	1.77	0.48
4:D:64:ARG:O	4:D:64:ARG:HG2	2.14	0.48
1:A:401:C:H1'	1:A:622:A:H1'	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:69:LEU:O	10:J:70:VAL:HB	2.13	0.48
1:A:738:C:OP2	6:F:92:LYS:HE2	2.13	0.48
3:C:179:ALA:HB1	3:C:181:ILE:HD11	1.96	0.48
7:G:17:TYR:HE2	7:G:58:LEU:HB2	1.78	0.48
4:D:56:ARG:HG3	4:D:56:ARG:NH1	2.29	0.48
11:K:24:ASP:HB2	11:K:25:PRO:HD2	1.96	0.48
1:A:376:G:H5"	16:P:5:ARG:HB2	1.95	0.48
3:C:156:ILE:HG21	3:C:163:ARG:HH21	1.78	0.48
14:N:10:LYS:C	14:N:12:THR:N	2.67	0.48
2:B:108:ARG:NH1	2:B:112:LEU:CG	2.72	0.48
2:B:86:TYR:HD1	2:B:86:TYR:N	2.12	0.48
18:R:44:SER:OG	18:R:47:GLU:HG3	2.13	0.48
5:E:27:LEU:HD22	5:E:39:LEU:HD22	1.95	0.48
1:A:1365:G:H5'	1:A:1365:G:H8	1.78	0.48
20:T:49:MET:CE	20:T:81:VAL:HG11	2.42	0.48
7:G:22:VAL:O	7:G:26:ILE:HG13	2.14	0.48
9:I:41:ARG:O	9:I:43:VAL:N	2.46	0.48
20:T:16:ARG:NH1	20:T:16:ARG:HG2	2.29	0.48
1:A:939:G:H2'	1:A:940:C:C6	2.49	0.47
1:A:272:C:C5'	1:A:272:C:H6	2.20	0.47
11:K:38:ILE:HD11	11:K:54:ALA:N	2.29	0.47
1:A:364:A:N6	12:L:24:LYS:HZ1	2.11	0.47
4:D:176:ASP:OD1	4:D:178:GLU:CG	2.62	0.47
3:C:149:LYS:HG3	3:C:168:ALA:HB2	1.95	0.47
3:C:190:THR:HG21	3:C:192:TYR:CE1	2.48	0.47
19:S:41:PRO:O	19:S:43:MET:N	2.47	0.47
1:A:38:G:N2	1:A:397:A:H5'	2.17	0.47
10:J:2:ILE:O	10:J:71:ASP:HA	2.14	0.47
7:G:36:ASN:HD21	9:I:40:VAL:HG23	1.77	0.47
10:J:30:ALA:HB2	10:J:74:ASN:HB3	1.95	0.47
1:A:1064:G:H1'	1:A:1190:G:N2	2.29	0.47
1:A:460:G:C2'	1:A:461:A:H5"	2.42	0.47
5:E:74:HIS:CE1	5:E:139:ARG:H	2.25	0.47
1:A:1286:A:H8	1:A:1286:A:H3'	1.79	0.47
4:D:120:VAL:O	4:D:133:ASP:HA	2.14	0.47
1:A:390:C:O3'	16:P:28:ARG:NH2	2.47	0.47
1:A:1346:A:N1	1:A:1374:A:H5"	2.29	0.47
1:A:607:A:O2'	1:A:608:A:H5'	2.13	0.47
4:D:127:VAL:HG12	4:D:128:ASN:ND2	2.28	0.47
1:A:182:U:C4	1:A:183:G:H1'	2.50	0.47
1:A:184:G:H5'	1:A:224:C:O2'	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:189:ARG:NH1	3:C:189:ARG:HB3	2.21	0.47
11:K:38:ILE:HD11	11:K:54:ALA:HA	1.95	0.47
6:F:99:ALA:O	6:F:101:ALA:N	2.47	0.47
9:I:98:LEU:HB2	9:I:100:PHE:HE1	1.79	0.47
1:A:1118:C:O4'	1:A:1179:A:H1'	2.14	0.47
14:N:59:SER:O	14:N:60:TRP:HB3	2.14	0.47
11:K:71:ASP:OD1	11:K:96:LYS:HB2	2.14	0.47
1:A:868:C:H2'	1:A:869:G:O4'	2.14	0.47
1:A:1439:C:P	20:T:31:LYS:HZ3	2.37	0.47
1:A:106:C:O2	1:A:379:C:H4'	2.14	0.47
3:C:71:LYS:HB3	3:C:71:LYS:NZ	2.29	0.47
17:Q:100:ARG:NE	17:Q:100:ARG:HA	2.29	0.47
1:A:389:A:N3	1:A:389:A:H2'	2.30	0.47
1:A:721:G:OP2	18:R:38:ARG:HG3	2.15	0.47
13:M:124:ARG:HH11	13:M:124:ARG:HG3	1.79	0.47
1:A:411:A:H2'	1:A:412:A:C5'	2.44	0.47
1:A:1366:C:H2'	1:A:1367:C:H6	1.79	0.47
1:A:299:G:H2'	1:A:300:A:C8	2.49	0.47
1:A:922:G:H2'	1:A:923:A:C8	2.49	0.47
1:A:5:U:H5"	1:A:5:U:O2	2.15	0.47
1:A:123:C:OP1	1:A:312:C:H5'	2.14	0.47
1:A:959:A:C2	1:A:1222:G:O4'	2.68	0.47
1:A:1013:G:N2	1:A:1016:A:OP2	2.48	0.47
1:A:649:G:C5'	1:A:649:G:H8	2.27	0.47
11:K:4:VAL:CG2	11:K:67:MET:HG2	2.45	0.47
1:A:328:C:O2	1:A:328:C:H2'	2.15	0.47
10:J:51:PRO:O	10:J:52:PHE:O	2.33	0.47
11:K:48:PRO:O	11:K:51:ALA:HB3	2.14	0.47
1:A:1126:U:C2'	1:A:1126:U:O2	2.61	0.47
7:G:112:GLU:HG3	7:G:117:VAL:HG12	1.97	0.47
14:N:25:ARG:CZ	14:N:46:LEU:HD21	2.44	0.47
1:A:997:U:H2'	1:A:998:G:O4'	2.13	0.47
10:J:25:ALA:HA	10:J:79:THR:HG23	1.97	0.47
9:I:9:ARG:HD2	9:I:10:LYS:H	1.80	0.47
23:Z:31:A:O2'	23:Z:32:U:H5'	2.14	0.47
9:I:105:ALA:O	9:I:107:VAL:HG23	2.14	0.47
1:A:143:A:H5'	1:A:144:G:O5'	2.15	0.47
1:A:643:C:H2'	1:A:644:G:H8	1.78	0.47
1:A:109:A:H2'	1:A:326:G:N2	2.29	0.47
1:A:1054:C:H42	23:Z:34:G:C1'	2.28	0.47
1:A:1277:C:H5'	1:A:1277:C:C6	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2:LYS:O	2:B:3:GLU:HB2	2.13	0.47
19:S:4:LEU:O	19:S:5:LYS:CB	2.50	0.47
13:M:51:GLU:HG2	13:M:54:ARG:NH2	2.27	0.47
5:E:76:ILE:HD13	5:E:87:LEU:HD12	1.96	0.47
3:C:7:ILE:HG23	3:C:15:ARG:HG2	1.97	0.47
3:C:154:GLY:O	3:C:155:ARG:CB	2.62	0.47
1:A:1111:A:N1	3:C:176:THR:HB	2.29	0.47
1:A:407:G:H2'	1:A:408:A:C8	2.49	0.47
8:H:24:THR:HG22	8:H:63:LEU:HD21	1.97	0.47
2:B:123:GLU:O	2:B:124:ARG:HB2	2.15	0.47
19:S:79:TYR:O	19:S:80:ARG:C	2.52	0.47
19:S:11:ASP:H	19:S:37:SER:HB3	1.80	0.47
1:A:1351:U:O4'	7:G:32:ASP:HB3	2.14	0.47
8:H:6:ILE:HD11	8:H:31:PHE:CD2	2.50	0.47
1:A:359:U:O2'	1:A:360:A:H5'	2.14	0.47
2:B:36:ILE:HD12	2:B:197:GLY:HA2	1.97	0.47
1:A:382:A:C2	1:A:383:A:C4	3.02	0.47
4:D:61:GLN:HA	4:D:61:GLN:NE2	2.30	0.47
19:S:42:GLU:H	19:S:42:GLU:CD	2.18	0.47
10:J:96:ILE:H	10:J:96:ILE:HD12	1.80	0.47
13:M:5:GLY:O	13:M:7:GLU:N	2.48	0.47
10:J:85:THR:C	10:J:86:LEU:HD12	2.35	0.47
5:E:32:ASP:O	5:E:33:ARG:HB2	2.15	0.47
3:C:163:ARG:NH2	3:C:165:GLU:OE1	2.44	0.47
1:A:1414:U:H2'	1:A:1415:G:H8	1.80	0.47
1:A:1423:G:O2'	1:A:1424:C:H5'	2.15	0.47
6:F:9:VAL:HB	6:F:87:ARG:HB2	1.97	0.47
1:A:1275:A:O2'	1:A:1276:G:H5'	2.15	0.47
2:B:2:LYS:HD2	2:B:2:LYS:C	2.35	0.47
3:C:69:VAL:O	3:C:105:VAL:HG23	2.15	0.47
1:A:1390:U:H2'	1:A:1391:U:C6	2.50	0.47
6:F:18:GLN:O	6:F:21:LEU:HB3	2.15	0.47
10:J:30:ALA:H	10:J:76:ASN:ND2	2.13	0.47
1:A:279:A:C8	1:A:279:A:H5'	2.50	0.47
4:D:172:TRP:CD2	4:D:188:PRO:HB3	2.50	0.47
5:E:72:ILE:HD12	5:E:138:LEU:HD11	1.96	0.47
2:B:13:HIS:HD2	2:B:199:ASP:OD1	1.97	0.47
4:D:29:LYS:O	4:D:31:ALA:N	2.47	0.47
1:A:872:A:C3'	1:A:873:A:C5'	2.92	0.47
1:A:224:C:C6	1:A:224:C:H5'	2.48	0.47
11:K:81:ARG:NH1	18:R:73:LYS:HE2	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:25:GLY:O	12:L:26:ALA:C	2.52	0.47
17:Q:3:LYS:CE	17:Q:5:LEU:HD21	2.45	0.47
1:A:1349:A:OP2	9:I:117:LYS:HE2	2.15	0.47
13:M:15:ASP:OD1	13:M:16:VAL:N	2.46	0.47
1:A:1074:G:O3'	2:B:97:THR:HG22	2.15	0.47
1:A:542:G:O2'	1:A:543:C:H5'	2.15	0.47
3:C:188:ALA:HB3	3:C:195:LEU:HB2	1.97	0.47
2:B:156:ILE:HG22	2:B:158:VAL:HG23	1.97	0.47
20:T:39:GLU:OE1	20:T:41:LYS:NZ	2.48	0.47
3:C:178:ARG:O	3:C:178:ARG:HG2	2.15	0.47
1:A:73:G:O2'	1:A:76:C:H5'	2.15	0.47
1:A:41:G:H2'	1:A:42:G:C8	2.50	0.47
2:B:1:VAL:CG2	2:B:215:LEU:HD23	2.31	0.46
2:B:189:ASP:O	8:H:68:ARG:NH2	2.47	0.46
6:F:101:ALA:HA	18:R:13:GLU:OE1	2.15	0.46
17:Q:3:LYS:HE3	17:Q:5:LEU:CD2	2.44	0.46
1:A:1353:G:O2'	1:A:1354:C:H5'	2.15	0.46
3:C:57:GLU:HB2	3:C:64:ALA:CB	2.45	0.46
16:P:20:VAL:CG1	16:P:21:VAL:N	2.77	0.46
8:H:26:VAL:O	8:H:27:PRO:C	2.52	0.46
1:A:1252:A:H61	1:A:1285:A:N6	2.13	0.46
1:A:18:C:H5"	5:E:123:ASN:HD21	1.79	0.46
1:A:627:G:H2'	1:A:628:G:H8	1.80	0.46
1:A:1203:C:H2'	1:A:1204:A:H8	1.79	0.46
4:D:17:LYS:HZ3	4:D:30:CYS:CB	2.15	0.46
19:S:76:THR:HG22	19:S:77:ARG:N	2.29	0.46
15:O:86:ILE:O	15:O:87:ARG:HB2	2.16	0.46
1:A:539:A:H2'	1:A:540:G:H8	1.78	0.46
18:R:40:ARG:HH11	18:R:40:ARG:CA	2.29	0.46
1:A:824:C:H2'	1:A:825:G:C8	2.47	0.46
1:A:384:G:H2'	1:A:385:C:H6	1.79	0.46
3:C:148:ALA:O	3:C:168:ALA:HB1	2.15	0.46
1:A:109:A:H5'	1:A:110:C:C5	2.50	0.46
1:A:687:A:H4'	1:A:688:G:O5'	2.15	0.46
7:G:102:TRP:CH2	7:G:140:VAL:HG21	2.50	0.46
9:I:31:ASP:O	9:I:34:GLU:HB3	2.15	0.46
2:B:56:ALA:C	2:B:58:ARG:H	2.19	0.46
1:A:1124:G:H4'	10:J:36:ILE:HD11	1.97	0.46
17:Q:91:ARG:NH1	17:Q:91:ARG:CB	2.72	0.46
1:A:970:C:N4	9:I:125:SER:OG	2.48	0.46
1:A:945:G:H2'	1:A:945:G:N3	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:954:G:H2'	1:A:955:U:H6	1.80	0.46
1:A:1151:A:O2'	1:A:1152:A:H8	1.98	0.46
20:T:67:LYS:HB2	20:T:68:ASN:H	1.32	0.46
9:I:24:LYS:HB3	9:I:24:LYS:HZ3	1.80	0.46
1:A:156:G:C3'	1:A:157:G:H5"	2.45	0.46
4:D:63:LEU:HD23	4:D:197:VAL:HG21	1.97	0.46
21:V:2:GLY:O	21:V:4:GLY:N	2.48	0.46
15:O:49:HIS:O	15:O:52:HIS:HB3	2.15	0.46
4:D:93:LEU:HA	4:D:96:LEU:HD12	1.98	0.46
12:L:115:LYS:O	12:L:116:TYR:HB2	2.15	0.46
13:M:76:ASN:O	13:M:79:ARG:HB3	2.15	0.46
1:A:484:G:OP2	1:A:484:G:H8	1.98	0.46
1:A:737:A:H2'	1:A:738:C:C6	2.50	0.46
5:E:70:GLY:CA	5:E:112:THR:HG22	2.46	0.46
14:N:30:ARG:NH1	14:N:30:ARG:HG3	2.31	0.46
7:G:61:PHE:HD1	7:G:123:LEU:HD21	1.81	0.46
1:A:1175:G:O2'	1:A:1176:A:H5'	2.15	0.46
8:H:112:LEU:HD12	8:H:112:LEU:N	2.30	0.46
19:S:12:ASP:HA	19:S:15:LEU:HB3	1.98	0.46
19:S:28:ARG:O	19:S:29:LEU:HB2	2.15	0.46
19:S:21:LEU:HD12	19:S:30:ILE:HD11	1.97	0.46
12:L:37:ARG:HG2	12:L:38:THR:N	2.24	0.46
1:A:129(A):G:C6	1:A:189(E):U:O2'	2.66	0.46
6:F:67:MET:HB2	6:F:68:PRO:HD2	1.95	0.46
17:Q:66:LYS:O	17:Q:67:ARG:CG	2.62	0.46
7:G:16:VAL:HG12	7:G:17:TYR:CE1	2.51	0.46
15:O:25:GLU:OE2	15:O:76:ARG:HD2	2.16	0.46
5:E:9:ILE:HA	5:E:25:GLY:O	2.16	0.46
20:T:37:ALA:HA	20:T:85:LEU:HD21	1.98	0.46
9:I:39:LEU:O	9:I:41:ARG:N	2.49	0.46
1:A:1082:G:O2'	1:A:1083:U:H5'	2.15	0.46
1:A:583:A:H2'	1:A:584:G:O4'	2.16	0.46
1:A:1281:U:O2	1:A:1281:U:O4'	2.33	0.46
19:S:18:VAL:HG13	19:S:19:LEU:N	2.31	0.46
5:E:47:VAL:O	5:E:50:ALA:HB3	2.16	0.46
4:D:195:LEU:HB2	4:D:196:PRO:HD2	1.97	0.46
1:A:364:A:N6	12:L:24:LYS:NZ	2.63	0.46
9:I:36:PHE:HB3	9:I:42:ALA:HB2	1.96	0.46
7:G:45:ALA:O	7:G:49:ILE:HG13	2.15	0.46
20:T:66:HIS:C	20:T:67:LYS:CG	2.83	0.46
1:A:1428:A:H2'	1:A:1429:C:C6	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:74:LEU:CD2	16:P:79:VAL:HG21	2.44	0.46
7:G:91:SER:HB2	7:G:92:PRO:HD2	1.98	0.46
1:A:651:C:O2'	1:A:652:U:H5'	2.16	0.46
1:A:1483:A:H2'	1:A:1484:C:O4'	2.16	0.46
1:A:607:A:H5'	1:A:607:A:H8	1.80	0.46
17:Q:16:LYS:HA	17:Q:45:ASP:O	2.14	0.46
9:I:48:PRO:HB3	9:I:81:ALA:HB2	1.96	0.46
3:C:137:VAL:O	3:C:141:MET:HB2	2.16	0.46
3:C:19:SER:O	14:N:53:PRO:HB3	2.15	0.46
5:E:36:ARG:HG2	5:E:36:ARG:HH11	1.80	0.46
23:Z:34:G:H2'	23:Z:35:A:H8	1.81	0.46
1:A:1126:U:H6	1:A:1280:A:N7	2.12	0.46
1:A:293:G:H5'	1:A:609:A:N6	2.26	0.46
10:J:24:ALA:O	10:J:83:LEU:HG	2.16	0.46
18:R:71:VAL:O	18:R:72:ARG:HG2	2.15	0.46
1:A:653:A:C8	8:H:56:LYS:HG2	2.51	0.46
6:F:62:TRP:CG	18:R:20:ARG:NH1	2.83	0.46
12:L:24:LYS:HD3	12:L:29:ARG:HH12	1.80	0.46
10:J:73:ILE:HG22	10:J:74:ASN:N	2.31	0.46
13:M:123:PRO:C	13:M:125:LYS:N	2.69	0.46
3:C:82:ARG:C	3:C:84:ARG:H	2.18	0.46
17:Q:80:ARG:HG3	17:Q:80:ARG:O	2.16	0.46
2:B:72:GLN:O	2:B:88:ASN:OD1	2.33	0.46
6:F:40:VAL:CG2	6:F:41:GLU:N	2.79	0.46
13:M:45:LYS:HG3	13:M:46:ASP:N	2.31	0.46
3:C:27:GLN:HA	3:C:30:HIS:HD2	1.81	0.46
3:C:69:VAL:C	3:C:105:VAL:HG23	2.35	0.46
2:B:4:LEU:O	2:B:6:GLU:N	2.49	0.46
10:J:4:ILE:HG12	10:J:4:ILE:O	2.15	0.46
10:J:96:ILE:N	10:J:96:ILE:HD12	2.31	0.46
2:B:183:ASP:OD2	2:B:199:ASP:OD1	2.34	0.46
1:A:310:G:H5"	16:P:31:LYS:HB2	1.98	0.46
1:A:18:C:H5"	5:E:123:ASN:ND2	2.31	0.46
15:O:65:LEU:O	15:O:68:TYR:HB3	2.16	0.46
12:L:31:GLY:HA3	12:L:54:VAL:CG1	2.46	0.46
1:A:107:G:C2'	1:A:108:G:H5'	2.46	0.46
1:A:1144:G:H21	1:A:1146:A:N6	2.13	0.46
14:N:7:GLU:C	14:N:7:GLU:OE1	2.55	0.46
9:I:63:THR:HG22	9:I:64:VAL:N	2.31	0.46
11:K:81:ARG:CZ	18:R:73:LYS:CE	2.92	0.46
11:K:38:ILE:HD13	11:K:53:LEU:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:64:LYS:HE3	13:M:68:GLU:CG	2.40	0.46
5:E:72:ILE:HG23	5:E:138:LEU:HD13	1.98	0.46
1:A:439:A:H2'	1:A:441:A:C5'	2.45	0.46
1:A:1471:G:O2'	1:A:1472:U:H5'	2.16	0.46
1:A:714:G:H2'	1:A:715:A:C8	2.50	0.46
12:L:30:ARG:O	12:L:57:THR:HG23	2.15	0.46
19:S:57:VAL:O	19:S:59:VAL:HG23	2.16	0.46
3:C:22:TYR:CD1	3:C:23:ALA:N	2.84	0.46
1:A:1044:A:H2'	1:A:1045:C:C4'	2.46	0.46
11:K:36:GLY:O	11:K:38:ILE:O	2.34	0.45
2:B:24:ARG:NH2	2:B:188:PRO:HB2	2.31	0.45
1:A:1129:C:O5'	1:A:1130:A:H5'	2.16	0.45
1:A:413:G:H21	1:A:428:G:H1'	1.80	0.45
15:O:35:ILE:HD12	15:O:59:VAL:HG23	1.97	0.45
1:A:1460:A:H2'	1:A:1461:G:O4'	2.16	0.45
15:O:7:LYS:O	15:O:11:ILE:HD12	2.16	0.45
1:A:1037:C:H2'	1:A:1038:C:C6	2.51	0.45
4:D:69:ILE:HG22	4:D:73:GLN:HB2	1.98	0.45
13:M:2:ARG:HG2	13:M:2:ARG:O	2.16	0.45
1:A:55:A:O2'	1:A:56:U:H5'	2.16	0.45
1:A:253:U:H2'	1:A:254:G:H8	1.78	0.45
14:N:25:ARG:HE	14:N:46:LEU:HD21	1.80	0.45
3:C:153:SER:CB	3:C:196:GLY:H	2.29	0.45
13:M:10:ARG:HA	13:M:44:VAL:HB	1.97	0.45
1:A:334:C:H2'	1:A:335:C:C6	2.52	0.45
1:A:455:C:H2'	1:A:456:C:C6	2.52	0.45
3:C:44:LYS:HB2	3:C:44:LYS:HE3	1.66	0.45
19:S:18:VAL:HG21	19:S:43:MET:HG2	1.98	0.45
1:A:483:C:C3'	1:A:484:G:H5"	2.38	0.45
1:A:880:C:O2'	1:A:881:G:H5'	2.16	0.45
5:E:112:THR:HG23	5:E:113:ASP:OD2	2.16	0.45
7:G:123:LEU:O	7:G:126:ALA:HB3	2.15	0.45
1:A:1161:C:H2'	1:A:1162:C:C6	2.51	0.45
16:P:67:THR:HG22	16:P:69:THR:H	1.81	0.45
17:Q:100:ARG:HA	17:Q:100:ARG:HE	1.81	0.45
1:A:715:A:H2'	1:A:716:A:C8	2.52	0.45
1:A:639:G:O2'	1:A:640:A:H5'	2.16	0.45
1:A:982:U:O4	1:A:1223:C:N3	2.50	0.45
19:S:4:LEU:C	19:S:4:LEU:HD23	2.37	0.45
14:N:28:ARG:HG2	14:N:39:CYS:HB2	1.98	0.45
21:V:6:ARG:CG	21:V:15:ARG:NH1	2.74	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:175:LEU:HG	4:D:176:ASP:N	2.31	0.45
1:A:1249:C:H4'	9:I:35:TYR:OH	2.17	0.45
2:B:22:PHE:HD1	2:B:188:PRO:HG3	1.81	0.45
1:A:1142:G:C2'	1:A:1143:G:H5'	2.47	0.45
12:L:84:GLY:H	12:L:94:TYR:HA	1.81	0.45
1:A:1346:A:C2	7:G:9:ARG:NH1	2.84	0.45
1:A:175:C:H2'	1:A:176:C:H6	1.81	0.45
2:B:37:ASP:OD1	2:B:39:GLN:HB2	2.15	0.45
2:B:150:LYS:HD3	2:B:150:LYS:O	2.15	0.45
1:A:977:A:O2'	1:A:978:A:H5"	2.16	0.45
13:M:80:LEU:O	13:M:85:CYS:HB3	2.16	0.45
1:A:1256:A:N6	1:A:1278:U:H3	2.05	0.45
3:C:46:LEU:CD2	3:C:67:VAL:HG11	2.47	0.45
10:J:30:ALA:HB2	10:J:74:ASN:CB	2.47	0.45
7:G:40:ARG:O	7:G:41:ILE:C	2.55	0.45
1:A:921:U:O2	5:E:15:MET:HB2	2.17	0.45
4:D:60:LYS:NZ	4:D:71:GLU:OE1	2.50	0.45
1:A:1032:G:H2'	1:A:1033:G:C8	2.52	0.45
6:F:43:LEU:N	6:F:43:LEU:HD22	2.32	0.45
3:C:118:ARG:CG	3:C:139:ARG:NH2	2.76	0.45
2:B:3:GLU:HG2	2:B:211:ARG:HH12	1.81	0.45
1:A:1335:C:H5"	1:A:1335:C:H6	1.81	0.45
1:A:1040:U:H2'	1:A:1041:A:H8	1.82	0.45
2:B:9:VAL:HG12	2:B:204:SER:HA	1.99	0.45
1:A:952:U:H2'	1:A:953:G:C8	2.52	0.45
2:B:19:ASN:HD22	2:B:21:LYS:H	1.65	0.45
11:K:4:VAL:O	11:K:5:ALA:HB3	2.16	0.45
2:B:82:ALA:C	2:B:84:MET:H	2.19	0.45
3:C:147:GLY:HA3	3:C:171:ARG:O	2.16	0.45
5:E:94:THR:HG22	5:E:97:ILE:HD11	1.98	0.45
1:A:1168:A:O2'	1:A:1169:A:H8	1.99	0.45
1:A:1402:C:H2'	1:A:1403:C:O4'	2.16	0.45
1:A:161:A:O2'	1:A:162:A:H5'	2.17	0.45
1:A:807:A:H2'	1:A:808:C:C6	2.51	0.45
1:A:1109:C:H2'	1:A:1110:A:O4'	2.17	0.45
19:S:12:ASP:OD1	19:S:12:ASP:N	2.49	0.45
2:B:129:GLN:O	2:B:133:LYS:HB2	2.16	0.45
2:B:130:VAL:HG12	2:B:134:HIS:CD2	2.52	0.45
1:A:1231:G:H4'	9:I:125:SER:HB2	1.98	0.45
12:L:25:GLY:O	12:L:26:ALA:O	2.34	0.45
6:F:72:VAL:CG1	6:F:90:VAL:HG11	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:38:ARG:HG2	18:R:48:GLN:OE1	2.17	0.45
1:A:954:G:H21	1:A:1227:A:H62	1.65	0.45
1:A:253:U:H2'	1:A:254:G:C8	2.52	0.45
2:B:81:ARG:HD3	2:B:228:PRO:HD2	1.98	0.45
3:C:82:ARG:C	3:C:84:ARG:N	2.70	0.45
6:F:94:GLN:HE21	18:R:17:ARG:NH1	2.12	0.45
4:D:63:LEU:HD12	4:D:74:PHE:HZ	1.82	0.45
1:A:19:C:H2'	1:A:20:U:C6	2.51	0.45
5:E:78:VAL:HG22	5:E:137:GLN:NE2	2.31	0.45
1:A:572:A:H5"	1:A:917:G:H4'	1.99	0.45
10:J:44:ARG:CG	10:J:44:ARG:NH1	2.76	0.45
2:B:109:LEU:HD11	2:B:140:GLN:NE2	2.32	0.45
4:D:110:ALA:HB2	4:D:119:LEU:HD12	1.99	0.45
1:A:173:U:H2'	1:A:197:A:N7	2.32	0.45
8:H:60:ARG:NH1	8:H:60:ARG:HG3	2.30	0.45
8:H:56:LYS:N	8:H:56:LYS:HD2	2.31	0.45
1:A:1438:G:H2'	1:A:1439:C:C6	2.51	0.45
11:K:116:ARG:O	11:K:117:LYS:HB2	2.17	0.45
6:F:50:TYR:CE1	18:R:62:GLY:HA2	2.51	0.45
5:E:149:LYS:O	5:E:151:GLU:N	2.50	0.45
1:A:1305:G:H22	1:A:1331:G:H1'	1.80	0.45
10:J:43:ARG:NH2	14:N:35:PHE:CD2	2.85	0.45
11:K:100:ASP:OD1	11:K:101:ASP:N	2.50	0.45
13:M:121:LYS:CD	13:M:122:ALA:H	2.29	0.45
15:O:16:ARG:HG3	15:O:16:ARG:NH1	2.32	0.45
1:A:892:A:H2'	1:A:893:C:C6	2.52	0.45
20:T:36:LEU:HD13	20:T:44:GLU:HG3	1.99	0.45
3:C:4:ILE:O	3:C:4:ILE:HD12	2.16	0.45
11:K:40:TYR:HB3	11:K:44:ARG:HB2	1.97	0.45
2:B:52:ILE:HD11	2:B:179:ILE:HD13	1.98	0.45
2:B:77:MET:HG3	2:B:229:SER:CB	2.45	0.45
4:D:110:ALA:HB1	4:D:115:GLN:HG2	1.99	0.45
18:R:32:THR:HG22	18:R:33:GLY:N	2.31	0.45
20:T:16:ARG:HH11	20:T:16:ARG:HG2	1.80	0.45
8:H:4:ASP:OD2	8:H:85:ARG:NH1	2.49	0.45
1:A:838:G:H1	1:A:848:C:N4	2.15	0.45
1:A:1401:G:OP2	1:A:1544:U:O2'	2.31	0.45
1:A:1099:G:H5'	1:A:1099:G:H8	1.81	0.44
10:J:32:VAL:HG12	10:J:33:SER:N	2.31	0.44
1:A:279:A:H8	1:A:279:A:H5'	1.83	0.44
2:B:231:ALA:C	2:B:233:VAL:N	2.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:22:VAL:HG23	18:R:23:GLU:N	2.33	0.44
13:M:34:GLU:C	13:M:36:THR:N	2.70	0.44
4:D:7:VAL:HG13	4:D:20:LEU:CD1	2.47	0.44
5:E:140:THR:HG22	5:E:142:ALA:H	1.81	0.44
1:A:130:A:C8	17:Q:62:ARG:HG3	2.52	0.44
14:N:23:CYS:HA	14:N:37:GLY:O	2.16	0.44
13:M:20:TYR:N	13:M:20:TYR:CD1	2.84	0.44
2:B:151:ARG:HG3	2:B:151:ARG:HH11	1.82	0.44
7:G:5:ARG:HG2	7:G:5:ARG:O	2.17	0.44
1:A:1036:G:O2'	1:A:1037:C:H5'	2.17	0.44
4:D:186:ARG:NH2	4:D:187:LEU:HG	2.32	0.44
2:B:18:TRP:N	2:B:18:TRP:CD1	2.85	0.44
20:T:46:LEU:HB2	20:T:93:ILE:HG21	1.96	0.44
1:A:1128:C:O2'	1:A:1129:C:P	2.75	0.44
10:J:85:THR:H	10:J:86:LEU:HD12	1.81	0.44
2:B:47:ARG:HG2	2:B:47:ARG:HH11	1.82	0.44
11:K:2:ARG:O	11:K:3:GLN:HB2	2.17	0.44
1:A:328:C:C2'	1:A:328:C:O2	2.63	0.44
1:A:107:G:C3'	1:A:108:G:H5'	2.47	0.44
2:B:39:GLN:O	2:B:42:MET:HB2	2.17	0.44
8:H:46:LYS:HG3	8:H:64:LYS:HG2	1.99	0.44
4:D:30:CYS:O	4:D:31:ALA:HB3	2.17	0.44
19:S:14:LEU:HD23	19:S:14:LEU:H	1.82	0.44
19:S:19:LEU:HA	19:S:22:ASN:ND2	2.31	0.44
2:B:1:VAL:HG11	2:B:215:LEU:HD23	2.00	0.44
1:A:485:G:O2'	1:A:486:U:P	2.75	0.44
2:B:194:ILE:HG22	2:B:195:ILE:N	2.32	0.44
18:R:38:ARG:HD2	18:R:43:LEU:O	2.17	0.44
1:A:949:A:H2'	1:A:950:U:O4'	2.18	0.44
7:G:15:LEU:HD22	7:G:15:LEU:H	1.82	0.44
7:G:119:ILE:CD1	7:G:119:ILE:H	2.31	0.44
1:A:1241:G:H2'	1:A:1242:C:C6	2.52	0.44
13:M:28:ARG:HB3	13:M:63:TRP:CH2	2.53	0.44
11:K:66:GLY:O	11:K:67:MET:C	2.56	0.44
2:B:13:HIS:CE1	2:B:200:ASP:HB3	2.51	0.44
5:E:140:THR:O	5:E:144:VAL:HG23	2.18	0.44
15:O:52:HIS:HE1	15:O:56:LEU:HD13	1.81	0.44
1:A:76:C:O2'	1:A:77:G:H5'	2.17	0.44
1:A:1236:A:H2'	1:A:1237:C:C6	2.52	0.44
8:H:86:ILE:HG13	8:H:133:LEU:HD22	1.99	0.44
1:A:39:G:O2'	1:A:40:C:H5'	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:110:ALA:HB3	8:H:121:ASP:HB3	1.99	0.44
13:M:83:ILE:CG2	19:S:73:PHE:HE2	2.28	0.44
8:H:83:ILE:O	8:H:83:ILE:HG23	2.18	0.44
1:A:613:C:C2'	1:A:614:A:H5'	2.48	0.44
1:A:1226:C:H4'	1:A:1227:A:OP2	2.18	0.44
1:A:146:G:C3'	1:A:147:G:C5'	2.96	0.44
2:B:96:LEU:N	2:B:96:LEU:CD1	2.81	0.44
16:P:72:ARG:HG2	16:P:72:ARG:HH11	1.82	0.44
1:A:1346:A:N1	7:G:9:ARG:NH1	2.65	0.44
3:C:35:ASP:OD1	3:C:56:ILE:HD12	2.17	0.44
1:A:911:U:H2'	1:A:912:C:C6	2.52	0.44
1:A:224:C:C6	1:A:224:C:C5'	2.95	0.44
1:A:1238:A:OP2	1:A:1335:C:H1'	2.17	0.44
1:A:965:A:C2	1:A:969:A:C2	3.06	0.44
4:D:69:ILE:HG22	4:D:70:SER:N	2.32	0.44
1:A:438:G:O2'	1:A:494:U:O4	2.35	0.44
1:A:1053:G:HO2'	1:A:1199:U:H5	1.66	0.44
1:A:189(E):U:C2'	1:A:189(E):U:O2	2.66	0.44
1:A:55:A:C2'	1:A:56:U:H5'	2.47	0.44
12:L:79:VAL:CG2	12:L:96:ILE:HG23	2.48	0.44
3:C:172:VAL:N	3:C:173:PRO:CD	2.80	0.44
3:C:194:VAL:HG12	3:C:195:LEU:H	1.82	0.44
2:B:91:TRP:CZ3	2:B:170:GLU:OE2	2.71	0.44
12:L:54:VAL:O	12:L:61:GLU:HA	2.17	0.44
1:A:46:G:O2'	1:A:365:U:H1'	2.18	0.44
1:A:200:G:H2'	1:A:201:C:O4'	2.18	0.44
1:A:1027:C:H2'	1:A:1028:C:H6	1.82	0.44
1:A:1054:C:O2'	1:A:1055:A:C5'	2.46	0.44
2:B:131:ARG:C	2:B:133:LYS:H	2.20	0.44
1:A:487:A:H2'	1:A:488:C:O4'	2.18	0.44
14:N:22:ARG:HA	14:N:32:VAL:HG21	1.99	0.44
10:J:59:GLU:OE2	14:N:57:LYS:NZ	2.44	0.44
4:D:6:PRO:HG2	4:D:9:ARG:HD2	1.99	0.44
1:A:35:G:H2'	1:A:36:C:H6	1.83	0.44
2:B:27:TYR:HB2	2:B:37:ASP:HA	1.99	0.44
5:E:78:VAL:CG2	5:E:137:GLN:HE21	2.31	0.44
4:D:156:LEU:HD11	4:D:160:ASN:HD21	1.83	0.44
1:A:1479:C:H2'	1:A:1480:G:O5'	2.18	0.44
2:B:136:LEU:O	2:B:140:GLN:OE1	2.36	0.44
18:R:44:SER:O	18:R:45:GLY:C	2.56	0.44
1:A:1300:G:H1'	1:A:1301:U:H5	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:735:C:O2'	1:A:736:C:H5'	2.17	0.44
1:A:194:C:OP2	20:T:54:SER:OG	2.29	0.44
1:A:567:G:H2'	1:A:568:G:O4'	2.18	0.44
4:D:79:GLU:OE1	4:D:79:GLU:HA	2.18	0.44
1:A:1392:G:N2	1:A:1502:A:C8	2.83	0.43
2:B:52:ILE:CD1	2:B:179:ILE:HD13	2.48	0.43
12:L:75:GLU:C	12:L:77:SER:H	2.21	0.43
11:K:1:LYS:H3	11:K:1:LYS:HD2	1.81	0.43
4:D:7:VAL:O	4:D:9:ARG:N	2.48	0.43
13:M:69:LEU:O	13:M:72:GLU:N	2.51	0.43
11:K:98:ILE:O	11:K:99:VAL:HG23	2.18	0.43
8:H:91:ARG:NH1	17:Q:32:GLY:HA3	2.33	0.43
1:A:923:A:OP2	5:E:17:ALA:HB2	2.18	0.43
13:M:97:VAL:HG12	13:M:97:VAL:O	2.17	0.43
20:T:69:ALA:O	20:T:73:ARG:CG	2.66	0.43
13:M:39:ASN:HD22	13:M:40:PRO:N	2.16	0.43
9:I:42:ALA:H	9:I:73:ILE:HD13	1.83	0.43
6:F:10:LEU:HD12	6:F:59:TYR:O	2.18	0.43
1:A:273:A:H1'	17:Q:15:GLN:OE1	2.18	0.43
17:Q:67:ARG:CG	17:Q:67:ARG:O	2.63	0.43
2:B:186:SER:O	2:B:188:PRO:HD3	2.18	0.43
11:K:42:GLY:H	11:K:45:LYS:HG3	1.83	0.43
2:B:36:ILE:CD1	2:B:197:GLY:HA2	2.48	0.43
1:A:524:G:H2'	1:A:525:C:C6	2.54	0.43
6:F:52:ILE:O	6:F:53:ALA:HB3	2.18	0.43
2:B:2:LYS:O	2:B:211:ARG:NH1	2.50	0.43
3:C:67:VAL:HG12	3:C:69:VAL:HG23	2.00	0.43
10:J:47:VAL:CG1	14:N:40:ARG:HB2	2.48	0.43
6:F:22:GLU:OE2	6:F:84:ASN:HB2	2.19	0.43
10:J:13:THR:HG22	10:J:92:VAL:CG2	2.48	0.43
9:I:116:HIS:O	9:I:117:LYS:HB3	2.18	0.43
3:C:111:SER:HB3	3:C:114:LEU:HD12	1.98	0.43
1:A:234:C:H2'	1:A:235:C:C6	2.53	0.43
1:A:974:A:OP1	14:N:31:SER:HB3	2.18	0.43
3:C:146:LYS:NZ	3:C:205:GLU:HB2	2.33	0.43
8:H:104:ARG:NH2	8:H:138:TRP:CZ3	2.86	0.43
8:H:114:THR:C	8:H:116:LYS:H	2.21	0.43
1:A:490:G:O2'	1:A:491:G:H5'	2.18	0.43
15:O:87:ARG:HE	15:O:87:ARG:CA	2.31	0.43
13:M:77:ILE:HG22	13:M:81:MET:HE3	2.00	0.43
3:C:69:VAL:CG1	3:C:70:ALA:N	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1399:C:C2	1:A:1502:A:N6	2.87	0.43
10:J:47:VAL:HG12	14:N:40:ARG:HB2	2.00	0.43
3:C:14:THR:O	3:C:15:ARG:CB	2.58	0.43
1:A:1326:C:C5'	21:V:12:LYS:NZ	2.76	0.43
3:C:171:ARG:NH1	3:C:171:ARG:HB3	2.30	0.43
15:O:2:ILE:CD1	15:O:2:ILE:N	2.81	0.43
11:K:1:LYS:HD2	11:K:1:LYS:H1	1.83	0.43
1:A:813:U:OP2	1:A:904:C:H5'	2.18	0.43
7:G:153:TYR:O	7:G:154:ARG:C	2.56	0.43
15:O:68:TYR:CE1	15:O:72:GLU:HG3	2.54	0.43
1:A:189:G:H2'	1:A:189(A):C:C6	2.53	0.43
14:N:12:THR:HG22	14:N:12:THR:O	2.18	0.43
2:B:210:SER:O	2:B:213:VAL:N	2.52	0.43
5:E:76:ILE:HD13	5:E:87:LEU:HB2	1.97	0.43
11:K:38:ILE:CD1	11:K:54:ALA:N	2.82	0.43
9:I:126:LYS:H	9:I:126:LYS:HD2	1.81	0.43
4:D:69:ILE:HG22	4:D:70:SER:H	1.84	0.43
13:M:2:ARG:HA	13:M:7:GLU:O	2.19	0.43
5:E:72:ILE:HG23	5:E:138:LEU:CD1	2.49	0.43
1:A:1381:U:C2'	1:A:1381:U:O2	2.67	0.43
1:A:913:A:H2'	1:A:914:A:H1'	2.01	0.43
21:V:2:GLY:C	21:V:4:GLY:N	2.72	0.43
20:T:31:LYS:O	20:T:35:GLN:HB2	2.18	0.43
1:A:1516:G:H2'	1:A:1518:A:OP2	2.18	0.43
1:A:656:C:O2'	15:O:27:GLN:OE1	2.30	0.43
9:I:54:ALA:O	9:I:56:GLY:N	2.49	0.43
1:A:1272:G:H2'	1:A:1273:G:O4'	2.19	0.43
14:N:11:ARG:C	14:N:13:PRO:CD	2.87	0.43
3:C:7:ILE:HD12	3:C:15:ARG:CZ	2.48	0.43
2:B:13:HIS:ND1	2:B:198:ASN:ND2	2.66	0.43
16:P:72:ARG:HG2	16:P:72:ARG:NH1	2.33	0.43
3:C:78:ARG:HH21	3:C:81:GLU:HG2	1.82	0.43
1:A:234:C:H2'	1:A:235:C:H6	1.83	0.43
11:K:114:LYS:HD3	11:K:115:PHE:CE1	2.53	0.43
17:Q:82:ASP:O	17:Q:85:GLU:HB2	2.19	0.43
1:A:517:G:OP1	1:A:517:G:H8	2.02	0.43
14:N:2:ARG:O	14:N:3:LYS:C	2.57	0.43
18:R:31:GLU:CD	18:R:31:GLU:N	2.66	0.43
3:C:179:ALA:CB	3:C:181:ILE:HD11	2.49	0.43
7:G:142:ARG:O	7:G:146:ALA:CB	2.67	0.43
1:A:996:A:H5'	1:A:996:A:C8	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:598:U:H2'	1:A:599:C:C6	2.54	0.43
1:A:247:G:OP1	17:Q:98:SER:HB2	2.18	0.43
16:P:27:LYS:NZ	16:P:27:LYS:HB3	2.34	0.43
1:A:1310:G:N7	19:S:1:PRO:HG3	2.33	0.43
7:G:49:ILE:HA	7:G:124:MET:HE1	2.00	0.43
1:A:1425:U:H3	1:A:1475:G:H1	1.65	0.43
3:C:133:ILE:HD12	3:C:152:VAL:HG23	2.00	0.43
4:D:120:VAL:HG22	4:D:125:ILE:HD12	2.00	0.43
17:Q:79:GLY:O	17:Q:80:ARG:HB3	2.19	0.43
20:T:89:GLY:O	20:T:90:ALA:CB	2.67	0.43
1:A:1203:C:O2'	1:A:1204:A:H5'	2.19	0.43
1:A:374:A:C6	1:A:375:U:C4	3.07	0.43
10:J:45:PHE:CE2	14:N:36:PHE:HE2	2.36	0.43
1:A:659:U:H2'	1:A:660:G:C8	2.53	0.43
13:M:107:ARG:HD3	13:M:113:ARG:NH1	2.34	0.43
5:E:96:VAL:O	5:E:103:ARG:NH2	2.52	0.43
3:C:51:LEU:CD2	3:C:51:LEU:H	2.32	0.43
14:N:20:TYR:O	14:N:20:TYR:CD1	2.72	0.43
10:J:58:ARG:NH1	10:J:58:ARG:HG2	2.33	0.43
12:L:51:VAL:HG13	12:L:52:ALA:N	2.34	0.43
1:A:1296:C:H5"	13:M:13:ARG:HD2	2.01	0.43
4:D:125:ILE:HG22	4:D:126:THR:N	2.33	0.43
2:B:122:GLU:O	2:B:123:GLU:C	2.58	0.43
18:R:19:TYR:HA	18:R:54:THR:HG23	1.99	0.43
1:A:501:C:H1'	1:A:549:C:O2'	2.19	0.43
16:P:21:VAL:HG21	16:P:59:TRP:CD1	2.54	0.43
18:R:29:LEU:CD1	18:R:64:LEU:HD22	2.49	0.43
19:S:35:ARG:HH21	19:S:74:ALA:HB3	1.84	0.43
1:A:985:C:H2'	1:A:986:A:C8	2.53	0.43
1:A:1527:C:O2'	1:A:1528:U:H5'	2.19	0.43
8:H:49:GLU:HG2	8:H:62:TYR:HE2	1.84	0.43
2:B:131:ARG:CB	2:B:131:ARG:NH1	2.82	0.43
2:B:131:ARG:HB3	2:B:131:ARG:NH1	2.33	0.43
14:N:12:THR:N	14:N:13:PRO:CD	2.82	0.43
1:A:1060:C:N4	3:C:1:GLY:HA3	2.34	0.43
13:M:122:ALA:O	13:M:123:PRO:C	2.57	0.43
2:B:19:ASN:ND2	2:B:19:ASN:C	2.70	0.43
8:H:68:ARG:NH1	8:H:68:ARG:HG2	2.34	0.43
1:A:1486:G:H8	1:A:1486:G:H5'	1.84	0.43
7:G:71:ARG:HH12	7:G:137:LYS:HZ1	1.63	0.43
1:A:1355:G:O2'	1:A:1356:G:H5'	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:11:ARG:HD3	5:E:22:PHE:CG	2.53	0.43
9:I:47:GLU:N	9:I:48:PRO:CD	2.81	0.43
1:A:231:G:C2'	1:A:232:G:H5'	2.48	0.43
15:O:28:VAL:HG12	15:O:84:LEU:CD1	2.48	0.43
1:A:707:C:H2'	1:A:708:C:H6	1.83	0.43
10:J:10:ASP:OD1	10:J:12:LYS:N	2.48	0.43
4:D:17:LYS:CE	4:D:32:MET:HB2	2.49	0.42
1:A:1223:C:P	19:S:77:ARG:NH1	2.92	0.42
4:D:186:ARG:NH1	4:D:187:LEU:HB2	2.34	0.42
2:B:163:LYS:O	2:B:163:LYS:HD3	2.18	0.42
7:G:144:ALA:C	7:G:146:ALA:N	2.73	0.42
20:T:43:GLU:N	20:T:92:LEU:HD12	2.34	0.42
2:B:63:LEU:HD23	2:B:63:LEU:C	2.39	0.42
1:A:1001:A:H61	1:A:1002:G:H1	1.67	0.42
1:A:934:C:C4	1:A:1345:U:C5	3.07	0.42
1:A:1441:G:H4'	1:A:1442:G:C5	2.54	0.42
1:A:33:A:H2'	1:A:34:C:C6	2.54	0.42
19:S:7:GLY:O	19:S:8:VAL:C	2.57	0.42
15:O:63:ARG:HB2	15:O:63:ARG:HH11	1.83	0.42
3:C:106:GLN:CD	3:C:106:GLN:H	2.21	0.42
14:N:5:LEU:C	14:N:7:GLU:H	2.23	0.42
3:C:11:LEU:O	3:C:15:ARG:O	2.36	0.42
1:A:251:G:H4'	1:A:252:U:O5'	2.18	0.42
1:A:129(A):G:N1	1:A:189(E):U:O2'	2.40	0.42
1:A:730:G:H3'	1:A:731:G:C5'	2.49	0.42
18:R:32:THR:HG23	18:R:68:GLU:H	1.84	0.42
10:J:21:ILE:HG23	10:J:83:LEU:HD22	2.02	0.42
16:P:28:ARG:NH1	16:P:29:ASP:OD1	2.51	0.42
1:A:1394:A:C6	1:A:1501:C:H4'	2.54	0.42
15:O:26:VAL:O	15:O:29:ALA:HB3	2.19	0.42
7:G:64:ALA:HB3	7:G:123:LEU:HD23	2.01	0.42
16:P:40:ASP:HB3	16:P:48:TRP:HB2	2.01	0.42
1:A:1337:G:H5"	1:A:1338:G:OP2	2.19	0.42
8:H:13:ILE:O	8:H:17:THR:HG23	2.19	0.42
1:A:862:C:O2'	1:A:863:U:H5'	2.18	0.42
1:A:1513:A:H2'	1:A:1514:C:C6	2.54	0.42
4:D:28:PRO:O	4:D:29:LYS:CG	2.61	0.42
1:A:1126:U:C6	1:A:1280:A:N7	2.87	0.42
4:D:154:LEU:HB2	4:D:157:ILE:HG12	2.01	0.42
1:A:620:C:C6	4:D:134:LEU:HD13	2.53	0.42
15:O:30:LEU:N	15:O:30:LEU:HD12	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:4:LYS:O	18:R:5:ALA:CB	2.67	0.42
3:C:205:GLU:O	3:C:207:ILE:N	2.52	0.42
1:A:443:C:O2'	1:A:444:C:H5'	2.20	0.42
1:A:649:G:C8	1:A:649:G:H5'	2.52	0.42
14:N:7:GLU:O	14:N:9:ALA:N	2.52	0.42
1:A:1244:C:C2'	1:A:1245:A:C5'	2.82	0.42
2:B:108:ARG:HH12	2:B:112:LEU:HG	1.80	0.42
4:D:172:TRP:HB2	4:D:186:ARG:O	2.19	0.42
9:I:12:ALA:CB	9:I:66:GLY:O	2.68	0.42
1:A:162:A:C2'	1:A:163:C:H5'	2.48	0.42
1:A:1176:A:H2'	1:A:1177:G:C8	2.54	0.42
1:A:457:C:H2'	1:A:458:C:H6	1.84	0.42
5:E:133:GLU:O	5:E:137:GLN:HG3	2.19	0.42
8:H:4:ASP:OD1	8:H:85:ARG:NH1	2.52	0.42
15:O:63:ARG:HB2	15:O:63:ARG:NH1	2.34	0.42
1:A:190:U:H3	20:T:98:SER:HB2	1.84	0.42
1:A:1477:C:H2'	1:A:1478:C:C6	2.54	0.42
1:A:1019:C:H2'	1:A:1020:U:O4'	2.19	0.42
19:S:21:LEU:HD22	19:S:27:LYS:HD2	2.01	0.42
1:A:1419:G:H1	1:A:1481:U:H3	1.67	0.42
14:N:13:PRO:C	14:N:15:PHE:H	2.23	0.42
11:K:12:HIS:CD2	11:K:12:HIS:O	2.73	0.42
6:F:35:ALA:HA	6:F:67:MET:HB3	2.01	0.42
9:I:126:LYS:N	9:I:126:LYS:CD	2.81	0.42
1:A:765:G:N1	1:A:812:C:H2'	2.32	0.42
20:T:92:LEU:C	20:T:94:GLY:H	2.23	0.42
2:B:110:GLU:HA	2:B:113:GLU:OE1	2.20	0.42
2:B:47:ARG:NH1	2:B:193:TYR:HD1	2.18	0.42
17:Q:75:LEU:HD23	17:Q:76:VAL:H	1.84	0.42
1:A:162:A:H2'	1:A:163:C:H5'	2.02	0.42
19:S:35:ARG:HB2	19:S:71:GLY:CA	2.50	0.42
1:A:328:C:H4'	1:A:329:A:H5"	2.00	0.42
19:S:79:TYR:CG	19:S:80:ARG:N	2.88	0.42
9:I:27:VAL:HG21	9:I:32:PHE:HD1	1.84	0.42
4:D:169:VAL:HG22	4:D:170:GLY:H	1.85	0.42
3:C:190:THR:HB	3:C:193:GLY:O	2.20	0.42
1:A:976:G:H4'	1:A:977:A:OP1	2.19	0.42
14:N:9:ALA:O	14:N:10:LYS:C	2.58	0.42
14:N:8:LYS:C	14:N:8:LYS:CD	2.87	0.42
16:P:52:ASP:OD1	16:P:52:ASP:O	2.37	0.42
14:N:28:ARG:HH22	14:N:40:ARG:HH12	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:51:VAL:HG13	12:L:63:THR:HG23	2.02	0.42
9:I:45:ALA:HB1	9:I:76:ILE:HG22	2.02	0.42
1:A:58:C:O2'	1:A:59:A:H5'	2.20	0.42
1:A:1308:U:OP2	13:M:96:PRO:HA	2.20	0.42
7:G:113:ARG:HG2	7:G:113:ARG:NH1	2.31	0.42
3:C:187:LEU:HD11	3:C:194:VAL:HG11	2.01	0.42
1:A:1178:G:H22	1:A:1180:A:H3'	1.82	0.42
2:B:85:PRO:HG3	2:B:149:LEU:HG	2.02	0.42
1:A:1540:U:HO2'	1:A:1541:U:H6	1.65	0.42
1:A:1168:A:O2'	1:A:1169:A:P	2.77	0.42
1:A:189(K):U:H2'	1:A:189(L):G:C8	2.55	0.42
8:H:46:LYS:N	8:H:64:LYS:HG3	2.35	0.42
3:C:51:LEU:HD23	3:C:51:LEU:H	1.85	0.42
1:A:707:C:H2'	1:A:708:C:C6	2.55	0.42
1:A:1087:G:H2'	1:A:1088:G:C8	2.54	0.42
1:A:437:U:O2'	4:D:122:HIS:CD2	2.73	0.42
12:L:7:VAL:HG22	17:Q:28:HIS:CD2	2.54	0.42
1:A:1270:C:O2'	1:A:1271:G:H5'	2.20	0.42
19:S:16:GLU:O	19:S:16:GLU:HG3	2.18	0.42
19:S:40:VAL:HG22	19:S:43:MET:HE3	2.00	0.42
1:A:1189:C:H5'	1:A:1189:C:C6	2.43	0.42
1:A:1182:G:O2'	1:A:1183:A:OP2	2.33	0.42
14:N:28:ARG:HG2	14:N:39:CYS:CB	2.50	0.42
8:H:10:LEU:HD22	8:H:83:ILE:HD11	2.01	0.42
1:A:281:G:H4'	1:A:282:A:OP1	2.18	0.42
2:B:17:ARG:NH1	2:B:185:ASP:HB3	2.34	0.42
11:K:4:VAL:HG23	11:K:67:MET:HG2	2.01	0.42
4:D:145:ILE:CD1	4:D:145:ILE:N	2.80	0.42
12:L:81:ILE:HG23	12:L:94:TYR:HB3	2.02	0.42
2:B:225:GLU:HB3	2:B:226:PRO:CD	2.50	0.42
20:T:77:LEU:O	20:T:81:VAL:HG23	2.20	0.42
1:A:537:G:OP1	12:L:109:ARG:NH2	2.49	0.42
1:A:1495:U:H2'	1:A:1496:C:C6	2.54	0.42
11:K:111:PRO:HG2	11:K:116:ARG:HG2	2.01	0.42
1:A:1234:C:O2'	1:A:1235:U:H5'	2.19	0.42
1:A:103:C:P	20:T:10:ARG:HH11	2.42	0.42
20:T:23:LYS:O	20:T:27:LYS:HG3	2.20	0.42
8:H:51:VAL:HG12	8:H:52:ASP:N	2.35	0.42
1:A:1221:G:O2'	1:A:1222:G:H5'	2.19	0.42
2:B:126:LYS:HG2	2:B:129:GLN:CD	2.40	0.42
2:B:133:LYS:O	2:B:137:GLU:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1123:A:O2'	10:J:36:ILE:HD13	2.18	0.42
1:A:1256:A:H2'	3:C:26:LYS:NZ	2.35	0.42
9:I:29:GLY:O	9:I:30:GLN:C	2.58	0.42
1:A:1292:U:P	7:G:40:ARG:NH2	2.89	0.42
9:I:78:LEU:HD22	9:I:82:ARG:CD	2.50	0.42
1:A:620:C:C1'	4:D:134:LEU:HD13	2.50	0.42
1:A:1405:G:O4'	1:A:1519:A:H4'	2.19	0.42
2:B:161:PRO:CD	2:B:182:ALA:HA	2.49	0.42
1:A:913:A:H2'	1:A:914:A:O4'	2.19	0.42
1:A:961:U:H2'	1:A:962:C:H5'	2.01	0.42
1:A:41:G:H2'	1:A:42:G:H8	1.85	0.42
1:A:1082:G:C2'	1:A:1083:U:H5'	2.50	0.42
21:V:5:ASP:O	21:V:11:GLY:HA3	2.18	0.42
1:A:265:G:H2'	1:A:267:C:H5	1.84	0.42
1:A:857:C:H2'	1:A:858:G:O4'	2.20	0.42
1:A:1328:C:O2'	1:A:1329:A:H5'	2.19	0.42
8:H:82:HIS:C	8:H:82:HIS:CD2	2.93	0.42
1:A:189(E):U:H2'	1:A:189(E):U:O2	2.20	0.42
1:A:1064:G:H1'	1:A:1190:G:H21	1.85	0.42
13:M:64:LYS:HG3	13:M:68:GLU:OE2	2.20	0.42
17:Q:5:LEU:HB2	17:Q:58:ILE:HG22	2.01	0.42
6:F:45:LEU:H	6:F:45:LEU:HD22	1.85	0.42
15:O:31:LEU:O	15:O:35:ILE:HG12	2.19	0.42
11:K:24:ASP:OD1	11:K:24:ASP:C	2.58	0.42
10:J:53:LYS:HG3	10:J:54:HIS:N	2.35	0.42
5:E:78:VAL:HG22	5:E:137:GLN:HE21	1.83	0.42
20:T:69:ALA:O	20:T:73:ARG:HG3	2.20	0.42
1:A:828:A:H2'	1:A:829:G:O4'	2.20	0.42
13:M:92:ARG:HE	13:M:92:ARG:HB2	1.62	0.42
1:A:977:A:O2'	1:A:978:A:H5'	2.18	0.42
19:S:15:LEU:C	19:S:17:LYS:N	2.73	0.42
2:B:48:THR:HG21	2:B:195:ILE:HD11	2.01	0.42
3:C:7:ILE:HD12	3:C:15:ARG:NE	2.35	0.42
9:I:76:ILE:O	9:I:80:ILE:HG12	2.20	0.42
6:F:22:GLU:C	6:F:24:GLU:H	2.23	0.42
7:G:49:ILE:HA	7:G:124:MET:HE3	2.00	0.42
1:A:952:U:O4	13:M:103:ARG:HD3	2.20	0.42
7:G:19:ASP:OD1	7:G:21:LEU:HB3	2.20	0.42
3:C:178:ARG:HG2	3:C:206:VAL:HA	2.00	0.42
3:C:178:ARG:HD3	3:C:206:VAL:HG22	2.02	0.42
3:C:149:LYS:HE2	3:C:151:ILE:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:G:H1'	1:A:608:A:C2	2.54	0.42
1:A:572:A:N3	1:A:917:G:H1'	2.35	0.42
1:A:91:C:H2'	1:A:92:C:H6	1.85	0.42
9:I:96:LYS:HB2	9:I:97:PRO:HD3	2.01	0.42
3:C:16:ASP:HB3	3:C:20:ARG:HH12	1.84	0.42
1:A:958:A:C6	1:A:959:A:N1	2.88	0.41
19:S:21:LEU:CD1	19:S:30:ILE:HD11	2.50	0.41
6:F:25:ILE:N	6:F:25:ILE:HD12	2.09	0.41
1:A:967:C:H4'	9:I:127:ARG:NE	2.35	0.41
11:K:81:ARG:CD	18:R:73:LYS:HE2	2.50	0.41
12:L:52:ALA:HB2	12:L:66:ILE:HD11	2.01	0.41
1:A:255:G:O6	1:A:266:G:O6	2.38	0.41
16:P:82:GLN:O	16:P:83:GLU:C	2.58	0.41
1:A:629:G:H2'	1:A:630:G:O4'	2.20	0.41
12:L:82:ARG:NH1	12:L:82:ARG:HG3	2.32	0.41
2:B:161:PRO:HG3	2:B:182:ALA:CB	2.50	0.41
5:E:8:LEU:O	5:E:8:LEU:HD13	2.20	0.41
7:G:151:ALA:C	7:G:153:TYR:H	2.24	0.41
4:D:63:LEU:HB2	4:D:197:VAL:HG11	2.01	0.41
16:P:67:THR:HG22	16:P:68:ASP:N	2.35	0.41
9:I:31:ASP:O	9:I:32:PHE:C	2.58	0.41
1:A:1303:C:N4	1:A:1304:G:C6	2.88	0.41
1:A:274:A:H4'	1:A:275:G:OP2	2.20	0.41
3:C:59:ALA:HB3	3:C:62:ASN:HD22	1.85	0.41
1:A:977:A:H8	1:A:982:U:O4	2.03	0.41
15:O:86:ILE:CG2	15:O:87:ARG:N	2.64	0.41
1:A:1145:C:H4'	1:A:1146:A:O5'	2.20	0.41
6:F:22:GLU:C	6:F:24:GLU:N	2.73	0.41
6:F:4:TYR:HD1	6:F:92:LYS:HA	1.85	0.41
2:B:15:ARG:HH11	2:B:17:ARG:CG	2.33	0.41
10:J:13:THR:O	10:J:15:ASP:N	2.53	0.41
4:D:110:ALA:HB3	4:D:116:ALA:HB2	2.01	0.41
5:E:94:THR:HG22	5:E:97:ILE:HD13	2.02	0.41
4:D:7:VAL:C	4:D:9:ARG:N	2.70	0.41
12:L:82:ARG:HD3	12:L:97:VAL:HG22	2.02	0.41
10:J:85:THR:N	10:J:86:LEU:HD12	2.35	0.41
17:Q:39:LYS:HG3	17:Q:40:LYS:N	2.34	0.41
5:E:145:GLU:O	5:E:149:LYS:HG3	2.21	0.41
1:A:568:G:O2'	1:A:574:A:N1	2.52	0.41
1:A:665:A:N3	1:A:732:C:H2'	2.35	0.41
13:M:74:ALA:O	13:M:78:LYS:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:135:LYS:C	7:G:135:LYS:HD2	2.40	0.41
2:B:53:GLU:CB	2:B:215:LEU:HD11	2.48	0.41
16:P:52:ASP:OD1	16:P:52:ASP:C	2.58	0.41
2:B:52:ILE:HD11	2:B:179:ILE:HG21	2.02	0.41
2:B:10:HIS:HB2	2:B:11:PHE:H	1.52	0.41
13:M:5:GLY:O	13:M:7:GLU:HG2	2.20	0.41
1:A:998:G:H2'	1:A:999:C:H5"	2.03	0.41
2:B:91:TRP:HZ3	2:B:170:GLU:OE2	2.03	0.41
20:T:88:ALA:O	20:T:89:GLY:C	2.58	0.41
1:A:1470:G:O2'	1:A:1471:G:H5'	2.21	0.41
17:Q:32:GLY:O	17:Q:33:LYS:C	2.58	0.41
1:A:563:A:H2'	1:A:567:G:C8	2.55	0.41
1:A:1020:U:O2'	1:A:1021:G:H5'	2.20	0.41
6:F:13:ASN:O	6:F:14:LEU:HD23	2.20	0.41
1:A:1009:G:O2'	1:A:1010:G:H5'	2.20	0.41
1:A:1145:C:O2'	1:A:1146:A:P	2.79	0.41
1:A:1217:C:H2'	1:A:1218:C:O4'	2.21	0.41
2:B:210:SER:OG	2:B:211:ARG:N	2.53	0.41
7:G:50:GLN:O	7:G:53:THR:O	2.38	0.41
7:G:49:ILE:O	7:G:53:THR:HB	2.20	0.41
5:E:88:LYS:O	5:E:114:ILE:HD13	2.21	0.41
17:Q:77:GLU:HG3	17:Q:77:GLU:O	2.20	0.41
1:A:1044:A:H2'	1:A:1045:C:C5'	2.50	0.41
1:A:456:C:H2'	1:A:457:C:C6	2.55	0.41
1:A:116:A:H8	1:A:116:A:O5'	2.03	0.41
1:A:769:G:H4'	1:A:1513:A:H4'	2.02	0.41
9:I:99:GLY:C	9:I:101:LEU:N	2.73	0.41
1:A:686:U:O4	1:A:703:G:H1'	2.20	0.41
1:A:1221:G:O3'	19:S:76:THR:HG21	2.21	0.41
1:A:1123:A:O3'	10:J:34:GLY:HA3	2.20	0.41
15:O:38:LEU:HD13	15:O:38:LEU:O	2.20	0.41
2:B:229:SER:C	2:B:231:ALA:H	2.24	0.41
1:A:1474:G:C2'	1:A:1475:G:C5'	2.94	0.41
1:A:731:G:H5'	1:A:766:A:H4'	2.03	0.41
1:A:1494:G:OP1	26:A:2733:3TS:NAC	2.51	0.41
26:A:2733:3TS:OAX	26:A:2733:3TS:H4'	2.21	0.41
2:B:158:VAL:HG11	2:B:161:PRO:HA	2.02	0.41
17:Q:68:LYS:C	17:Q:69:ARG:HD2	2.40	0.41
7:G:22:VAL:HG12	7:G:26:ILE:CD1	2.51	0.41
1:A:473:G:C2'	1:A:474:G:H5'	2.51	0.41
3:C:119:VAL:O	3:C:123:ILE:HG13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:176:ILE:O	2:B:177:PRO:C	2.58	0.41
13:M:83:ILE:CG2	19:S:65:MET:HB3	2.51	0.41
14:N:4:ALA:O	14:N:7:GLU:CG	2.69	0.41
1:A:1113:C:H6	1:A:1113:C:O5'	2.03	0.41
2:B:76:ARG:O	2:B:80:GLU:HG3	2.21	0.41
13:M:32:ALA:HA	13:M:58:TYR:CE2	2.55	0.41
18:R:68:GLU:OE1	18:R:68:GLU:HA	2.21	0.41
11:K:60:LYS:O	11:K:61:LYS:C	2.59	0.41
1:A:663:A:H5'	1:A:836:G:OP2	2.19	0.41
4:D:130:ARG:NH1	4:D:130:ARG:HG3	2.35	0.41
7:G:92:PRO:HA	7:G:95:GLN:HE21	1.84	0.41
1:A:642:A:C6	1:A:643:C:C4	3.08	0.41
1:A:491:G:O2'	1:A:492:G:H5'	2.19	0.41
19:S:62:THR:H	19:S:65:MET:CG	2.34	0.41
11:K:38:ILE:HD11	11:K:54:ALA:CA	2.51	0.41
13:M:47:LEU:HB3	13:M:52:VAL:HG23	2.01	0.41
10:J:6:LEU:O	10:J:67:ASN:HA	2.21	0.41
9:I:80:ILE:O	9:I:84:LEU:HB2	2.21	0.41
4:D:186:ARG:HH22	4:D:187:LEU:CG	2.33	0.41
1:A:953:G:C1'	13:M:124:ARG:HA	2.48	0.41
3:C:10:ARG:NH1	3:C:176:THR:O	2.54	0.41
5:E:72:ILE:HD12	5:E:138:LEU:CD1	2.51	0.41
7:G:43:TYR:O	7:G:46:CYS:N	2.54	0.41
4:D:198:ASN:C	4:D:198:ASN:ND2	2.71	0.41
8:H:12:ARG:NH1	8:H:27:PRO:HD3	2.36	0.41
1:A:801:U:O2'	1:A:802:A:H5'	2.21	0.41
18:R:1:PRO:HG2	18:R:2:SER:H	1.86	0.41
1:A:832:C:O2'	1:A:833:U:H5'	2.21	0.41
1:A:933:G:OP1	7:G:2:ARG:HB3	2.20	0.41
13:M:109:ARG:CG	13:M:109:ARG:HH11	2.34	0.41
3:C:153:SER:HB3	3:C:196:GLY:H	1.84	0.41
2:B:81:ARG:O	2:B:82:ALA:CB	2.67	0.41
4:D:161:LEU:HD13	4:D:180:MET:CE	2.51	0.41
1:A:1491:G:H5"	12:L:42:LYS:HB3	2.01	0.41
1:A:1409:C:O2'	1:A:1410:G:H5'	2.21	0.41
1:A:168:G:O2'	1:A:169:C:H5'	2.21	0.41
3:C:142:GLU:C	3:C:144:GLY:H	2.23	0.41
1:A:811:C:O2'	1:A:901:A:N1	2.48	0.41
9:I:3:TYR:CD1	9:I:3:TYR:N	2.89	0.41
4:D:34:ARG:N	4:D:34:ARG:CD	2.83	0.41
10:J:55:LYS:C	10:J:55:LYS:HD2	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:41:PRO:C	19:S:43:MET:N	2.74	0.41
1:A:1479:C:O2	1:A:1479:C:C2'	2.69	0.41
7:G:78:ARG:HH11	7:G:78:ARG:CB	2.11	0.41
1:A:1502:A:C2	1:A:1504:G:C2	3.09	0.41
16:P:19:ILE:HG22	16:P:36:ILE:HG13	2.03	0.41
1:A:1113:C:H4'	3:C:13:ILE:HD11	2.02	0.41
6:F:67:MET:CE	6:F:72:VAL:HG22	2.51	0.41
6:F:92:LYS:HE3	6:F:92:LYS:HB2	1.86	0.41
6:F:4:TYR:CE2	6:F:72:VAL:HG21	2.56	0.41
1:A:1226:C:N4	13:M:103:ARG:HG3	2.35	0.41
2:B:19:ASN:HD22	2:B:20:PRO:N	2.19	0.41
6:F:101:ALA:HA	18:R:13:GLU:CD	2.41	0.41
1:A:1307:U:H2'	1:A:1308:U:C6	2.56	0.41
10:J:78:LYS:HG3	10:J:78:LYS:O	2.21	0.41
1:A:812:C:OP2	1:A:903:G:H1'	2.21	0.41
20:T:92:LEU:C	20:T:94:GLY:N	2.74	0.41
15:O:69:LEU:HD23	15:O:69:LEU:HA	1.90	0.41
5:E:140:THR:O	5:E:141:LYS:C	2.58	0.41
6:F:33:TYR:HB2	6:F:75:LEU:HD23	2.03	0.41
1:A:1316:G:H4'	14:N:17:VAL:HG11	2.03	0.41
1:A:191:G:O2'	1:A:192:U:H5'	2.21	0.41
2:B:54:ASP:OD1	2:B:58:ARG:NH2	2.54	0.41
1:A:32:A:H2'	1:A:33:A:C8	2.56	0.41
1:A:685:G:C2	1:A:686:U:C4	3.09	0.41
13:M:18:LEU:O	13:M:21:ILE:HG13	2.21	0.41
20:T:9:HIS:CE1	20:T:13:LEU:HD11	2.56	0.41
18:R:6:LYS:O	18:R:9:ALA:HB3	2.19	0.41
18:R:24:VAL:O	18:R:27:ARG:HB2	2.21	0.41
1:A:724:G:O2'	1:A:725:G:H5'	2.21	0.41
16:P:8:ARG:HH11	16:P:8:ARG:HG2	1.86	0.41
15:O:44:VAL:O	15:O:45:HIS:C	2.59	0.41
2:B:11:PHE:O	2:B:12:GLY:C	2.59	0.41
1:A:1475:G:H5'	1:A:1475:G:H8	1.85	0.41
3:C:133:ILE:HG21	3:C:166:TRP:O	2.21	0.41
7:G:16:VAL:HG12	7:G:17:TYR:CD1	2.55	0.41
18:R:40:ARG:HB3	18:R:40:ARG:CZ	2.51	0.41
1:A:502:G:H2'	1:A:503:C:C6	2.56	0.41
6:F:38:GLU:O	6:F:39:LYS:CB	2.69	0.41
1:A:1160:G:O2'	1:A:1161:C:H5'	2.21	0.41
1:A:1320:C:N3	19:S:35:ARG:HG3	2.36	0.41
1:A:1088:G:O5'	1:A:1088:G:H8	2.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:222:GLY:O	2:B:223:VAL:C	2.58	0.41
7:G:38:ALA:O	7:G:39:ALA:C	2.59	0.41
1:A:559:A:P	5:E:122:ARG:HH22	2.44	0.41
2:B:116:PHE:CZ	2:B:133:LYS:HG2	2.56	0.40
14:N:7:GLU:O	14:N:8:LYS:C	2.59	0.40
6:F:10:LEU:HD11	6:F:59:TYR:HD2	1.85	0.40
10:J:29:GLY:CA	10:J:76:ASN:ND2	2.84	0.40
1:A:1300:G:C2'	1:A:1301:U:OP2	2.69	0.40
1:A:1286:A:C3'	1:A:1286:A:C8	3.05	0.40
1:A:836:G:C6	1:A:851:G:C6	3.09	0.40
17:Q:21:LEU:HD13	17:Q:40:LYS:HG2	2.02	0.40
1:A:1366:C:O2'	1:A:1367:C:H5'	2.21	0.40
17:Q:14:MET:HB2	17:Q:17:THR:HB	2.03	0.40
1:A:1469:G:O2'	1:A:1470:G:H5'	2.20	0.40
12:L:69:GLU:HA	12:L:69:GLU:OE1	2.20	0.40
16:P:67:THR:CG2	16:P:68:ASP:N	2.84	0.40
1:A:437:U:O2'	4:D:122:HIS:HD2	2.04	0.40
9:I:113:TYR:CE1	10:J:57:SER:O	2.74	0.40
1:A:399:G:H2'	1:A:400:C:C6	2.57	0.40
1:A:976:G:N7	1:A:1358:U:N3	2.69	0.40
1:A:1272:G:O2'	1:A:1273:G:H5'	2.21	0.40
1:A:1053:G:H4'	1:A:1054:C:H5'	2.02	0.40
3:C:106:GLN:O	3:C:107:ASN:HB3	2.20	0.40
1:A:1309:G:C2'	1:A:1310:G:H5"	2.51	0.40
3:C:25:LYS:HZ2	3:C:25:LYS:H	1.62	0.40
2:B:191:VAL:CB	2:B:194:ILE:HG13	2.51	0.40
2:B:6:GLU:OE1	2:B:9:VAL:HG21	2.21	0.40
1:A:279:A:H4'	1:A:281:G:C8	2.56	0.40
4:D:154:LEU:O	4:D:155:GLU:C	2.59	0.40
1:A:182:U:O4	1:A:183:G:N3	2.53	0.40
1:A:909:A:H2'	1:A:910:C:O4'	2.21	0.40
1:A:84:U:H2'	1:A:88:A:O4'	2.21	0.40
1:A:1124:G:O2'	1:A:1145:C:N4	2.54	0.40
1:A:1182:G:C4'	1:A:1183:A:H5'	2.40	0.40
18:R:43:LEU:HD11	18:R:51:LEU:HD22	2.02	0.40
1:A:229:U:O2'	1:A:230:G:H5'	2.22	0.40
8:H:90:GLY:O	8:H:91:ARG:CB	2.69	0.40
8:H:4:ASP:CG	8:H:85:ARG:HH11	2.23	0.40
8:H:86:ILE:HG12	8:H:135:CYS:HA	2.02	0.40
14:N:7:GLU:OE1	14:N:8:LYS:N	2.54	0.40
5:E:75:GLU:HA	5:E:87:LEU:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:81:ARG:HD3	18:R:73:LYS:HE2	2.03	0.40
1:A:403:C:OP2	4:D:135:PRO:HD2	2.21	0.40
2:B:11:PHE:CD1	2:B:11:PHE:C	2.95	0.40
1:A:952:U:O2'	1:A:953:G:H5'	2.21	0.40
1:A:998:G:H2'	1:A:999:C:C5'	2.51	0.40
6:F:94:GLN:HB3	18:R:17:ARG:NH1	2.36	0.40
1:A:764:C:H2'	1:A:765:G:O4'	2.22	0.40
20:T:87:ALA:O	20:T:88:ALA:CB	2.68	0.40
11:K:17:ASN:ND2	11:K:45:LYS:CD	2.83	0.40
7:G:64:ALA:HB1	7:G:126:ALA:HB3	2.03	0.40
20:T:37:ALA:HB2	20:T:81:VAL:HG13	2.03	0.40
15:O:35:ILE:HD11	15:O:58:MET:CB	2.50	0.40
15:O:35:ILE:HD11	15:O:58:MET:HB2	2.03	0.40
1:A:16:A:N1	1:A:919:A:H2	2.18	0.40
13:M:66:GLU:CG	13:M:67:GLY:H	2.19	0.40
19:S:41:PRO:HA	19:S:44:VAL:HG23	2.03	0.40
1:A:485:G:O2'	1:A:486:U:C6	2.73	0.40
7:G:49:ILE:CG2	7:G:60:VAL:HG21	2.52	0.40
1:A:953:G:H1'	13:M:124:ARG:CA	2.49	0.40
1:A:1128:C:O2'	1:A:1129:C:OP1	2.40	0.40
7:G:142:ARG:O	7:G:146:ALA:HB2	2.21	0.40
1:A:1135:U:O2	1:A:1135:U:C2'	2.67	0.40
2:B:91:TRP:HZ2	2:B:96:LEU:CD1	2.33	0.40
16:P:28:ARG:HG2	16:P:28:ARG:NH1	2.34	0.40
7:G:119:ILE:N	7:G:119:ILE:CD1	2.85	0.40
11:K:72:VAL:HB	11:K:98:ILE:HA	2.04	0.40
4:D:24:ARG:C	4:D:26:TYR:H	2.25	0.40
1:A:186:C:H2'	1:A:187:C:C6	2.57	0.40
4:D:14:GLU:O	4:D:16:VAL:HG23	2.21	0.40
3:C:94:THR:HG23	3:C:94:THR:O	2.22	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	233/256 (91%)	168 (72%)	40 (17%)	25 (11%)	0 2
3	C	205/239 (86%)	139 (68%)	48 (23%)	18 (9%)	1 4
4	D	206/208 (99%)	167 (81%)	29 (14%)	10 (5%)	3 16
5	E	149/161 (92%)	141 (95%)	5 (3%)	3 (2%)	9 41
6	F	99/101 (98%)	83 (84%)	15 (15%)	1 (1%)	19 61
7	G	153/155 (99%)	115 (75%)	31 (20%)	7 (5%)	3 18
8	H	136/138 (99%)	120 (88%)	15 (11%)	1 (1%)	26 70
9	I	125/128 (98%)	95 (76%)	14 (11%)	16 (13%)	0 1
10	J	97/104 (93%)	67 (69%)	14 (14%)	16 (16%)	0 1
11	K	117/129 (91%)	91 (78%)	19 (16%)	7 (6%)	2 11
12	L	123/132 (93%)	98 (80%)	17 (14%)	8 (6%)	1 8
13	M	123/126 (98%)	88 (72%)	20 (16%)	15 (12%)	0 2
14	N	58/60 (97%)	40 (69%)	13 (22%)	5 (9%)	1 4
15	O	86/88 (98%)	72 (84%)	13 (15%)	1 (1%)	16 56
16	P	82/88 (93%)	73 (89%)	7 (8%)	2 (2%)	7 35
17	Q	102/104 (98%)	86 (84%)	10 (10%)	6 (6%)	2 11
18	R	71/88 (81%)	62 (87%)	7 (10%)	2 (3%)	6 30
19	S	79/92 (86%)	53 (67%)	20 (25%)	6 (8%)	1 6
20	T	97/106 (92%)	74 (76%)	15 (16%)	8 (8%)	1 5
21	V	23/26 (88%)	19 (83%)	3 (13%)	1 (4%)	3 19
All	All	2364/2529 (94%)	1851 (78%)	355 (15%)	158 (7%)	1 8

All (158) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	12	GLY
2	B	18	TRP
2	B	117	ALA
3	C	14	THR
3	C	15	ARG
3	C	100	LEU
3	C	153	SER
4	D	28	PRO

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Mol	Chain	Res	Type
4	D	35	ARG
4	D	174	SER
7	G	6	ALA
7	G	32	ASP
8	H	91	ARG
9	I	10	LYS
9	I	22	ASN
9	I	30	GLN
9	I	42	ALA
9	I	57	ARG
9	I	117	LYS
9	I	126	LYS
10	J	32	VAL
10	J	52	PHE
10	J	88	LEU
12	L	23	LEU
12	L	76	HIS
13	M	3	ILE
13	M	22	TYR
13	M	66	GLU
14	N	21	THR
16	P	83	GLU
17	Q	79	GLY
17	Q	80	ARG
19	S	5	LYS
19	S	8	VAL
2	B	3	GLU
2	B	5	LEU
2	B	9	VAL
2	B	11	PHE
2	B	14	GLU
2	B	82	ALA
2	B	223	VAL
3	C	75	VAL
3	C	87	ARG
3	C	145	ALA
3	C	155	ARG
3	C	206	VAL
4	D	29	LYS
4	D	89	GLY
5	E	149	LYS
6	F	39	LYS

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Mol	Chain	Res	Type
7	G	66	GLU
9	I	54	ALA
9	I	118	ALA
10	J	28	SER
10	J	70	VAL
11	K	118	ALA
12	L	24	LYS
12	L	25	GLY
13	M	5	GLY
13	M	23	GLY
13	M	35	LYS
13	M	105	ASN
13	M	123	PRO
15	O	86	ILE
17	Q	11	SER
18	R	72	ARG
19	S	42	GLU
19	S	80	ARG
20	T	89	GLY
20	T	92	LEU
20	T	95	GLY
21	V	3	LYS
2	B	17	ARG
2	B	70	GLN
2	B	71	ALA
3	C	46	LEU
3	C	180	ASN
4	D	30	CYS
9	I	41	ARG
10	J	37	PRO
10	J	53	LYS
10	J	58	ARG
11	K	2	ARG
11	K	3	GLN
11	K	79	ALA
13	M	4	ALA
13	M	37	GLY
14	N	8	LYS
17	Q	52	LEU
17	Q	103	LYS
19	S	4	LEU
20	T	87	ALA

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Mol	Chain	Res	Type
20	T	91	PRO
2	B	4	LEU
2	B	15	ARG
2	B	57	MET
2	B	77	MET
2	B	123	GLU
3	C	21	TRP
3	C	60	ALA
3	C	80	GLY
5	E	18	GLY
7	G	65	VAL
9	I	23	GLY
9	I	43	VAL
10	J	34	GLY
10	J	38	LEU
10	J	55	LYS
10	J	71	ASP
11	K	80	GLY
11	K	108	GLY
13	M	31	GLU
16	P	27	LYS
18	R	5	ALA
19	S	23	ALA
20	T	4	SER
2	B	2	LYS
2	B	124	ARG
2	B	149	LEU
3	C	3	LYS
3	C	99	ALA
4	D	4	ILE
4	D	8	CYS
4	D	196	PRO
7	G	61	PHE
7	G	148	ARG
9	I	40	VAL
10	J	25	ALA
10	J	39	PRO
10	J	75	PRO
12	L	26	ALA
12	L	47	ALA
12	L	117	GLY
13	M	11	ASN

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Mol	Chain	Res	Type
13	M	67	GLY
14	N	55	VAL
20	T	90	ALA
3	C	107	ASN
7	G	89	GLU
9	I	99	GLY
10	J	14	LEU
11	K	25	PRO
12	L	75	GLU
13	M	121	LYS
14	N	22	ARG
20	T	2	ASN
2	B	177	PRO
3	C	102	VAL
13	M	6	VAL
2	B	221	GLY
2	B	226	PRO
4	D	87	VAL
9	I	108	VAL
5	E	150	GLY
9	I	52	VAL
17	Q	63	PRO
2	B	159	VAL
14	N	17	VAL

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	202/220 (92%)	184 (91%)	18 (9%)	12 42
3	C	160/188 (85%)	148 (92%)	12 (8%)	17 51
4	D	180/180 (100%)	166 (92%)	14 (8%)	16 49
5	E	115/122 (94%)	105 (91%)	10 (9%)	13 43
6	F	90/90 (100%)	86 (96%)	4 (4%)	35 74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
7	G	126/126 (100%)	121 (96%)	5 (4%)	38 77
8	H	119/119 (100%)	113 (95%)	6 (5%)	30 70
9	I	98/99 (99%)	88 (90%)	10 (10%)	9 33
10	J	88/91 (97%)	81 (92%)	7 (8%)	15 47
11	K	90/99 (91%)	83 (92%)	7 (8%)	16 49
12	L	104/109 (95%)	99 (95%)	5 (5%)	31 71
13	M	100/101 (99%)	84 (84%)	16 (16%)	3 15
14	N	49/49 (100%)	44 (90%)	5 (10%)	9 33
15	O	78/79 (99%)	74 (95%)	4 (5%)	29 69
16	P	72/74 (97%)	66 (92%)	6 (8%)	14 46
17	Q	96/96 (100%)	88 (92%)	8 (8%)	14 46
18	R	64/77 (83%)	63 (98%)	1 (2%)	70 92
19	S	71/79 (90%)	66 (93%)	5 (7%)	19 55
20	T	76/82 (93%)	64 (84%)	12 (16%)	3 15
21	V	19/21 (90%)	19 (100%)	0	100 100
All	All	1997/2101 (95%)	1842 (92%)	155 (8%)	16 49

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

Mol	Chain	Res	Type
2	B	2	LYS
2	B	10	HIS
2	B	17	ARG
2	B	18	TRP
2	B	19	ASN
2	B	76	ARG
2	B	86	TYR
2	B	91	TRP
2	B	138	ARG
2	B	151	ARG
2	B	162	THR
2	B	164	GLU
2	B	172	ARG
2	B	179	ILE
2	B	181	LEU
2	B	194	ILE
2	B	218	GLN

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Mol	Chain	Res	Type
2	B	230	TYR
3	C	2	ASN
3	C	25	LYS
3	C	33	LEU
3	C	51	LEU
3	C	84	ARG
3	C	103	GLN
3	C	106	GLN
3	C	126	ARG
3	C	155	ARG
3	C	189	ARG
3	C	191	THR
3	C	195	LEU
4	D	7	VAL
4	D	8	CYS
4	D	28	PRO
4	D	35	ARG
4	D	60	LYS
4	D	121	ARG
4	D	126	THR
4	D	155	GLU
4	D	161	LEU
4	D	186	ARG
4	D	190	ARG
4	D	192	ASP
4	D	195	LEU
4	D	198	ASN
5	E	8	LEU
5	E	12	THR
5	E	30	VAL
5	E	37	VAL
5	E	39	LEU
5	E	62	MET
5	E	69	ASN
5	E	76	ILE
5	E	114	ILE
5	E	140	THR
6	F	10	LEU
6	F	25	ILE
6	F	47	ARG
6	F	100	ASN
7	G	7	GLU

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Mol	Chain	Res	Type
7	G	10	GLN
7	G	34	LYS
7	G	135	LYS
7	G	139	ASP
8	H	2	LEU
8	H	26	VAL
8	H	63	LEU
8	H	84	ARG
8	H	85	ARG
8	H	105	ARG
9	I	15	ARG
9	I	22	ASN
9	I	24	LYS
9	I	28	ASN
9	I	37	GLN
9	I	55	LEU
9	I	78	LEU
9	I	90	ASP
9	I	98	LEU
9	I	126	LYS
10	J	4	ILE
10	J	43	ARG
10	J	55	LYS
10	J	63	LEU
10	J	71	ASP
10	J	81	GLU
10	J	96	ILE
11	K	8	ARG
11	K	19	ILE
11	K	25	PRO
11	K	44	ARG
11	K	82	GLU
11	K	83	GLN
11	K	106	HIS
12	L	38	THR
12	L	42	LYS
12	L	49	ARG
12	L	108	ASP
12	L	122	LYS
13	M	11	ASN
13	M	13	ARG
13	M	39	ASN

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Mol	Chain	Res	Type
13	M	42	THR
13	M	43	ARG
13	M	55	LEU
13	M	79	ARG
13	M	80	LEU
13	M	83	ILE
13	M	101	ARG
13	M	105	ASN
13	M	109	ARG
13	M	114	LYS
13	M	116	VAL
13	M	123	PRO
13	M	124	ARG
14	N	2	ARG
14	N	7	GLU
14	N	21	THR
14	N	30	ARG
14	N	43	LEU
15	O	5	GLU
15	O	33	LEU
15	O	69	LEU
15	O	80	LEU
16	P	1	MET
16	P	2	VAL
16	P	4	ILE
16	P	42	ARG
16	P	52	ASP
16	P	72	ARG
17	Q	33	LYS
17	Q	37	ARG
17	Q	58	ILE
17	Q	69	ARG
17	Q	73	LEU
17	Q	75	LEU
17	Q	91	ARG
17	Q	95	GLN
18	R	13	GLU
19	S	6	LYS
19	S	12	ASP
19	S	19	LEU
19	S	35	ARG
19	S	61	ILE

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Mol	Chain	Res	Type
20	T	2	ASN
20	T	6	LEU
20	T	18	ARG
20	T	24	SER
20	T	35	GLN
20	T	50	ARG
20	T	61	LYS
20	T	66	HIS
20	T	67	LYS
20	T	73	ARG
20	T	82	ARG
20	T	86	GLU

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

Mol	Chain	Res	Type
2	B	19	ASN
2	B	72	GLN
2	B	88	ASN
2	B	129	GLN
2	B	206	GLN
3	C	2	ASN
3	C	5	HIS
3	C	27	GLN
3	C	30	HIS
3	C	62	ASN
3	C	103	GLN
3	C	106	GLN
3	C	107	ASN
3	C	109	ASN
3	C	117	GLN
3	C	122	GLN
3	C	138	GLN
3	C	175	HIS
4	D	41	GLN
4	D	61	GLN
4	D	73	GLN
4	D	115	GLN
4	D	122	HIS
4	D	159	GLN
4	D	160	ASN
4	D	198	ASN

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Mol	Chain	Res	Type
5	E	69	ASN
5	E	74	HIS
5	E	123	ASN
5	E	137	GLN
6	F	18	GLN
6	F	27	GLN
6	F	32	ASN
6	F	73	ASN
6	F	94	GLN
6	F	100	ASN
7	G	36	ASN
7	G	55	GLN
7	G	63	GLN
7	G	67	ASN
7	G	95	GLN
7	G	105	GLN
9	I	22	ASN
9	I	72	GLN
10	J	54	HIS
10	J	60	HIS
10	J	76	ASN
10	J	82	GLN
11	K	12	HIS
11	K	52	GLN
11	K	83	GLN
12	L	45	ASN
12	L	71	HIS
13	M	39	ASN
13	M	61	ASN
15	O	12	GLN
15	O	36	ASN
15	O	45	HIS
16	P	76	GLN
17	Q	15	GLN
19	S	22	ASN
19	S	52	ASN
20	T	2	ASN
20	T	9	HIS

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1510/1521 (99%)	272 (18%)	58 (3%)
22	W	3/6 (50%)	0	0
23	Z	14/16 (87%)	2 (14%)	0
All	All	1527/1543 (98%)	274 (17%)	58 (3%)

All (274) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	G
1	A	8	A
1	A	9	G
1	A	32	A
1	A	39	G
1	A	47	C
1	A	48	C
1	A	51	A
1	A	52	G
1	A	60	A
1	A	61	G
1	A	65	U
1	A	69	G
1	A	105	G
1	A	121	C
1	A	131	C
1	A	144	G
1	A	146	G
1	A	147	G
1	A	156	G
1	A	157	G
1	A	173	U
1	A	174	C
1	A	189(E)	U
1	A	189(F)	U
1	A	189(G)	G
1	A	189(H)	G
1	A	195	A
1	A	196	A
1	A	197	A
1	A	202	U
1	A	203	U
1	A	204	U
1	A	216	G
1	A	224	C

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Mol	Chain	Res	Type
1	A	244	U
1	A	247	G
1	A	251	G
1	A	257	G
1	A	258	G
1	A	266	G
1	A	267	C
1	A	272	C
1	A	281	G
1	A	282	A
1	A	289	G
1	A	292	G
1	A	293	G
1	A	305	G
1	A	306	G
1	A	321	A
1	A	328	C
1	A	329	A
1	A	332	G
1	A	345	C
1	A	351	G
1	A	352	C
1	A	353	A
1	A	354	G
1	A	357	G
1	A	367	U
1	A	369	C
1	A	373	A
1	A	381	C
1	A	388	G
1	A	389	A
1	A	397	A
1	A	406	G
1	A	413	G
1	A	414	A
1	A	421	U
1	A	422	C
1	A	423	G
1	A	426	G
1	A	429	U
1	A	430	A
1	A	453	A

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Mol	Chain	Res	Type
1	A	461	A
1	A	481	G
1	A	484	G
1	A	485	G
1	A	486	U
1	A	487	A
1	A	488	C
1	A	496	A
1	A	498	U
1	A	511	C
1	A	517	G
1	A	518	C
1	A	531	U
1	A	532	A
1	A	545	C
1	A	547	A
1	A	548	G
1	A	561	U
1	A	562	C
1	A	564	C
1	A	572	A
1	A	573	A
1	A	576	G
1	A	577	G
1	A	591	U
1	A	596	C
1	A	607	A
1	A	625	G
1	A	631	G
1	A	632	A
1	A	649	G
1	A	653	A
1	A	654	G
1	A	665	A
1	A	687	A
1	A	688	G
1	A	721	G
1	A	723	U
1	A	731	G
1	A	734	G
1	A	751	U
1	A	755	G

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Mol	Chain	Res	Type
1	A	777	A
1	A	793	U
1	A	794	A
1	A	813	U
1	A	817	C
1	A	819	A
1	A	836	G
1	A	840	C
1	A	848	C
1	A	859	A
1	A	865	A
1	A	870	U
1	A	872	A
1	A	873	A
1	A	874	G
1	A	885	G
1	A	896	C
1	A	913	A
1	A	914	A
1	A	926	G
1	A	927	G
1	A	934	C
1	A	935	A
1	A	951	G
1	A	960	U
1	A	968	A
1	A	969	A
1	A	971	G
1	A	974	A
1	A	975	A
1	A	976	G
1	A	977	A
1	A	978	A
1	A	982	U
1	A	983	A
1	A	992	U
1	A	993	G
1	A	996	A
1	A	998	G
1	A	999	C
1	A	1001(A)	G
1	A	1003	G

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Mol	Chain	Res	Type
1	A	1004	A
1	A	1007	C
1	A	1009	G
1	A	1012	U
1	A	1013	G
1	A	1025	U
1	A	1026	G
1	A	1030	C
1	A	1045	C
1	A	1048	G
1	A	1049	U
1	A	1053	G
1	A	1054	C
1	A	1055	A
1	A	1065	U
1	A	1068	G
1	A	1081	G
1	A	1085	U
1	A	1086	U
1	A	1094	G
1	A	1095	U
1	A	1099	G
1	A	1101	A
1	A	1102	A
1	A	1106	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	1135	U
1	A	1136	U
1	A	1137	C
1	A	1138	G
1	A	1139	G
1	A	1141	C
1	A	1144	G
1	A	1146	A
1	A	1159	U
1	A	1169	A

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Mol	Chain	Res	Type
1	A	1179	A
1	A	1183	A
1	A	1184	G
1	A	1189	C
1	A	1190	G
1	A	1196	U
1	A	1197	G
1	A	1202	G
1	A	1212	U
1	A	1213	A
1	A	1214	C
1	A	1215	G
1	A	1227	A
1	A	1238	A
1	A	1240	U
1	A	1241	G
1	A	1245	A
1	A	1250	A
1	A	1253	G
1	A	1256	A
1	A	1257	U
1	A	1260	C
1	A	1272	G
1	A	1277	C
1	A	1279	A
1	A	1280	A
1	A	1282	C
1	A	1287	A
1	A	1297	C
1	A	1299	A
1	A	1300	G
1	A	1301	U
1	A	1302	U
1	A	1310	G
1	A	1320	C
1	A	1324	A
1	A	1330	U
1	A	1331	G
1	A	1335	C
1	A	1336	C
1	A	1338	G
1	A	1346	A

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Mol	Chain	Res	Type
1	A	1347	G
1	A	1363(A)	A
1	A	1365	G
1	A	1401	G
1	A	1442	G
1	A	1442(B)	A
1	A	1443	G
1	A	1452	C
1	A	1456	G
1	A	1475	G
1	A	1479	C
1	A	1480	G
1	A	1481	U
1	A	1486	G
1	A	1492	A
1	A	1497	G
1	A	1503	A
1	A	1504	G
1	A	1506	U
1	A	1517	G
1	A	1520	G
1	A	1529	G
1	A	1530	G
1	A	1531	A
1	A	1533	C
1	A	1540	U
1	A	1541	U
23	Z	30	G
23	Z	34	G

All (58) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	7	G
1	A	47	C
1	A	51	A
1	A	173	U
1	A	189(E)	U
1	A	189(G)	G
1	A	196	A
1	A	203	U
1	A	250	A

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Mol	Chain	Res	Type
1	A	281	G
1	A	292	G
1	A	305	G
1	A	353	A
1	A	366	C
1	A	372	C
1	A	388	G
1	A	422	C
1	A	429	U
1	A	452	A
1	A	485	G
1	A	495	A
1	A	517	G
1	A	547	A
1	A	572	A
1	A	575	G
1	A	624	C
1	A	631	G
1	A	653	A
1	A	687	A
1	A	733	A
1	A	793	U
1	A	812	C
1	A	819	A
1	A	872	A
1	A	873	A
1	A	884	U
1	A	913	A
1	A	968	A
1	A	974	A
1	A	975	A
1	A	982	U
1	A	1048	G
1	A	1085	U
1	A	1128	C
1	A	1135	U
1	A	1145	C
1	A	1182	G
1	A	1201	A
1	A	1214	C
1	A	1240	U
1	A	1330	U

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Mol	Chain	Res	Type
1	A	1335	C
1	A	1345	U
1	A	1400	C
1	A	1442(A)	G
1	A	1447	A
1	A	1452	C
1	A	1479	C

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 (i)

Of 239 ligands modelled in this entry, 238 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
26	3TS	A	2733	24	54,54,54	1.41	10 (18%)	72,79,79	1.00	2 (2%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	3TS	A	2733	24	-	0/23/99/99	0/5/5/5

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	2733	3TS	CAU-CBE	-3.84	1.41	1.50
26	A	2733	3TS	OAX-CBR	2.20	1.47	1.41
26	A	2733	3TS	CBK-CBX	2.28	1.58	1.52
26	A	2733	3TS	CAP-CAN	2.29	1.42	1.38
26	A	2733	3TS	CAQ-CBE	2.34	1.43	1.38
26	A	2733	3TS	CBX-CBV	2.38	1.57	1.52
26	A	2733	3TS	CAP-CBE	2.48	1.44	1.38
26	A	2733	3TS	CAN-CBD	2.60	1.43	1.38
26	A	2733	3TS	CAQ-CAO	3.03	1.44	1.38
26	A	2733	3TS	CAO-CBD	3.32	1.44	1.38

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	A	2733	3TS	OAX-CBO-CAR	2.50	110.98	106.10
26	A	2733	3TS	O4-CAU-CBE	3.07	117.31	109.99

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	A	2733	3TS	6	0

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	1512/1521 (99%)	-0.20	10 (0%) 89 70	45, 72, 141, 193	0
2	B	235/256 (91%)	-0.00	7 (2%) 54 25	57, 105, 165, 195	0
3	C	207/239 (86%)	-0.17	0 100 100	57, 93, 132, 162	0
4	D	208/208 (100%)	-0.19	6 (2%) 55 26	54, 81, 136, 191	0
5	E	151/161 (93%)	-0.44	0 100 100	43, 63, 99, 176	0
6	F	101/101 (100%)	-0.23	0 100 100	72, 101, 132, 163	0
7	G	155/155 (100%)	-0.24	4 (2%) 59 29	60, 95, 152, 191	0
8	H	138/138 (100%)	-0.52	1 (0%) 89 70	38, 60, 89, 144	0
9	I	127/128 (99%)	-0.09	1 (0%) 87 67	55, 100, 134, 161	0
10	J	99/104 (95%)	0.59	13 (13%) 5 2	45, 125, 180, 195	0
11	K	119/129 (92%)	-0.03	4 (3%) 49 21	44, 77, 127, 174	0
12	L	125/132 (94%)	-0.13	3 (2%) 62 32	39, 69, 113, 181	0
13	M	125/126 (99%)	0.30	8 (6%) 23 8	58, 87, 151, 196	0
14	N	60/60 (100%)	-0.07	0 100 100	58, 83, 110, 157	0
15	O	88/88 (100%)	-0.31	1 (1%) 82 58	51, 79, 117, 174	0
16	P	84/88 (95%)	-0.33	1 (1%) 81 55	49, 63, 98, 180	0
17	Q	104/104 (100%)	0.08	5 (4%) 34 14	42, 70, 129, 200	0
18	R	73/88 (82%)	-0.20	1 (1%) 78 51	57, 86, 163, 193	0
19	S	81/92 (88%)	0.17	3 (3%) 45 19	73, 104, 145, 175	0
20	T	99/106 (93%)	-0.23	0 100 100	45, 73, 111, 129	0
21	V	25/26 (96%)	0.32	1 (4%) 42 17	56, 73, 113, 137	0
22	W	4/6 (66%)	0.09	0 100 100	85, 86, 87, 102	0
23	Z	15/16 (93%)	0.66	0 100 100	78, 118, 179, 180	0
All	All	3935/4072 (96%)	-0.14	69 (1%) 71 43	38, 79, 146, 200	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	M	122	ALA	14.4
13	M	123	PRO	13.9
17	Q	102	GLY	9.9
13	M	121	LYS	9.7
17	Q	103	LYS	9.6
13	M	120	LYS	8.8
11	K	119	SER	8.8
17	Q	104	ALA	8.1
11	K	118	ALA	7.4
13	M	124	ARG	7.3
17	Q	100	ARG	7.1
13	M	119	LYS	6.9
2	B	127	LYS	6.5
10	J	31	GLN	6.4
17	Q	101	GLY	6.3
10	J	32	VAL	6.0
12	L	125	ALA	5.6
13	M	125	LYS	5.3
12	L	124	ALA	5.3
2	B	128	GLU	5.0
4	D	36	PRO	4.6
2	B	125	PRO	4.6
10	J	73	ILE	4.6
11	K	117	LYS	4.2
1	A	630	G	4.2
18	R	1	PRO	4.1
2	B	126	LYS	4.0
1	A	1003	G	3.7
4	D	34	ARG	3.6
1	A	1539	C	3.6
1	A	1001(A)	G	3.6
10	J	70	VAL	3.5
2	B	132	LEU	3.4
10	J	83	LEU	3.4
19	S	2	ARG	3.4
19	S	81	GLY	3.4
12	L	15	ARG	3.4
7	G	155	TRP	3.4
7	G	79	VAL	3.3
1	A	1533	C	3.2
10	J	72	ILE	3.2
16	P	83	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
9	I	127	ARG	3.0
11	K	79	ALA	3.0
13	M	6	VAL	3.0
10	J	33	SER	2.9
8	H	1	MET	2.9
1	A	1129	C	2.8
1	A	202	U	2.8
19	S	26	GLU	2.7
4	D	44	GLN	2.6
7	G	80	GLY	2.5
15	O	88	GLY	2.5
10	J	2	ILE	2.4
21	V	24	ARG	2.4
10	J	97	LYS	2.3
10	J	4	ILE	2.3
10	J	3	ARG	2.3
4	D	22	GLY	2.3
1	A	841	U	2.2
10	J	68	ARG	2.2
2	B	232	LEU	2.2
2	B	124	ARG	2.2
4	D	1	GLY	2.1
1	A	723	U	2.1
7	G	82	ALA	2.1
1	A	631	G	2.1
4	D	32	MET	2.0
10	J	22	VAL	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)

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	2554	1/1	0.75	0.73	72.04	67,67,67,67	0
24	MG	A	2562	1/1	0.81	0.61	43.87	66,66,66,66	0
24	MG	A	2689	1/1	0.91	0.62	43.10	65,65,65,65	0
24	MG	A	3813	1/1	0.94	0.83	32.94	55,55,55,55	0
24	MG	A	3923	1/1	0.92	0.98	32.42	86,86,86,86	0
24	MG	A	2574	1/1	0.98	0.75	32.36	50,50,50,50	0
24	MG	A	2568	1/1	0.91	0.50	27.72	54,54,54,54	0
24	MG	A	2617	1/1	0.90	0.67	26.50	58,58,58,58	0
25	K	A	2671	1/1	0.65	0.52	21.36	135,135,135,135	0
24	MG	A	2609	1/1	0.61	0.41	18.23	94,94,94,94	0
24	MG	A	2717	1/1	0.75	0.71	17.77	66,66,66,66	0
24	MG	A	2565	1/1	0.86	0.38	16.80	63,63,63,63	0
25	K	A	2672	1/1	0.76	0.43	15.05	107,107,107,107	0
24	MG	A	2718	1/1	0.84	0.81	13.83	85,85,85,85	0
24	MG	A	2662	1/1	0.91	0.57	13.29	52,52,52,52	0
24	MG	A	2601	1/1	0.98	0.75	12.23	51,51,51,51	0
24	MG	A	2585	1/1	0.97	0.73	11.42	61,61,61,61	0
24	MG	A	2632	1/1	0.80	0.26	10.76	65,65,65,65	0
24	MG	G	1156	1/1	0.42	0.49	9.73	80,80,80,80	0
24	MG	A	2659	1/1	0.97	0.27	9.11	28,28,28,28	0
24	MG	A	2578	1/1	0.95	0.34	8.88	52,52,52,52	0
24	MG	A	2598	1/1	0.89	0.31	8.53	46,46,46,46	0
24	MG	A	2695	1/1	0.72	0.34	8.48	54,54,54,54	0
24	MG	A	2702	1/1	0.44	0.31	8.34	65,65,65,65	0
24	MG	A	2705	1/1	0.81	0.29	7.95	52,52,52,52	0
24	MG	A	2649	1/1	0.94	0.25	7.53	34,34,34,34	0
24	MG	A	2569	1/1	0.94	0.32	7.04	61,61,61,61	0
24	MG	A	2599	1/1	0.94	0.29	6.50	58,58,58,58	0
24	MG	A	2612	1/1	0.77	0.34	6.29	55,55,55,55	0
24	MG	A	2729	1/1	0.66	0.30	6.12	70,70,70,70	0
24	MG	A	2637	1/1	0.45	0.33	5.96	80,80,80,80	0
24	MG	A	2605	1/1	0.56	0.25	5.88	55,55,55,55	0
24	MG	A	2706	1/1	0.84	0.20	5.76	69,69,69,69	0
24	MG	A	2704	1/1	0.59	0.30	5.62	62,62,62,62	0
24	MG	A	2723	1/1	0.58	0.27	5.47	65,65,65,65	0
24	MG	A	2610	1/1	0.94	0.21	5.47	53,53,53,53	0
24	MG	A	2582	1/1	0.98	0.23	4.74	52,52,52,52	0
24	MG	A	2576	1/1	0.84	0.20	4.70	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
24	MG	A	2665	1/1	0.92	0.25	4.46	63,63,63,63	0
24	MG	A	2623	1/1	0.81	0.22	4.03	44,44,44,44	0
24	MG	A	2584	1/1	0.95	0.31	3.74	60,60,60,60	0
26	3TS	A	2733	50/50	0.89	0.26	3.72	61,68,89,90	0
24	MG	A	2693	1/1	0.91	0.19	3.27	61,61,61,61	0
24	MG	A	2710	1/1	0.99	0.22	3.17	58,58,58,58	0
24	MG	A	2647	1/1	0.92	0.20	3.06	39,39,39,39	0
24	MG	A	2549	1/1	0.70	0.32	2.95	61,61,61,61	0
24	MG	A	2651	1/1	0.83	0.24	2.27	50,50,50,50	0
24	MG	C	1207	1/1	0.87	0.25	2.07	66,66,66,66	0
24	MG	A	2640	1/1	0.80	0.21	2.01	52,52,52,52	0
24	MG	A	2661	1/1	0.58	0.22	1.73	69,69,69,69	0
24	MG	A	2660	1/1	0.30	0.22	1.50	71,71,71,71	0
24	MG	N	1062	1/1	0.90	0.29	1.31	65,65,65,65	0
24	MG	A	2708	1/1	0.82	0.32	1.17	64,64,64,64	0
25	K	A	2678	1/1	0.88	0.17	1.08	97,97,97,97	0
24	MG	H	1139	1/1	0.89	0.19	0.98	48,48,48,48	0
24	MG	A	2650	1/1	0.95	0.20	0.96	58,58,58,58	0
24	MG	A	2618	1/1	0.88	0.18	0.80	53,53,53,53	0
24	MG	A	2725	1/1	0.96	0.20	0.62	68,68,68,68	0
24	MG	A	2622	1/1	0.87	0.25	0.52	60,60,60,60	0
24	MG	A	2615	1/1	0.94	0.20	0.52	47,47,47,47	0
24	MG	A	2653	1/1	0.89	0.19	0.25	76,76,76,76	0
24	MG	A	2590	1/1	0.95	0.16	0.08	43,43,43,43	0
24	MG	A	2726	1/1	0.93	0.18	0.03	53,53,53,53	0
24	MG	A	2638	1/1	0.91	0.19	-0.13	57,57,57,57	0
24	MG	A	2587	1/1	0.95	0.17	-0.15	52,52,52,52	0
24	MG	A	2644	1/1	0.87	0.14	-0.19	46,46,46,46	0
27	ZN	D	1209	1/1	0.98	0.22	-0.31	106,106,106,106	0
24	MG	A	2691	1/1	0.94	0.15	-0.33	55,55,55,55	0
24	MG	A	2616	1/1	0.84	0.16	-0.36	49,49,49,49	0
24	MG	A	2641	1/1	0.90	0.15	-0.56	45,45,45,45	0
24	MG	A	2602	1/1	0.96	0.18	-0.57	46,46,46,46	0
24	MG	L	1126	1/1	0.93	0.17	-0.57	59,59,59,59	0
27	ZN	N	1061	1/1	0.99	0.17	-0.60	131,131,131,131	0
24	MG	M	1126	1/1	0.95	0.15	-0.63	61,61,61,61	0
24	MG	L	1125	1/1	0.98	0.18	-0.93	63,63,63,63	0
24	MG	A	2648	1/1	0.98	0.15	-1.42	49,49,49,49	0
24	MG	D	1210	1/1	0.93	0.07	-1.57	60,60,60,60	0
24	MG	A	2631	1/1	0.75	0.10	-1.74	45,45,45,45	0
24	MG	A	2645	1/1	0.93	0.08	-3.86	23,23,23,23	0
24	MG	A	2624	1/1	0.93	0.07	-4.94	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
24	MG	A	2570	1/1	0.95	0.08	-4.95	49,49,49,49	0
24	MG	A	2558	1/1	0.99	0.13	-5.68	50,50,50,50	0
25	K	A	2669	1/1	0.81	0.12	-9.54	99,99,99,99	0
24	MG	A	2724	1/1	0.95	0.22	-	64,64,64,64	0
24	MG	A	3734	1/1	0.92	0.48	-	49,49,49,49	0
24	MG	A	3911	1/1	0.58	1.04	-	83,83,83,83	0
24	MG	A	2606	1/1	0.87	0.55	-	77,77,77,77	0
24	MG	A	3743	1/1	0.77	0.26	-	98,98,98,98	0
24	MG	A	2719	1/1	0.81	1.06	-	74,74,74,74	0
24	MG	T	1101	1/1	0.93	0.23	-	49,49,49,49	0
24	MG	A	3933	1/1	0.79	0.63	-	73,73,73,73	0
24	MG	A	2656	1/1	0.90	0.34	-	69,69,69,69	0
24	MG	A	2716	1/1	0.88	0.41	-	67,67,67,67	0
24	MG	A	2699	1/1	0.75	0.19	-	74,74,74,74	0
24	MG	A	2707	1/1	0.93	0.26	-	48,48,48,48	0
24	MG	A	2630	1/1	0.67	0.22	-	76,76,76,76	0
24	MG	A	2664	1/1	0.89	0.23	-	64,64,64,64	0
24	MG	A	3941	1/1	0.91	1.03	-	84,84,84,84	0
24	MG	A	2730	1/1	0.40	0.37	-	84,84,84,84	0
24	MG	A	2553	1/1	0.68	0.43	-	108,108,108,108	0
24	MG	A	2593	1/1	0.62	0.55	-	77,77,77,77	0
24	MG	A	2731	1/1	0.74	0.53	-	80,80,80,80	0
25	K	A	2683	1/1	0.84	0.13	-	103,103,103,103	0
24	MG	A	2589	1/1	0.80	0.13	-	88,88,88,88	0
24	MG	A	2625	1/1	0.92	0.14	-	48,48,48,48	0
24	MG	T	1100	1/1	0.90	0.20	-	70,70,70,70	0
24	MG	A	2712	1/1	0.81	0.29	-	80,80,80,80	0
24	MG	A	2657	1/1	0.81	0.19	-	57,57,57,57	0
25	K	A	2677	1/1	0.72	0.35	-	109,109,109,109	0
24	MG	A	2614	1/1	0.69	0.26	-	85,85,85,85	0
24	MG	A	2714	1/1	0.61	0.37	-	81,81,81,81	0
25	K	A	2681	1/1	0.89	0.14	-	107,107,107,107	0
24	MG	L	1127	1/1	0.87	0.95	-	81,81,81,81	0
24	MG	A	3954	1/1	0.91	0.48	-	75,75,75,75	0
24	MG	A	2643	1/1	0.99	0.29	-	43,43,43,43	0
24	MG	A	2552	1/1	0.60	0.50	-	75,75,75,75	0
24	MG	A	3804	1/1	0.92	0.34	-	66,66,66,66	0
24	MG	A	2575	1/1	0.38	0.56	-	76,76,76,76	0
24	MG	A	2546	1/1	0.62	0.36	-	94,94,94,94	0
24	MG	A	2628	1/1	0.84	0.14	-	49,49,49,49	0
24	MG	A	2583	1/1	0.95	0.40	-	49,49,49,49	0
24	MG	A	2709	1/1	0.77	0.28	-	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
24	MG	A	2547	1/1	0.83	0.70	-	81,81,81,81	0
24	MG	A	3927	1/1	0.93	0.26	-	59,59,59,59	0
24	MG	A	2646	1/1	0.83	0.25	-	59,59,59,59	0
24	MG	A	2580	1/1	0.63	0.83	-	79,79,79,79	0
24	MG	A	2572	1/1	0.80	0.42	-	164,164,164,164	0
24	MG	A	2634	1/1	0.92	0.13	-	63,63,63,63	0
24	MG	A	3928	1/1	0.97	1.12	-	64,64,64,64	0
24	MG	A	3735	1/1	0.96	0.75	-	72,72,72,72	0
24	MG	A	2732	1/1	0.59	0.42	-	82,82,82,82	0
24	MG	A	2694	1/1	0.92	0.57	-	71,71,71,71	0
25	K	A	2674	1/1	0.93	0.08	-	101,101,101,101	0
24	MG	A	2626	1/1	0.94	0.36	-	74,74,74,74	0
24	MG	A	2557	1/1	0.69	0.20	-	67,67,67,67	0
24	MG	A	2633	1/1	0.83	0.15	-	72,72,72,72	0
24	MG	A	2697	1/1	0.63	0.44	-	94,94,94,94	0
24	MG	A	3822	1/1	0.66	0.73	-	83,83,83,83	0
24	MG	A	3907	1/1	0.86	0.31	-	64,64,64,64	0
24	MG	A	2621	1/1	0.83	0.23	-	75,75,75,75	0
24	MG	A	2701	1/1	0.71	0.45	-	78,78,78,78	0
24	MG	A	2577	1/1	0.72	0.30	-	55,55,55,55	0
24	MG	A	2586	1/1	0.81	0.13	-	122,122,122,122	0
24	MG	A	2727	1/1	0.95	0.29	-	77,77,77,77	0
24	MG	A	2635	1/1	0.95	0.13	-	37,37,37,37	0
24	MG	A	2588	1/1	0.60	0.18	-	74,74,74,74	0
24	MG	A	2597	1/1	0.83	0.24	-	50,50,50,50	0
24	MG	A	2545	1/1	0.83	0.16	-	78,78,78,78	0
24	MG	A	2567	1/1	0.87	0.54	-	69,69,69,69	0
24	MG	E	2148	1/1	0.96	0.15	-	66,66,66,66	0
24	MG	A	2685	1/1	0.86	0.53	-	63,63,63,63	0
25	K	A	3892	1/1	0.86	0.20	-	103,103,103,103	0
24	MG	A	2639	1/1	0.92	0.23	-	62,62,62,62	0
24	MG	A	2713	1/1	0.84	1.06	-	90,90,90,90	0
25	K	A	2673	1/1	0.77	0.21	-	112,112,112,112	0
24	MG	A	2696	1/1	0.68	0.24	-	76,76,76,76	0
24	MG	A	3910	1/1	0.74	0.84	-	83,83,83,83	0
24	MG	A	3774	1/1	0.97	0.70	-	69,69,69,69	0
24	MG	A	3963	1/1	0.77	0.89	-	92,92,92,92	0
24	MG	A	3749	1/1	0.55	0.45	-	90,90,90,90	0
24	MG	A	2571	1/1	0.30	0.87	-	90,90,90,90	0
24	MG	A	2592	1/1	0.97	0.32	-	47,47,47,47	0
24	MG	A	3789	1/1	0.91	0.88	-	73,73,73,73	0
24	MG	A	2596	1/1	0.95	0.41	-	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
24	MG	A	3757	1/1	0.92	0.45	-	51,51,51,51	0
24	MG	A	3740	1/1	0.78	0.40	-	83,83,83,83	0
24	MG	A	2642	1/1	0.81	0.30	-	68,68,68,68	0
24	MG	A	2722	1/1	0.63	0.44	-	76,76,76,76	0
24	MG	P	1084	1/1	0.86	0.54	-	63,63,63,63	0
24	MG	A	2611	1/1	0.96	0.12	-	55,55,55,55	0
24	MG	A	2573	1/1	0.56	0.71	-	75,75,75,75	0
24	MG	A	2721	1/1	0.82	0.33	-	82,82,82,82	0
24	MG	A	2560	1/1	0.79	0.31	-	87,87,87,87	0
24	MG	A	2550	1/1	0.67	0.24	-	63,63,63,63	0
24	MG	A	2686	1/1	0.81	0.51	-	65,65,65,65	0
24	MG	A	2700	1/1	0.65	0.46	-	73,73,73,73	0
24	MG	A	2688	1/1	0.89	0.34	-	58,58,58,58	0
24	MG	A	2720	1/1	0.88	0.32	-	80,80,80,80	0
24	MG	A	2629	1/1	0.76	0.41	-	77,77,77,77	0
24	MG	A	2652	1/1	0.66	0.31	-	56,56,56,56	0
24	MG	A	3780	1/1	0.93	0.41	-	84,84,84,84	0
24	MG	A	2711	1/1	0.82	0.71	-	81,81,81,81	0
24	MG	A	2594	1/1	0.87	0.32	-	64,64,64,64	0
25	K	E	1151	1/1	0.86	0.30	-	101,101,101,101	0
24	MG	A	2600	1/1	0.69	0.32	-	76,76,76,76	0
24	MG	A	2654	1/1	0.90	0.25	-	59,59,59,59	0
24	MG	A	3753	1/1	0.97	0.44	-	46,46,46,46	0
24	MG	A	2603	1/1	0.90	0.91	-	90,90,90,90	0
24	MG	A	2561	1/1	0.84	0.48	-	74,74,74,74	0
24	MG	A	3750	1/1	0.94	1.01	-	68,68,68,68	0
24	MG	A	3795	1/1	0.93	0.62	-	77,77,77,77	0
24	MG	A	2566	1/1	0.93	0.41	-	56,56,56,56	0
24	MG	A	2663	1/1	0.91	0.28	-	54,54,54,54	0
24	MG	A	3748	1/1	0.97	0.98	-	61,61,61,61	0
24	MG	A	2620	1/1	0.83	0.20	-	63,63,63,63	0
24	MG	A	3810	1/1	0.88	0.38	-	53,53,53,53	0
24	MG	A	2619	1/1	0.74	0.24	-	65,65,65,65	0
24	MG	A	2581	1/1	0.96	0.42	-	44,44,44,44	0
24	MG	A	2563	1/1	0.96	0.35	-	53,53,53,53	0
24	MG	A	2604	1/1	0.99	0.27	-	37,37,37,37	0
24	MG	A	2564	1/1	0.98	0.38	-	51,51,51,51	0
24	MG	E	1152	1/1	0.85	0.48	-	66,66,66,66	0
24	MG	Q	2217	1/1	0.94	0.20	-	62,62,62,62	0
24	MG	A	2559	1/1	0.94	0.61	-	51,51,51,51	0
24	MG	A	2595	1/1	0.82	0.23	-	61,61,61,61	0
24	MG	A	2607	1/1	0.47	0.24	-	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
24	MG	A	3909	1/1	0.93	0.57	-	77,77,77,77	0
24	MG	A	3828	1/1	0.88	0.37	-	68,68,68,68	0
24	MG	A	2636	1/1	0.69	0.46	-	76,76,76,76	0
24	MG	A	2692	1/1	0.89	0.43	-	71,71,71,71	0
24	MG	A	2698	1/1	0.73	0.32	-	76,76,76,76	0
24	MG	A	2655	1/1	0.93	0.14	-	73,73,73,73	0
24	MG	A	2555	1/1	0.87	0.24	-	77,77,77,77	0
24	MG	A	2728	1/1	0.89	0.10	-	77,77,77,77	0
24	MG	A	2613	1/1	0.82	0.71	-	61,61,61,61	0
24	MG	A	2715	1/1	0.85	0.38	-	70,70,70,70	0
24	MG	A	2667	1/1	0.87	0.14	-	56,56,56,56	0
24	MG	A	2668	1/1	0.95	0.19	-	117,117,117,117	0
25	K	A	2680	1/1	0.62	0.28	-	113,113,113,113	0
24	MG	A	2666	1/1	0.68	0.65	-	106,106,106,106	0
24	MG	A	2703	1/1	0.65	0.23	-	76,76,76,76	0
24	MG	A	2684	1/1	0.93	0.09	-	46,46,46,46	0
24	MG	A	2627	1/1	0.88	0.20	-	51,51,51,51	0
24	MG	A	2690	1/1	0.84	0.34	-	73,73,73,73	0
24	MG	A	2591	1/1	0.94	0.50	-	39,39,39,39	0
24	MG	A	2551	1/1	0.89	0.20	-	39,39,39,39	0
25	K	A	2682	1/1	0.83	0.16	-	106,106,106,106	0
24	MG	A	2687	1/1	0.93	0.34	-	12,12,12,12	0
25	K	A	2679	1/1	0.91	0.20	-	104,104,104,104	0
24	MG	A	2579	1/1	0.93	0.35	-	53,53,53,53	0
24	MG	A	3759	1/1	0.95	0.54	-	66,66,66,66	0
24	MG	A	2548	1/1	0.92	0.27	-	48,48,48,48	0
24	MG	A	2658	1/1	0.89	0.09	-	58,58,58,58	0
25	K	A	2676	1/1	0.94	0.16	-	96,96,96,96	0
24	MG	A	2608	1/1	0.90	0.54	-	52,52,52,52	0
24	MG	A	3967	1/1	0.94	0.21	-	83,83,83,83	0
24	MG	A	2556	1/1	0.66	0.71	-	82,82,82,82	0
25	K	A	2670	1/1	0.90	0.12	-	105,105,105,105	0
25	K	A	2675	1/1	0.73	0.23	-	100,100,100,100	0

6.5 Other polymers (i)

There are no such residues in this entry.