



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:01 PM UTC

PDB ID : 4DR5 / pdb_00004dr5
Title : Crystal structure of the *Thermus thermophilus* (HB8) 30S ribosomal subunit with codon, crystallographically disordered cognate transfer RNA anticodon stem-loop and streptomycin bound
Authors : Demirci, H.; Murphy IV, F.; Murphy, E.; Gregory, S.T.; Dahlberg, A.E.; Jogl, G.
Deposited on : 2012-02-16
Resolution : 3.45 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

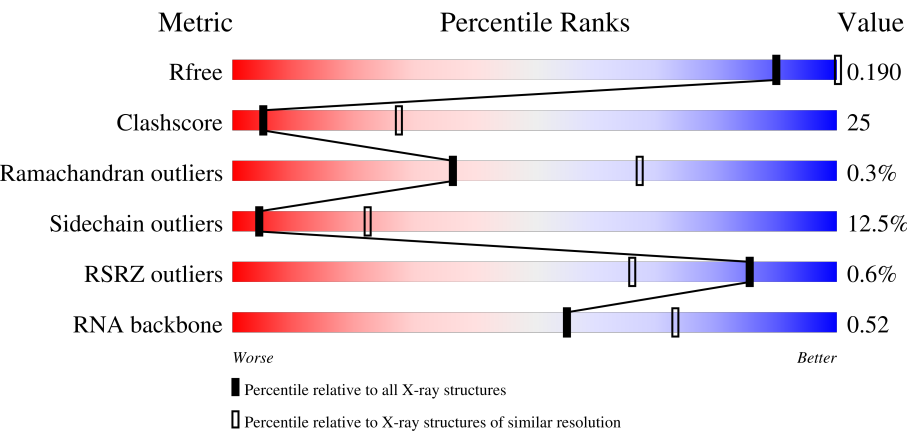
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.45 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1070 (3.50-3.42)
Clashscore	190562	1128 (3.50-3.42)
Ramachandran outliers	187476	1101 (3.50-3.42)
Sidechain outliers	187428	1102 (3.50-3.42)
RSRZ outliers	180081	1070 (3.50-3.42)
RNA backbone	3983	1186 (3.92-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	1522	37% 49% 13% .
2	B	256	36% 50% 6% 8%
3	C	239	43% 36% 8% 13%
4	D	209	4% 51% 43% 6%

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Mol	Chain	Length	Quality of chain
5	E	162	
6	F	101	
7	G	156	
8	H	138	
9	I	128	
10	J	105	
11	K	129	
12	L	135	
13	M	126	
14	N	61	
15	O	89	
16	P	88	
17	Q	105	
18	R	88	
19	S	93	
20	T	106	
21	U	27	
22	V	3	
23	W	15	

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
1	UR3	A	1498	-	-	X	-
1	MA6	A	1518[B]	-	-	X	-
24	MG	A	1717	-	-	-	X
24	MG	A	1729	-	-	-	X
24	MG	A	1732	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	MG	A	1746	-	-	-	X
24	MG	A	1766	-	-	-	X
24	MG	A	1851	-	-	-	X

2 Entry composition

There are 27 unique types of molecules in this entry. The entry contains 53065 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 rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1512	Total	C	N	O	P	0	6	0
			32641	14540	6039	10545	1517			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1534	C	A	conflict	GB M26923.1
A	1535	A	C	conflict	GB M26923.1

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	236	Total	C	N	O	S	0	0	1
			1896	1211	337	343	5			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	151	Total	C	N	O	S	0	0	1
			1147	724	218	201	4			

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	I	127	Total	C	N	O	0	0	0
			1010	639	197	174			

- 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
			793	498	157	137	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
			973	612	196	163	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	118	Total	C	N	O	S	0	0	0
			937	579	193	163	2			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	P	84	Total	C	N	O	S	0	0	1
			701	443	140	117	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	100	Total	C	N	O	S	0	0	0
			834	534	156	142	2			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	96	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
			598	381	118	99				

- 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
			763	470	162	129	2			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	V	3	Total	C	N	O	P	0	0	0
			57	27	6	22	2			

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

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

- Molecule 24 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

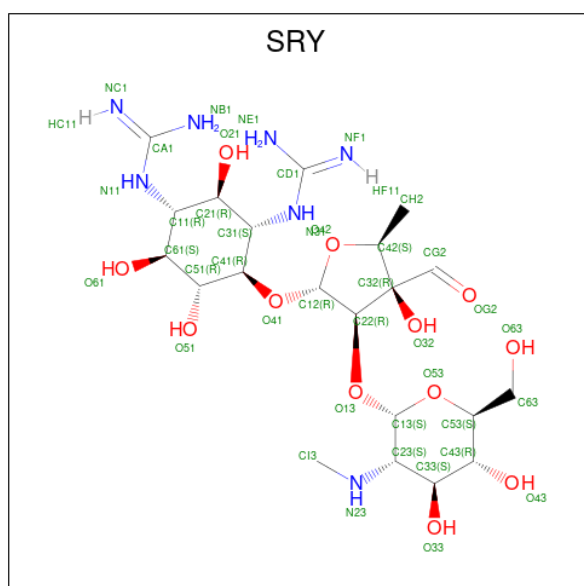
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	A	259	Total	Mg	0	0
			259	259		
24	D	2	Total	Mg	0	0
			2	2		
24	E	1	Total	Mg	0	0
			1	1		
24	F	1	Total	Mg	0	0
			1	1		
24	G	1	Total	Mg	0	0
			1	1		
24	H	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	L	1	Total	Mg	0	0
			1	1		
24	N	1	Total	Mg	0	0
			1	1		
24	P	3	Total	Mg	0	0
			3	3		
24	Q	1	Total	Mg	0	0
			1	1		
24	S	1	Total	Mg	0	0
			1	1		

- Molecule 25 is STREPTOMYCIN (CCD ID: SRY) (formula: $C_{21}H_{39}N_7O_{12}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	A	1	Total	C	N	O	0	0
			40	21	7	12		

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

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

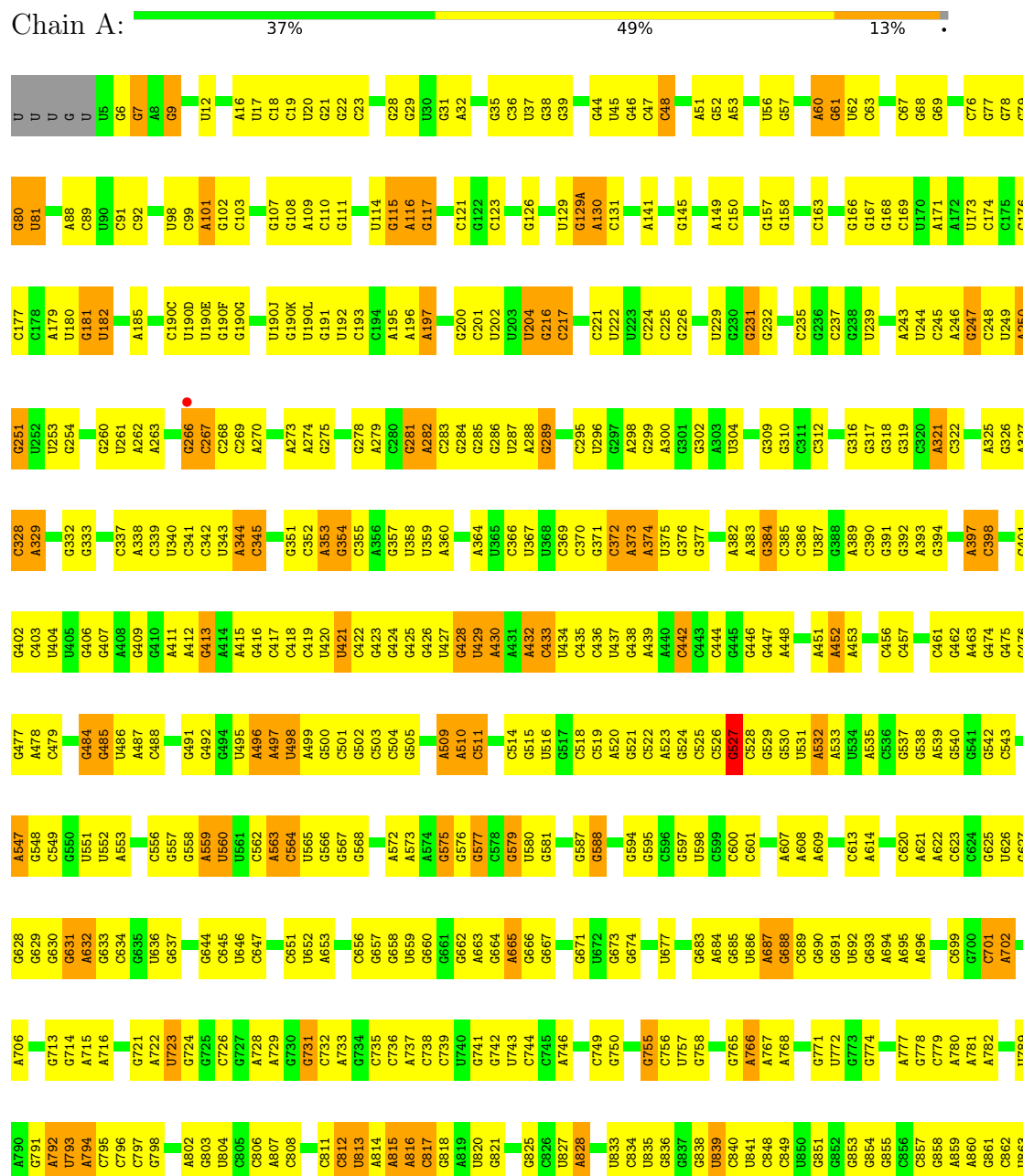
- Molecule 27 is water.

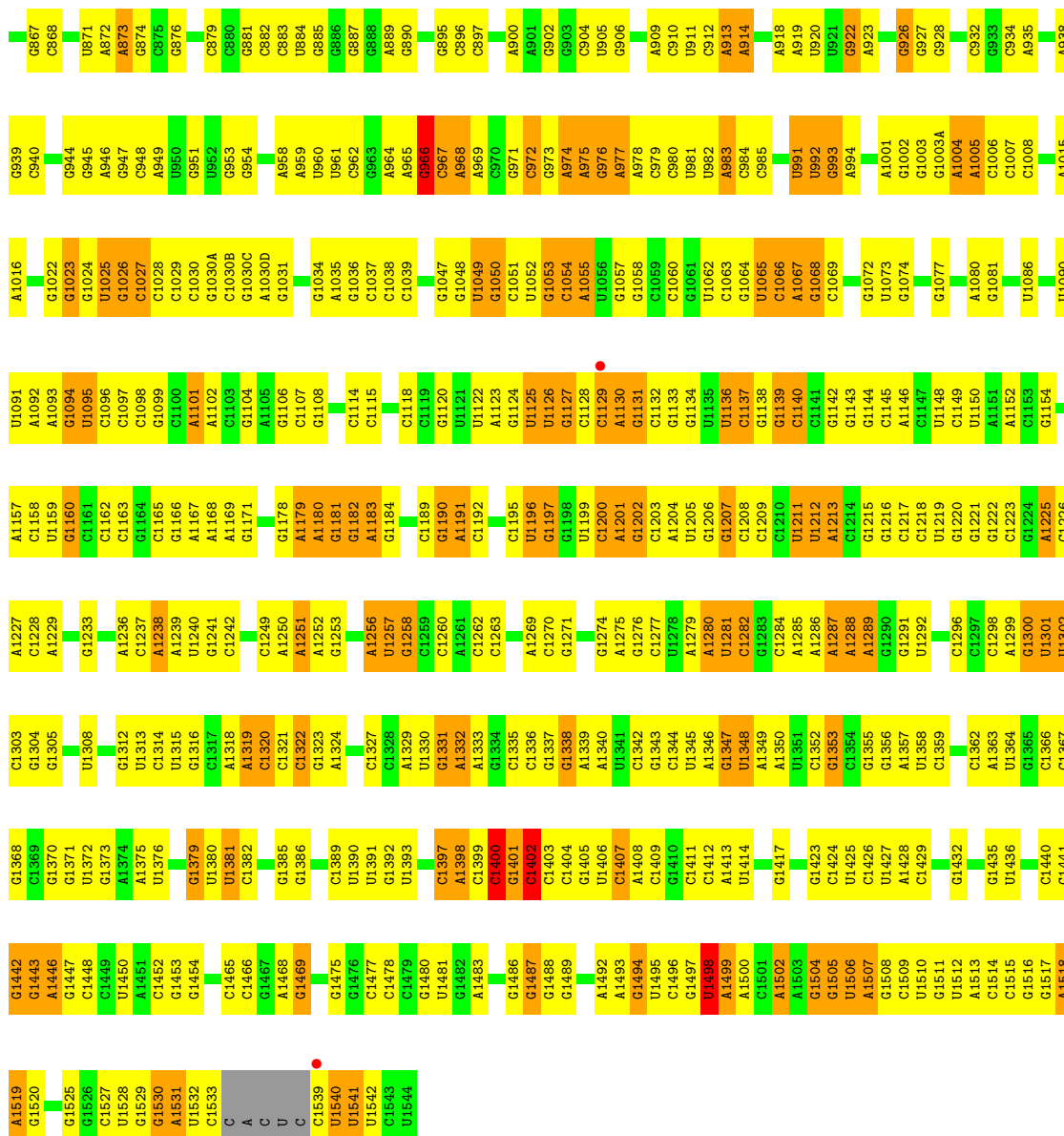
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
27	A	572	Total 572	O 572	0	0
27	D	2	Total 2	O 2	0	0
27	E	3	Total 3	O 3	0	0
27	L	1	Total 1	O 1	0	0
27	O	1	Total 1	O 1	0	0
27	P	1	Total 1	O 1	0	0
27	Q	1	Total 1	O 1	0	0
27	T	1	Total 1	O 1	0	0

3 Residue-property plots

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

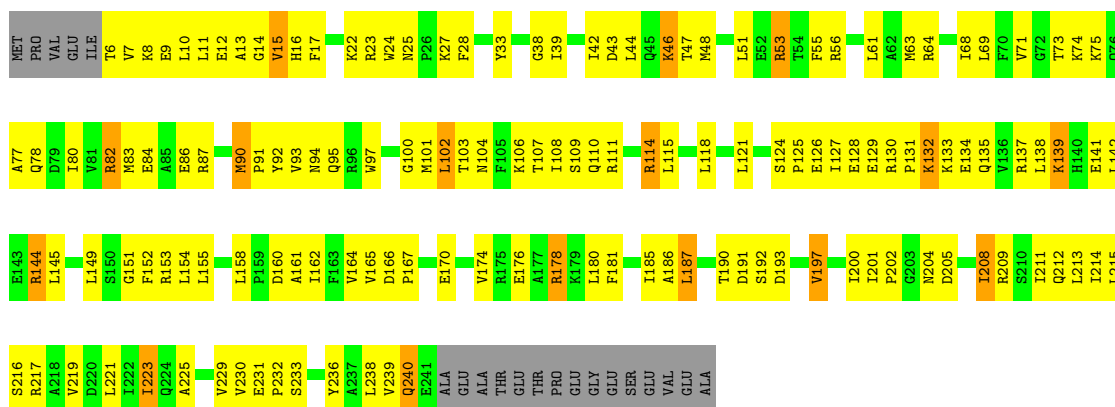
• Molecule 1: 16S rRNA



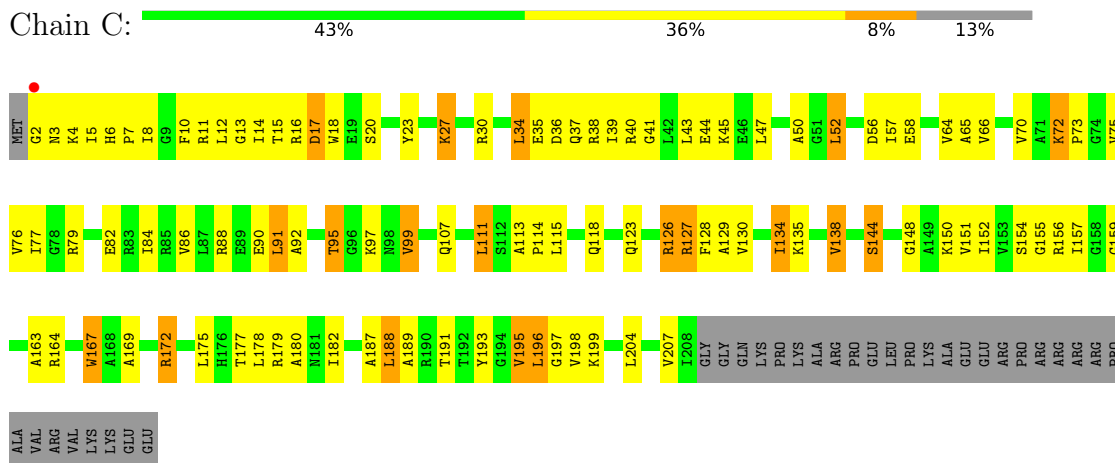


- Molecule 2: 30S ribosomal protein S2

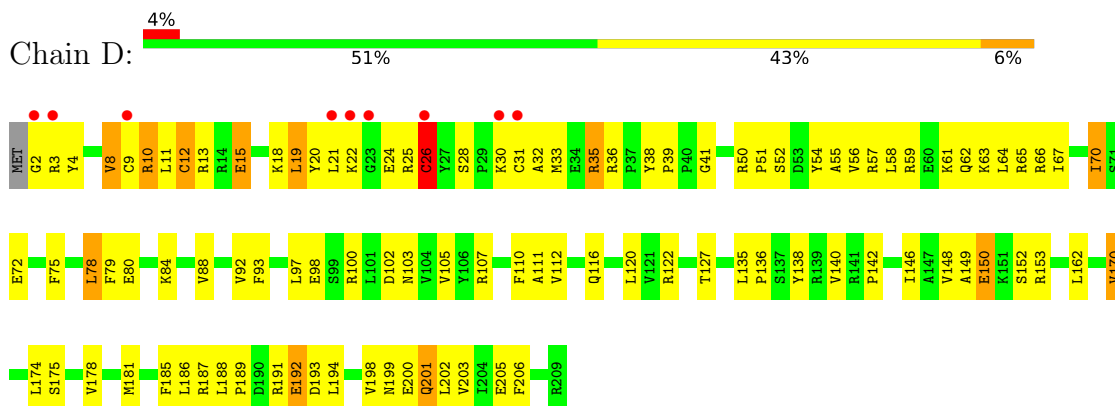
Chain B: 36% 50% 6% 8%



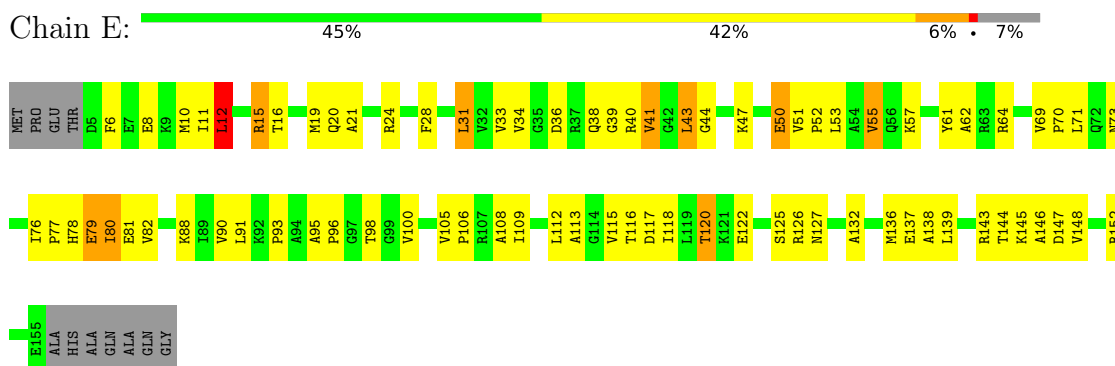
- Molecule 3: 30S ribosomal protein S3



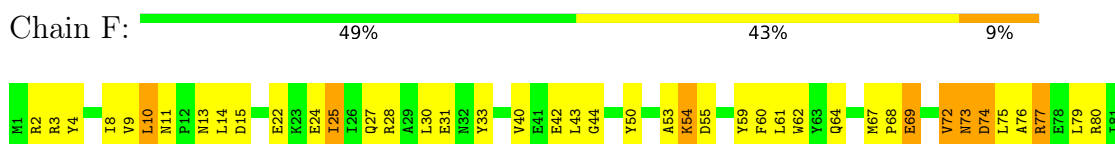
- Molecule 4: 30S ribosomal protein S4

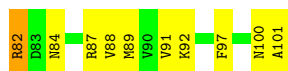


- Molecule 5: 30S ribosomal protein S5



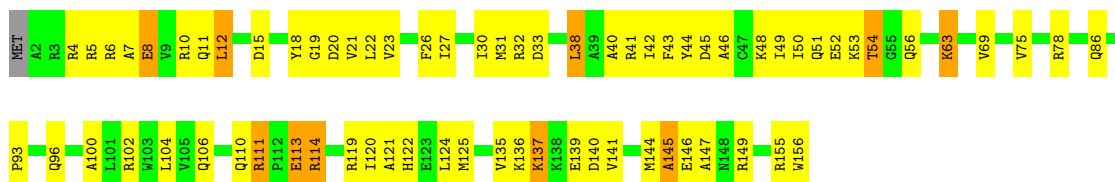
- Molecule 6: 30S ribosomal protein S6





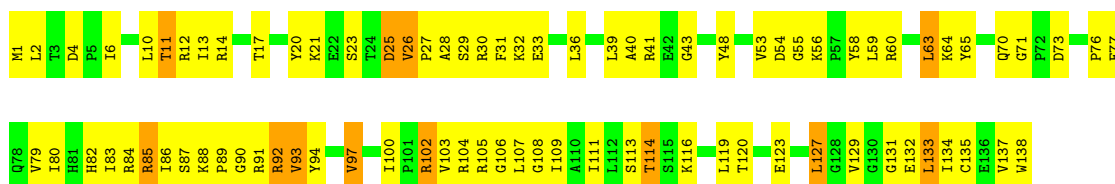
• Molecule 7: 30S ribosomal protein S7

Chain G: 54% 39% 6% •



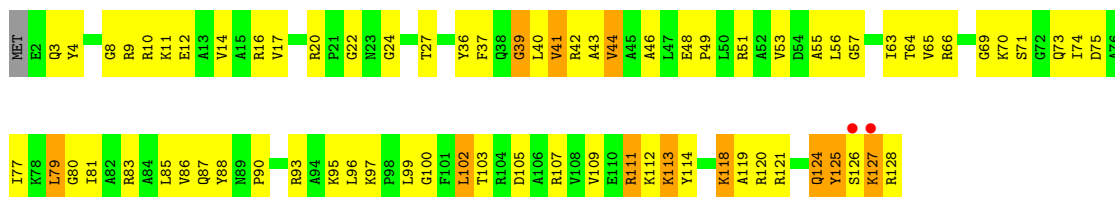
• Molecule 8: 30S ribosomal protein S8

Chain H: 39% 52% 9%



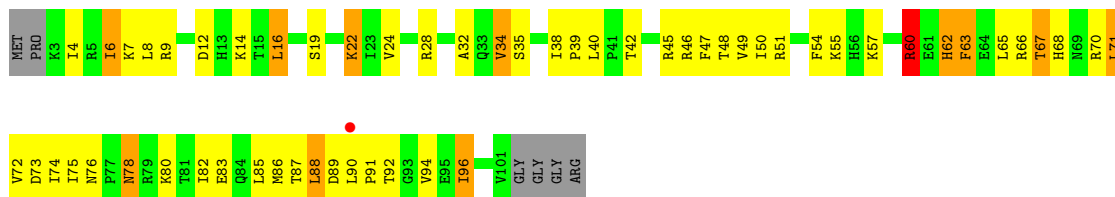
• Molecule 9: 30S ribosomal protein S9

Chain I: 2% 41% 49% 9% •



• Molecule 10: 30S ribosomal protein S10

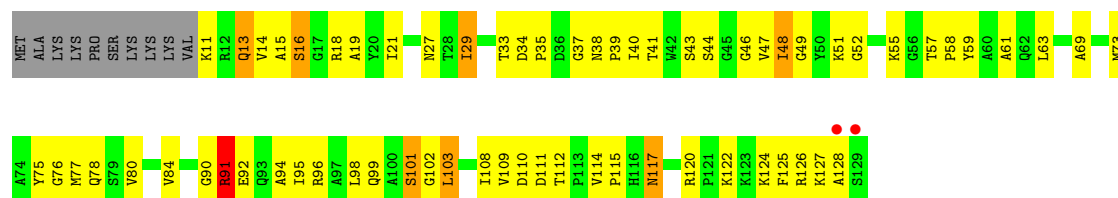
Chain J: 2% 40% 43% 10% 6% •



• Molecule 11: 30S ribosomal protein S11

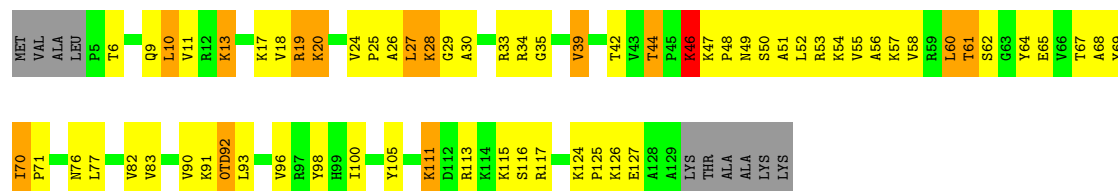
Chain K: 2% 41% 45% 5% 8% •





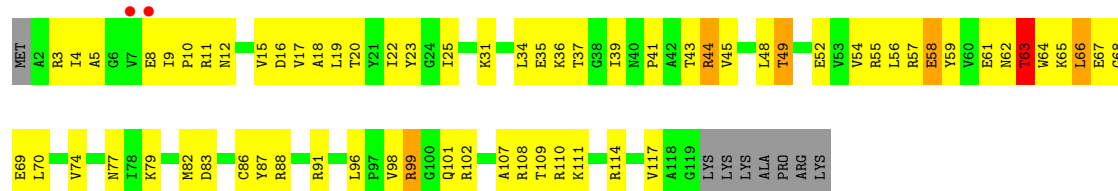
• Molecule 12: 30S ribosomal protein S12

Chain L: 44% 39% 10% 7%



• Molecule 13: 30S ribosomal protein S13

Chain M: 40% 48% 2% 6%



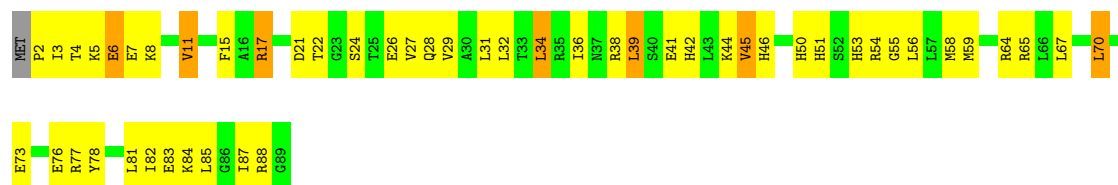
• Molecule 14: 30S ribosomal protein S14

Chain N: 49% 43% 2% 7%



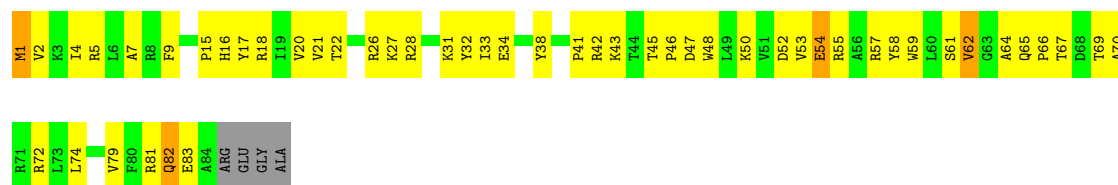
• Molecule 15: 30S ribosomal protein S15

Chain O: 42% 49% 8% 1%

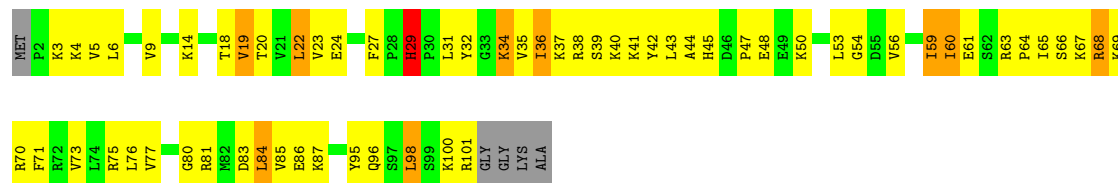


• Molecule 16: 30S ribosomal protein S16

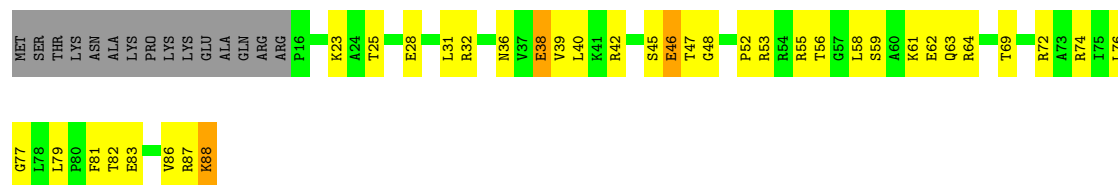
Chain P: 39% 52% 5% 5%



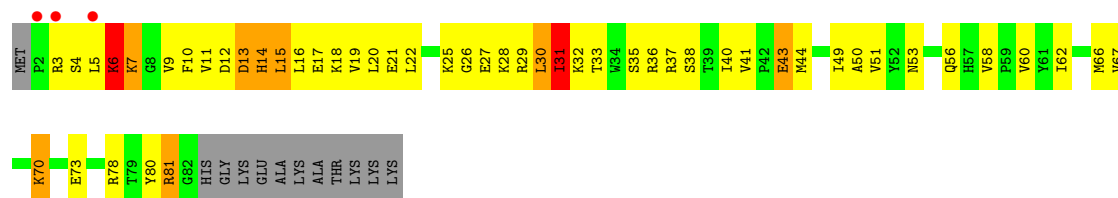
• Molecule 17: 30S ribosomal protein S17



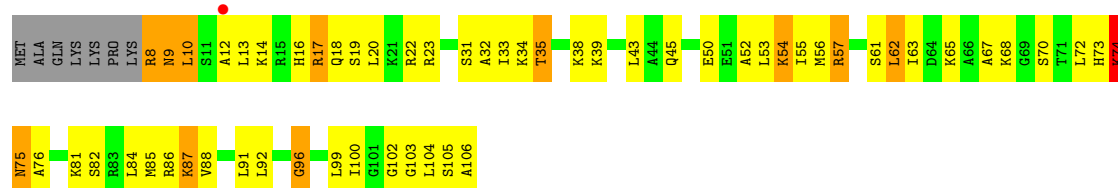
• Molecule 18: 30S ribosomal protein S18



• Molecule 19: 30S ribosomal protein S19



• Molecule 20: 30S ribosomal protein S20

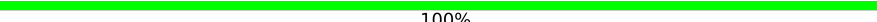


• Molecule 21: 30S ribosomal protein THX

Chain U:  63% 22% 7% 7%



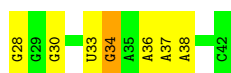
- Molecule 22: 5'-R(*UP*UP*U)-3'

Chain V:  100%

There are no outlier residues recorded for this chain.

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

Chain W:  53% 40% 7%



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	400.51Å 400.51Å 175.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.90 – 3.45 19.90 – 3.45	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.90-3.45) 99.4 (19.90-3.45)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.53 (at 3.44Å)	Xtriage
Refinement program	PHENIX dev_978	Depositor
R, R_{free}	0.152 , 0.192 0.151 , 0.190	Depositor DCC
R_{free} test set	9323 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	111.7	Xtriage
Anisotropy	0.223	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 104.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	53065	wwPDB-VP
Average B, all atoms (Å ²)	117.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.55% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 0TD, SRY, 4OC, UR3, M2G, 7MG, MG, MA6, 2MG, ZN, 5MC, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.29	0/36136	0.40	0/56392
2	B	0.39	0/1931	0.86	2/2607 (0.1%)
3	C	0.41	0/1637	0.81	0/2207
4	D	0.43	0/1733	0.90	2/2318 (0.1%)
5	E	0.59	0/1163	0.96	3/1566 (0.2%)
6	F	0.38	0/856	0.82	0/1154
7	G	0.43	0/1276	0.90	4/1709 (0.2%)
8	H	0.52	0/1136	1.06	8/1527 (0.5%)
9	I	0.39	0/1029	0.93	2/1379 (0.1%)
10	J	0.42	0/806	0.94	2/1084 (0.2%)
11	K	0.52	0/900	1.02	5/1213 (0.4%)
12	L	0.52	0/978	1.13	10/1308 (0.8%)
13	M	0.41	0/947	0.82	1/1270 (0.1%)
14	N	0.39	0/501	0.81	0/664
15	O	0.47	0/745	0.81	0/992
16	P	0.51	0/717	0.89	0/965
17	Q	0.55	0/847	1.02	2/1131 (0.2%)
18	R	0.42	0/604	0.88	0/801
19	S	0.37	0/662	0.93	2/892 (0.2%)
20	T	0.53	0/765	0.96	4/1007 (0.4%)
21	U	0.39	0/213	0.82	0/279
22	V	0.15	0/62	0.29	0/94
23	W	0.10	0/357	0.25	0/555
All	All	0.35	0/56001	0.61	47/83114 (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
2	B	0	1
8	H	0	1
12	L	0	1
All	All	0	3

There are no bond length outliers.

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
9	I	39	GLY	N-CA-C	-12.68	97.73	114.85
12	L	26	ALA	N-CA-C	-9.92	101.34	113.15
4	D	26	CYS	N-CA-C	-9.24	101.43	112.89
8	H	73	ASP	CA-C-N	7.55	127.72	119.87
8	H	73	ASP	C-N-CA	7.55	127.72	119.87
8	H	56	LYS	CA-C-N	7.10	127.35	119.90
8	H	56	LYS	C-N-CA	7.10	127.35	119.90
20	T	96	GLY	N-CA-C	7.10	121.91	111.76
7	G	147	ALA	N-CA-C	-7.07	104.66	113.28
2	B	15	VAL	N-CA-C	6.97	117.06	110.30
11	K	102	GLY	N-CA-C	-6.91	106.86	115.08
19	S	30	LEU	CB-CA-C	-6.58	107.96	115.79
11	K	91	ARG	N-CA-C	-6.37	103.62	111.40
7	G	111	ARG	CA-C-N	6.37	125.99	119.56
7	G	111	ARG	C-N-CA	6.37	125.99	119.56
8	H	100	ILE	CA-C-N	6.23	126.19	120.21
8	H	100	ILE	C-N-CA	6.23	126.19	120.21
20	T	74	LYS	CB-CA-C	-6.20	108.42	115.79
8	H	80	ILE	CB-CA-C	-6.13	103.41	111.81
11	K	99	GLN	CA-C-N	-6.06	113.71	123.23
11	K	99	GLN	C-N-CA	-6.06	113.71	123.23
4	D	12	CYS	N-CA-C	-5.97	103.95	111.11
12	L	44	THR	CA-C-N	5.86	127.16	119.84
12	L	44	THR	C-N-CA	5.86	127.16	119.84
12	L	70	ILE	CA-C-N	5.76	125.67	119.85
12	L	70	ILE	C-N-CA	5.76	125.67	119.85
2	B	90	MET	N-CA-C	5.69	117.06	109.83
19	S	29	ARG	N-CA-C	5.68	117.68	108.26
5	E	20	GLN	N-CA-C	-5.67	101.36	110.14
10	J	60	ARG	N-CA-C	5.59	118.13	110.24
9	I	22	GLY	N-CA-C	5.56	118.36	110.74
7	G	145	ALA	N-CA-C	-5.56	102.79	110.35
17	Q	29	HIS	CA-C-N	5.51	126.73	119.84
17	Q	29	HIS	C-N-CA	5.51	126.73	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	L	105	TYR	CB-CA-C	-5.47	110.28	116.63
11	K	101	SER	N-CA-C	-5.37	106.11	113.30
12	L	61	THR	N-CA-C	-5.35	106.01	112.54
5	E	41	VAL	CB-CA-C	-5.30	103.27	110.90
20	T	76	ALA	N-CA-C	-5.17	105.33	110.97
8	H	131	GLY	N-CA-C	5.15	117.14	110.45
10	J	96	ILE	N-CA-C	5.07	115.20	108.11
12	L	27	LEU	CB-CA-C	-5.06	109.76	115.79
13	M	63	THR	N-CA-C	-5.06	100.02	110.80
5	E	12	LEU	N-CA-C	5.06	115.72	108.74
20	T	9	ASN	N-CA-C	5.05	118.18	110.36
12	L	115	LYS	CA-C-N	-5.02	115.34	122.77
12	L	115	LYS	C-N-CA	-5.02	115.34	122.77

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	14	GLY	Peptide
8	H	90	GLY	Peptide
12	L	46	LYS	Peptide

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	32641	0	16508	1074	1
2	B	1896	0	1936	129	0
3	C	1613	0	1677	109	0
4	D	1703	0	1763	89	0
5	E	1147	0	1207	77	0
6	F	843	0	857	47	0
7	G	1257	0	1296	70	0
8	H	1116	0	1177	74	0
9	I	1010	0	1037	78	0
10	J	793	0	835	69	0
11	K	885	0	904	52	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	L	973	0	1058	67	0
13	M	937	0	995	74	0
14	N	492	0	529	37	0
15	O	734	0	771	52	0
16	P	701	0	720	48	0
17	Q	834	0	906	72	0
18	R	598	0	670	39	0
19	S	648	0	673	61	0
20	T	763	0	861	72	0
21	U	209	0	221	11	0
22	V	57	0	32	0	0
23	W	319	0	164	8	0
24	A	259	0	0	0	0
24	D	2	0	0	0	0
24	E	1	0	0	0	0
24	F	1	0	0	0	0
24	G	1	0	0	0	0
24	H	1	0	0	0	0
24	L	1	0	0	0	0
24	N	1	0	0	0	0
24	P	3	0	0	0	0
24	Q	1	0	0	0	0
24	S	1	0	0	0	0
25	A	40	0	37	9	0
26	D	1	0	0	0	0
26	N	1	0	0	0	0
27	A	572	0	0	22	0
27	D	2	0	0	0	0
27	E	3	0	0	0	0
27	L	1	0	0	0	0
27	O	1	0	0	0	0
27	P	1	0	0	0	0
27	Q	1	0	0	0	0
27	T	1	0	0	0	0
All	All	53065	0	36834	2192	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 25.

All (2192) 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)
11:K:15:ALA:HA	11:K:77:MET:HA	1.32	1.12
15:O:39:LEU:HD12	15:O:56:LEU:HB2	1.29	1.06
15:O:87:ILE:HG22	15:O:88:ARG:H	1.18	1.06
1:A:1498:UR3:O2'	1:A:1499:A:OP2	1.75	1.04
3:C:27:LYS:H	3:C:27:LYS:HD3	1.19	1.04
1:A:1129:C:H4'	1:A:1130:A:OP2	1.55	1.04
10:J:49:VAL:HG23	14:N:41:ARG:HB2	1.39	1.01
19:S:33:THR:HG22	19:S:35:SER:H	1.26	1.01
1:A:1540:PSU:H3'	1:A:1540:PSU:H6	1.25	1.01
1:A:250:A:H4'	1:A:251:G:O5'	1.59	0.99
1:A:1005:A:N3	1:A:1026:G:N2	2.11	0.98
1:A:235:C:H5'	17:Q:70:ARG:HG2	1.46	0.97
1:A:1057:G:H5''	3:C:154:SER:HB2	1.42	0.97
1:A:1399:C:H4'	1:A:1400:5MC:H5''	1.47	0.97
1:A:1182:G:O2'	1:A:1183:A:OP2	1.82	0.97
1:A:413:G:N2	1:A:429:U:OP2	1.99	0.96
3:C:127:ARG:HH12	3:C:193:TYR:HE2	1.10	0.95
1:A:1054:C:H42	23:W:34:G:C1'	1.78	0.95
2:B:77:ALA:HB2	2:B:211:ILE:HD13	1.48	0.94
1:A:442:C:H42	1:A:492:G:H1	1.13	0.94
2:B:7:VAL:HG13	2:B:48:MET:HE1	1.48	0.94
4:D:150:GLU:H	4:D:150:GLU:CD	1.76	0.94
12:L:6:THR:OG1	12:L:9:GLN:HG3	1.67	0.93
15:O:17:ARG:HG3	15:O:17:ARG:HH11	1.33	0.93
1:A:664:G:H22	1:A:741:G:H1	1.12	0.92
1:A:1497:G:H2'	1:A:1498:UR3:H5'	1.52	0.91
1:A:609:A:N6	27:A:2206:HOH:O	2.04	0.91
1:A:975:A:H5'	1:A:975:A:H8	1.35	0.91
1:A:1443:G:H4'	1:A:1446:A:O5'	1.70	0.90
3:C:91:LEU:HD21	3:C:99:VAL:HG22	1.53	0.90
1:A:204:U:H5'	1:A:216:G:OP1	1.72	0.89
1:A:344:A:H5'	1:A:345:C:H5	1.37	0.89
1:A:975:A:H4'	1:A:976:G:H5''	1.53	0.88
2:B:130:ARG:HB3	2:B:131:PRO:HD2	1.53	0.88
1:A:328:C:O2	1:A:328:C:H2'	1.70	0.88
1:A:279:A:OP2	17:Q:95:TYR:OH	1.92	0.87
1:A:932:C:H4'	7:G:4:ARG:HH21	1.39	0.87
1:A:974:A:OP2	14:N:41:ARG:NH1	2.06	0.87
13:M:49:THR:HG22	13:M:52:GLU:H	1.38	0.87
18:R:25:THR:HG21	18:R:42:ARG:NH2	1.89	0.87
1:A:1412:C:H2'	1:A:1413:A:C8	2.10	0.87
1:A:1086:U:H3	1:A:1099:G:H22	1.17	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1331:G:O2'	1:A:1332:A:OP2	1.91	0.86
3:C:14:ILE:HG22	3:C:15:THR:HG23	1.57	0.86
12:L:27:LEU:O	12:L:29:GLY:N	2.07	0.86
17:Q:27:PHE:CE1	17:Q:36:ILE:HD11	2.09	0.86
9:I:24:GLY:HA3	9:I:57:GLY:HA2	1.57	0.86
11:K:40:ILE:HG22	11:K:41:THR:HG23	1.58	0.86
1:A:1435:G:H2'	1:A:1436:U:C6	2.12	0.85
3:C:156:ARG:H	3:C:163:ALA:HA	1.42	0.84
7:G:15:ASP:OD2	7:G:44:TYR:OH	1.95	0.84
21:U:6:ARG:HD2	21:U:15:ARG:HH22	1.41	0.84
8:H:41:ARG:NH1	8:H:123:GLU:OE2	2.11	0.84
1:A:371:G:O2'	1:A:372:C:H5'	1.77	0.83
1:A:353:A:H5'	1:A:353:A:H8	1.43	0.83
6:F:2:ARG:NE	6:F:69:GLU:HG2	1.93	0.83
10:J:50:ILE:HG22	10:J:60:ARG:HD3	1.61	0.83
1:A:1212:U:O2'	1:A:1213:A:O5'	1.97	0.83
3:C:150:LYS:HG3	3:C:169:ALA:HB2	1.58	0.83
1:A:1285:A:H4'	1:A:1286:A:O5'	1.77	0.82
1:A:1095:U:H2'	1:A:1096:C:C6	2.14	0.82
18:R:32:ARG:HA	18:R:69:THR:HG21	1.61	0.82
6:F:97:PHE:HB2	18:R:32:ARG:NH1	1.94	0.82
10:J:91:PRO:HB2	10:J:94:VAL:HB	1.62	0.82
1:A:1498:UR3:O4'	1:A:1519[A]:MA6:H2	1.80	0.81
1:A:1136:U:H5''	1:A:1137:C:OP2	1.80	0.81
9:I:10:ARG:NH1	9:I:75:ASP:OD2	2.12	0.81
7:G:75:VAL:HG11	7:G:144:MET:HE3	1.62	0.81
16:P:26:ARG:HD2	16:P:31:LYS:O	1.80	0.81
17:Q:40:LYS:HD2	17:Q:42:TYR:CZ	2.14	0.81
1:A:737:A:H1'	6:F:73:ASN:ND2	1.95	0.81
10:J:63:PHE:HB3	14:N:58:LYS:HA	1.63	0.81
18:R:25:THR:HG21	18:R:42:ARG:HH21	1.43	0.81
20:T:50:GLU:HB2	20:T:99:LEU:HD12	1.63	0.81
13:M:19:LEU:O	13:M:22:ILE:HG12	1.81	0.81
3:C:64:VAL:HB	3:C:99:VAL:HB	1.62	0.81
1:A:266:G:H5'	1:A:268:C:H41	1.44	0.80
6:F:25:ILE:HD13	6:F:82:ARG:HD2	1.64	0.80
1:A:372:C:H4'	1:A:373:A:O5'	1.80	0.80
7:G:146:GLU:HA	7:G:149:ARG:HG2	1.62	0.80
1:A:1251:A:H4'	9:I:12:GLU:OE1	1.82	0.80
1:A:1366:C:O2'	10:J:60:ARG:NH1	2.13	0.80
8:H:28:ALA:HA	8:H:59:LEU:HD11	1.64	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:50:ILE:HA	10:J:60:ARG:HA	1.63	0.80
1:A:932:C:H4'	7:G:4:ARG:NH2	1.96	0.80
1:A:1406:U:O2'	1:A:1517[B]:G:N2	2.15	0.79
1:A:537:G:OP1	12:L:113:ARG:NH2	2.16	0.79
1:A:975:A:H5'	1:A:975:A:C8	2.18	0.79
1:A:983:A:OP1	14:N:3:ARG:NH2	2.15	0.79
2:B:197:VAL:HB	2:B:200:ILE:HG12	1.64	0.79
1:A:266:G:H5''	1:A:267:C:C5	2.16	0.79
1:A:1035:A:H2'	1:A:1036:G:H8	1.47	0.79
2:B:97:TRP:HH2	2:B:176:GLU:CD	1.90	0.79
12:L:19:ARG:HD3	12:L:19:ARG:H	1.47	0.79
1:A:432:A:H2'	1:A:433:C:O4'	1.82	0.79
1:A:1200:C:O2'	1:A:1205:U:O4	2.00	0.79
1:A:1540:PSU:H3'	1:A:1540:PSU:C6	2.11	0.79
11:K:101:SER:OG	11:K:103:LEU:HB2	1.82	0.79
21:U:10:ARG:HH11	21:U:10:ARG:HG3	1.46	0.79
1:A:673:G:H2'	1:A:674:G:C8	2.19	0.78
10:J:82:ILE:HA	10:J:85:LEU:HB2	1.62	0.78
1:A:737:A:H1'	6:F:73:ASN:HD21	1.48	0.78
1:A:946:A:H2'	1:A:947:G:C8	2.18	0.78
19:S:18:LYS:HG2	19:S:31:ILE:HD11	1.66	0.78
1:A:1054:C:O2	1:A:1054:C:H3'	1.84	0.78
1:A:1054:C:H42	23:W:34:G:H1'	1.48	0.78
1:A:1129:C:C4'	1:A:1130:A:OP2	2.32	0.78
8:H:87:SER:HA	8:H:93:VAL:HG23	1.66	0.77
1:A:103:C:OP1	20:T:17:ARG:NH1	2.18	0.77
1:A:1327:C:H5	21:U:6:ARG:HH22	1.32	0.77
1:A:677:U:H3	1:A:713:G:H22	1.30	0.77
1:A:1497:G:C2'	1:A:1498:UR3:H5'	2.15	0.77
2:B:124:SER:HB2	2:B:125:PRO:HD2	1.67	0.77
1:A:60:A:H4'	1:A:61:G:O5'	1.85	0.77
1:A:107:G:H2'	1:A:108:G:H5'	1.67	0.77
1:A:427:U:OP1	4:D:13:ARG:NH2	2.17	0.77
1:A:1028:C:N3	1:A:1034:G:N2	2.33	0.77
3:C:16:ARG:HD2	3:C:17:ASP:H	1.47	0.77
13:M:10:PRO:HB2	13:M:18:ALA:HB1	1.67	0.76
1:A:939:G:H2'	1:A:940:C:C6	2.20	0.76
1:A:390:C:O3'	16:P:28:ARG:NH2	2.17	0.76
17:Q:66:SER:O	17:Q:70:ARG:NH1	2.18	0.76
1:A:1397:C:H4'	1:A:1398:A:OP2	1.86	0.76
1:A:1331:G:O2'	1:A:1332:A:P	2.44	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1541:PSU:O4	1:A:1541:PSU:H2'	1.86	0.75
2:B:13:ALA:HB1	2:B:209:ARG:HB3	1.68	0.75
21:U:6:ARG:HD2	21:U:15:ARG:NH2	2.01	0.75
7:G:46:ALA:O	7:G:50:ILE:HG12	1.87	0.75
1:A:923:A:OP1	5:E:21:ALA:HB2	1.86	0.74
1:A:1128:C:H42	1:A:1143:G:H1	1.34	0.74
1:A:1281:U:O2'	1:A:1282:C:OP1	2.04	0.74
15:O:70:LEU:HD13	15:O:78:TYR:HA	1.69	0.74
20:T:57:ARG:HE	20:T:102:GLY:HA2	1.51	0.74
1:A:216:G:O2'	1:A:217:C:O5'	2.05	0.74
14:N:27:CYS:SG	14:N:29:ARG:HB2	2.27	0.74
1:A:656:C:O2'	15:O:28:GLN:OE1	2.04	0.74
3:C:5:ILE:HD13	3:C:10:PHE:HB2	1.69	0.74
7:G:38:LEU:O	7:G:42:ILE:HG13	1.87	0.74
1:A:699:C:N4	27:A:2306:HOH:O	2.19	0.74
15:O:87:ILE:O	15:O:88:ARG:HB2	1.86	0.74
3:C:27:LYS:HD3	3:C:27:LYS:N	2.00	0.74
9:I:90:PRO:O	9:I:93:ARG:HG3	1.87	0.74
1:A:1101:A:H4'	1:A:1102:A:O5'	1.87	0.74
1:A:21:G:H2'	1:A:22:G:C8	2.23	0.74
1:A:631:G:O2'	27:A:2340:HOH:O	2.05	0.74
1:A:1313:U:O4	19:S:4:SER:OG	2.03	0.74
7:G:12:LEU:H	7:G:12:LEU:HD12	1.52	0.74
1:A:1532:U:H2'	1:A:1533:C:H5''	1.71	0.73
1:A:1148:U:H2'	1:A:1149:C:O4'	1.88	0.73
11:K:69:ALA:O	11:K:73:MET:HG2	1.88	0.73
15:O:55:GLY:HA2	15:O:58:MET:HE2	1.70	0.73
4:D:20:TYR:HD2	4:D:26:CYS:HB3	1.53	0.73
1:A:107:G:C2'	1:A:108:G:H5'	2.18	0.73
1:A:1291:G:H4'	9:I:39:GLY:HA3	1.69	0.73
1:A:1352:C:H2'	1:A:1353:G:C8	2.23	0.73
1:A:1530:G:H4'	1:A:1530:G:OP1	1.89	0.73
20:T:14:LYS:HA	20:T:17:ARG:HG3	1.70	0.73
20:T:75:ASN:N	20:T:75:ASN:OD1	2.21	0.73
1:A:299:G:H2'	1:A:300:A:C8	2.24	0.73
12:L:111:LYS:NZ	12:L:111:LYS:HA	2.04	0.73
2:B:16:HIS:HB3	2:B:44:LEU:HD11	1.69	0.73
9:I:43:ALA:HA	9:I:74:ILE:HD13	1.68	0.73
1:A:370:C:C2'	1:A:371:G:H5'	2.19	0.73
4:D:102:ASP:OD1	4:D:103:ASN:N	2.21	0.73
20:T:82:SER:O	20:T:86:ARG:HG3	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:509:A:O2'	1:A:510:A:OP1	2.06	0.73
1:A:812:C:H4'	1:A:813:U:O5'	1.89	0.72
2:B:47:THR:HA	2:B:202:PRO:HG2	1.71	0.72
1:A:1347:G:O2'	1:A:1348:U:P	2.47	0.72
10:J:48:THR:HA	10:J:62:HIS:CB	2.20	0.72
16:P:22:THR:HA	16:P:33:ILE:HG13	1.69	0.72
1:A:328:C:O2'	1:A:329:A:OP2	2.08	0.72
1:A:1366:C:HO2'	10:J:60:ARG:HH12	1.37	0.72
1:A:1504:G:OP1	1:A:1507:A:H4'	1.90	0.72
3:C:34:LEU:HD21	3:C:38:ARG:NH2	2.04	0.72
5:E:144:THR:O	5:E:148:VAL:HG23	1.88	0.72
1:A:370:C:O2'	1:A:371:G:H5'	1.88	0.72
1:A:1131:G:H8	1:A:1131:G:OP2	1.72	0.72
1:A:1242:C:O2'	27:A:2149:HOH:O	2.08	0.72
1:A:1003(A):G:N2	1:A:1038:C:O2	2.23	0.72
3:C:138:VAL:HG23	3:C:151:VAL:HG23	1.71	0.72
4:D:98:GLU:OE2	4:D:107:ARG:NE	2.23	0.72
12:L:20:LYS:H	12:L:20:LYS:HD2	1.53	0.72
18:R:74:ARG:HB3	18:R:81:PHE:CE1	2.25	0.72
4:D:70:ILE:HD11	4:D:100:ARG:CZ	2.19	0.72
15:O:87:ILE:HG22	15:O:88:ARG:N	2.00	0.72
1:A:1180:A:H5''	1:A:1181:G:OP2	1.90	0.71
3:C:6:HIS:CD2	3:C:7:PRO:HD2	2.25	0.71
13:M:11:ARG:HG2	13:M:12:ASN:N	2.04	0.71
16:P:74:LEU:O	16:P:79:VAL:HG23	1.90	0.71
1:A:7:G:H5'	1:A:298:A:O4'	1.90	0.71
1:A:689:C:OP1	11:K:27:ASN:ND2	2.23	0.71
5:E:15:ARG:HB2	5:E:28:PHE:CE2	2.24	0.71
1:A:428:G:H1'	1:A:429:U:OP2	1.89	0.71
17:Q:67:LYS:HA	17:Q:70:ARG:HH12	1.53	0.71
19:S:11:VAL:HG13	19:S:38:SER:HB2	1.71	0.71
1:A:660:G:OP2	15:O:5:LYS:HE2	1.90	0.71
1:A:839:U:O2	1:A:839:U:H2'	1.89	0.71
20:T:13:LEU:HD12	20:T:14:LYS:N	2.05	0.71
1:A:1392:G:H21	1:A:1502:A:H8	1.36	0.71
1:A:1508:G:OP1	27:A:1927:HOH:O	2.07	0.71
12:L:33:ARG:HG2	12:L:62:SER:HB2	1.72	0.71
2:B:91:PRO:HG2	2:B:155:LEU:HD23	1.71	0.71
20:T:85:MET:HE2	20:T:104:LEU:HD23	1.71	0.71
18:R:47:THR:HG22	18:R:48:GLY:H	1.56	0.71
12:L:24:VAL:HG13	12:L:98:TYR:HE2	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:111:LYS:HA	12:L:111:LYS:HZ1	1.54	0.71
19:S:40:ILE:HG23	19:S:62:ILE:HD11	1.73	0.71
1:A:397:A:H5'	1:A:398:C:OP1	1.91	0.70
1:A:344:A:H5'	1:A:345:C:C5	2.25	0.70
1:A:792:A:H4'	1:A:793:U:O5'	1.90	0.70
1:A:1240:U:H1'	7:G:38:LEU:HD21	1.73	0.70
2:B:118:LEU:HB3	2:B:142:LEU:HD12	1.73	0.70
1:A:542:G:OP1	4:D:10:ARG:NH2	2.19	0.70
1:A:196:A:OP1	20:T:68:LYS:NZ	2.19	0.70
2:B:101:MET:HE2	2:B:152:PHE:CD1	2.26	0.70
1:A:231:G:O2'	1:A:232:G:H5'	1.91	0.70
1:A:1095:U:H2'	1:A:1096:C:H6	1.56	0.70
1:A:1392:G:N2	1:A:1502:A:H8	1.89	0.70
7:G:50:ILE:HD11	7:G:121:ALA:HA	1.74	0.70
10:J:86:MET:HA	10:J:86:MET:HE3	1.73	0.70
1:A:1160:G:O6	1:A:1181:G:O6	2.10	0.70
1:A:141:A:H1'	1:A:182:U:O2	1.91	0.70
17:Q:66:SER:HB3	17:Q:69:LYS:HB2	1.73	0.69
3:C:155:GLY:HA2	3:C:164:ARG:O	1.92	0.69
5:E:144:THR:HG22	5:E:146:ALA:H	1.57	0.69
15:O:39:LEU:CD1	15:O:56:LEU:HB2	2.17	0.69
14:N:41:ARG:HG3	14:N:42:ILE:N	2.05	0.69
16:P:26:ARG:CD	16:P:31:LYS:O	2.41	0.69
9:I:3:GLN:HG3	9:I:20:ARG:HG2	1.75	0.69
1:A:1314:C:OP2	19:S:6:LYS:HD3	1.92	0.69
13:M:88:ARG:HG3	19:S:3:ARG:HH22	1.58	0.69
1:A:254:G:OP1	17:Q:67:LYS:O	2.09	0.69
1:A:1191:A:H5''	3:C:4:LYS:NZ	2.08	0.69
20:T:13:LEU:HD12	20:T:13:LEU:C	2.17	0.69
1:A:1442:G:C6	1:A:1446:A:N6	2.60	0.69
1:A:204:U:O2	1:A:204:U:H2'	1.93	0.68
1:A:1207:2MG:HM23	1:A:1208:C:H1'	1.75	0.68
1:A:1286:A:H2'	1:A:1287:A:H4'	1.74	0.68
1:A:1371:G:O3'	9:I:69:GLY:HA3	1.93	0.68
10:J:49:VAL:CG2	14:N:41:ARG:HB2	2.20	0.68
1:A:1054:C:H5	1:A:1196:U:C5	2.12	0.68
2:B:10:LEU:HD22	2:B:15:VAL:HG21	1.75	0.68
3:C:58:GLU:HB3	10:J:92:THR:HG21	1.74	0.68
19:S:40:ILE:HG22	19:S:67:VAL:HA	1.75	0.68
20:T:57:ARG:HE	20:T:102:GLY:CA	2.07	0.68
1:A:1435:G:H2'	1:A:1436:U:H6	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:180:ALA:HB1	3:C:182:ILE:HG13	1.76	0.68
15:O:78:TYR:CZ	15:O:82:ILE:HD11	2.27	0.68
1:A:835:U:OP1	18:R:64:ARG:NH2	2.26	0.68
4:D:111:ALA:HB2	4:D:120:LEU:HD12	1.76	0.68
5:E:76:ILE:HG12	5:E:118:ILE:HD12	1.76	0.68
10:J:63:PHE:HA	14:N:59:ALA:H	1.58	0.68
10:J:87:THR:O	10:J:88:LEU:HD23	1.94	0.68
1:A:560:U:H6	1:A:560:U:H5'	1.59	0.68
1:A:983:A:O2'	1:A:1050:G:OP2	2.12	0.68
1:A:1347:G:O2'	1:A:1348:U:OP2	2.12	0.68
7:G:93:PRO:HA	7:G:96:GLN:HG3	1.74	0.68
1:A:1256:A:H5'	1:A:1258:G:H1'	1.75	0.68
2:B:53:ARG:HA	2:B:56:ARG:NH1	2.09	0.68
1:A:499:A:H4'	1:A:500:G:OP1	1.94	0.67
4:D:189:PRO:HB2	4:D:194:LEU:HD21	1.76	0.67
12:L:24:VAL:HG13	12:L:98:TYR:CE2	2.28	0.67
1:A:795:C:H5''	1:A:796:C:OP2	1.95	0.67
6:F:9:VAL:HB	6:F:87:ARG:HB2	1.76	0.67
14:N:9:LYS:HD2	14:N:9:LYS:C	2.19	0.67
16:P:38:TYR:OH	16:P:47:ASP:OD1	2.10	0.67
1:A:1300:G:O2'	1:A:1301:U:P	2.52	0.67
18:R:46:GLU:H	18:R:46:GLU:CD	2.02	0.67
20:T:65:LYS:HA	20:T:68:LYS:HG3	1.76	0.67
1:A:1366:C:H2'	1:A:1367:C:C6	2.30	0.67
20:T:81:LYS:O	20:T:85:MET:HG3	1.94	0.67
1:A:1279:A:H5''	1:A:1280:A:OP1	1.94	0.67
1:A:1305:G:H22	1:A:1331:G:C2'	2.08	0.67
6:F:30:LEU:HD23	6:F:75:LEU:HD11	1.74	0.67
1:A:965:A:H4'	1:A:966:M2G:O5'	1.95	0.67
3:C:111:LEU:HD21	3:C:144:SER:O	1.94	0.67
1:A:304:U:O4	27:A:2271:HOH:O	2.13	0.67
1:A:976:G:H5'	1:A:1358:U:O2'	1.95	0.67
1:A:1366:C:H2'	1:A:1367:C:H6	1.59	0.67
1:A:527:7MG:OP2	25:A:1860:SRY:O32	2.07	0.67
1:A:1065:U:H4'	1:A:1066:C:O5'	1.95	0.67
3:C:43:LEU:O	3:C:47:LEU:HB2	1.95	0.67
1:A:61:G:O2'	27:A:1902:HOH:O	2.13	0.66
2:B:11:LEU:HD12	2:B:11:LEU:H	1.58	0.66
8:H:28:ALA:HA	8:H:59:LEU:CD1	2.25	0.66
21:U:5:ASP:O	21:U:11:GLY:HA3	1.94	0.66
1:A:833:U:H2'	1:A:834:C:C6	2.30	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1540:PSU:C6	1:A:1540:PSU:C3'	2.75	0.66
5:E:152:ARG:O	8:H:64:LYS:NZ	2.29	0.66
8:H:116:LYS:HG3	8:H:127:LEU:HD12	1.77	0.66
12:L:113:ARG:NH1	12:L:116:SER:H	1.93	0.66
1:A:560:U:H5''	1:A:566:G:N2	2.11	0.66
1:A:914:A:P	25:A:1860:SRV:HI33	2.36	0.66
11:K:78:GLN:O	11:K:103:LEU:HD23	1.96	0.66
18:R:38:GLU:H	18:R:38:GLU:CD	2.01	0.66
7:G:75:VAL:HG21	7:G:86:GLN:HB3	1.76	0.66
1:A:91:C:H2'	1:A:92:C:H6	1.61	0.66
18:R:88:LYS:OXT	18:R:88:LYS:HD3	1.94	0.66
1:A:1190:G:O2'	1:A:1191:A:P	2.54	0.66
9:I:81:ILE:O	9:I:85:LEU:HB2	1.95	0.66
1:A:1442:G:H5''	1:A:1443:G:OP1	1.96	0.66
3:C:128:PHE:HD2	3:C:129:ALA:N	1.93	0.66
1:A:266:G:H5''	1:A:267:C:H5	1.59	0.66
1:A:547:A:H4'	1:A:548:G:O5'	1.96	0.66
1:A:687:A:H4'	1:A:688:G:O5'	1.95	0.66
8:H:54:ASP:CG	8:H:55:GLY:H	2.03	0.66
1:A:646:U:H2'	1:A:647:C:C6	2.31	0.65
1:A:731:G:OP1	1:A:766:A:H1'	1.96	0.65
1:A:1006:C:H42	1:A:1024:G:H22	1.44	0.65
1:A:1054:C:N4	23:W:34:G:H1'	2.11	0.65
1:A:1229:A:OP2	13:M:114:ARG:HD3	1.95	0.65
2:B:114:ARG:NH1	2:B:118:LEU:HD21	2.11	0.65
1:A:825:G:H21	8:H:11:THR:HG21	1.61	0.65
1:A:1331:G:HO2'	1:A:1332:A:P	2.18	0.65
1:A:560:U:H5'	1:A:560:U:C6	2.31	0.65
1:A:765:G:H5''	1:A:766:A:OP1	1.95	0.65
1:A:1139:G:N2	1:A:1142:G:O6	2.29	0.65
3:C:34:LEU:HD13	14:N:25:VAL:HG21	1.78	0.65
7:G:45:ASP:O	7:G:49:ILE:HG13	1.96	0.65
10:J:16:LEU:HD13	10:J:70:ARG:HG2	1.79	0.65
1:A:1212:U:O2'	1:A:1213:A:P	2.54	0.65
10:J:39:PRO:HB3	10:J:70:ARG:NH1	2.10	0.65
17:Q:40:LYS:HD2	17:Q:42:TYR:CE1	2.32	0.65
20:T:10:LEU:C	20:T:10:LEU:HD12	2.22	0.65
1:A:651:C:O2'	1:A:652:U:H5'	1.97	0.65
1:A:1168:A:H2'	1:A:1169:A:C8	2.32	0.65
10:J:32:ALA:O	10:J:34:VAL:HG23	1.97	0.65
1:A:1515[B]:C:N4	1:A:1520[B]:G:O6	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:64:LEU:HD12	4:D:75:PHE:HZ	1.62	0.65
20:T:74:LYS:HB3	20:T:74:LYS:NZ	2.11	0.65
1:A:1005:A:C2	1:A:1026:G:N2	2.65	0.65
14:N:4:LYS:O	14:N:7:ILE:HG12	1.97	0.65
1:A:1350:A:OP2	9:I:118:LYS:HE2	1.96	0.65
2:B:174:VAL:O	2:B:178:ARG:HG2	1.97	0.65
12:L:25:PRO:C	12:L:27:LEU:H	2.03	0.65
8:H:82:HIS:ND1	8:H:138:TRP:NE1	2.44	0.65
10:J:63:PHE:HZ	14:N:45:ARG:HA	1.62	0.65
1:A:1314:C:C5	19:S:6:LYS:HE2	2.33	0.64
3:C:72:LYS:HD3	3:C:75:VAL:HG21	1.79	0.64
1:A:983:A:H5'	1:A:984:C:OP2	1.96	0.64
1:A:1047:G:H2'	1:A:1048:G:H5'	1.79	0.64
8:H:86:ILE:HD12	8:H:133:LEU:HD22	1.79	0.64
10:J:32:ALA:HB3	10:J:75:ILE:O	1.98	0.64
1:A:262:A:H5'	20:T:74:LYS:HG3	1.80	0.64
1:A:918:A:H2'	1:A:919:A:C8	2.32	0.64
1:A:1182:G:O2'	1:A:1183:A:P	2.55	0.64
3:C:130:VAL:O	3:C:134:ILE:HG13	1.98	0.64
9:I:126:SER:C	9:I:128:ARG:H	2.03	0.64
11:K:126:ARG:O	11:K:127:LYS:HE2	1.97	0.64
12:L:53:ARG:HH12	12:L:92:OTD:CG	2.10	0.64
21:U:10:ARG:HH11	21:U:10:ARG:CG	2.11	0.64
1:A:99:C:H2'	1:A:101:A:C8	2.33	0.64
7:G:51:GLN:O	7:G:52:GLU:HG2	1.98	0.64
17:Q:63:ARG:HG2	17:Q:64:PRO:HD2	1.79	0.64
18:R:36:ASN:OD1	18:R:39:VAL:HG12	1.96	0.64
13:M:88:ARG:HG2	13:M:98:VAL:CG1	2.28	0.64
1:A:353:A:H5'	1:A:353:A:C8	2.29	0.64
1:A:580:U:H2'	1:A:581:G:O4'	1.98	0.64
1:A:620:C:H2'	1:A:621:A:O4'	1.97	0.64
1:A:928:G:O2'	1:A:1533:C:OP1	2.16	0.64
1:A:1347:G:C2'	1:A:1348:U:OP2	2.45	0.64
4:D:36:ARG:HB3	4:D:38:TYR:CE2	2.33	0.64
8:H:82:HIS:NE2	8:H:84:ARG:HB2	2.13	0.64
1:A:1399:C:O2	1:A:1401:G:C5	2.51	0.64
1:A:1443:G:H4'	1:A:1446:A:C5'	2.27	0.64
1:A:966:M2G:HM22	1:A:967:5MC:O2	1.98	0.64
1:A:1003(A):G:N2	1:A:1038:C:C2	2.66	0.64
5:E:51:VAL:O	5:E:55:VAL:HG23	1.98	0.64
5:E:71:LEU:HD21	5:E:115:VAL:HG22	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:630:G:H5'	1:A:631:G:OP2	1.98	0.64
1:A:1510:U:H2'	1:A:1511:G:C8	2.32	0.64
3:C:5:ILE:O	3:C:5:ILE:HD12	1.98	0.64
6:F:50:TYR:CE1	18:R:77:GLY:HA2	2.33	0.64
12:L:42:THR:OG1	12:L:52:LEU:HB3	1.98	0.64
13:M:37:THR:HG23	13:M:55:ARG:HD2	1.79	0.64
17:Q:65:ILE:HD12	17:Q:65:ILE:N	2.13	0.64
12:L:28:LYS:C	12:L:30:ALA:N	2.55	0.63
18:R:46:GLU:OE2	18:R:46:GLU:N	2.23	0.63
1:A:45:U:H2'	1:A:46:G:C8	2.33	0.63
1:A:1443:G:C4'	1:A:1446:A:O5'	2.45	0.63
2:B:69:LEU:HD22	2:B:71:VAL:HG23	1.80	0.63
3:C:6:HIS:HD2	3:C:7:PRO:HD2	1.61	0.63
6:F:4:TYR:CE1	6:F:92:LYS:HG2	2.33	0.63
20:T:74:LYS:HA	20:T:74:LYS:HZ3	1.62	0.63
13:M:34:LEU:HD13	13:M:41:PRO:HA	1.79	0.63
20:T:67:ALA:HA	20:T:73:HIS:H	1.62	0.63
1:A:192:U:H1'	20:T:103:GLY:HA2	1.80	0.63
3:C:130:VAL:HG21	3:C:157:ILE:HG23	1.80	0.63
1:A:972:C:OP1	10:J:57:LYS:NZ	2.19	0.63
1:A:598:U:H4'	8:H:94:TYR:CD1	2.34	0.63
4:D:32:ALA:HA	4:D:35:ARG:HG3	1.81	0.63
1:A:509:A:N3	1:A:543:C:O2'	2.29	0.63
5:E:43:LEU:HB2	5:E:136:MET:HE2	1.81	0.63
19:S:31:ILE:HG21	19:S:49:ILE:HG23	1.79	0.63
4:D:188:LEU:HD23	4:D:189:PRO:HD2	1.80	0.63
1:A:359:U:H2'	1:A:360:A:C8	2.33	0.63
1:A:1493:A:N1	23:W:36:A:O2'	2.26	0.62
2:B:44:LEU:H	2:B:44:LEU:HD22	1.64	0.62
8:H:86:ILE:HG13	8:H:135:CYS:HA	1.79	0.62
1:A:359:U:H2'	1:A:360:A:H8	1.64	0.62
1:A:882:C:O2'	1:A:883:C:H5'	2.00	0.62
12:L:60:LEU:HB2	12:L:64:TYR:O	1.98	0.62
1:A:1296:C:H4'	1:A:1302:U:C5	2.34	0.62
4:D:22:LYS:HB2	4:D:26:CYS:SG	2.39	0.62
3:C:151:VAL:O	3:C:167:TRP:O	2.16	0.62
6:F:22:GLU:OE2	6:F:82:ARG:HD3	1.98	0.62
2:B:74:LYS:HD2	2:B:166:ASP:HB2	1.82	0.62
7:G:111:ARG:HB3	7:G:113:GLU:HG2	1.81	0.62
15:O:87:ILE:CG2	15:O:88:ARG:H	2.01	0.62
1:A:376:G:H2'	1:A:377:G:H8	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:814:A:H2'	1:A:816:A:C5'	2.29	0.62
1:A:1047:G:C2'	1:A:1048:G:H5'	2.29	0.62
1:A:1304:G:C6	1:A:1305:G:N1	2.67	0.62
2:B:144:ARG:HD2	2:B:145:LEU:HD23	1.82	0.62
9:I:70:LYS:O	9:I:74:ILE:HG13	1.99	0.62
13:M:63:THR:HG23	13:M:64:TRP:H	1.63	0.62
13:M:66:LEU:O	13:M:69:GLU:HB2	1.99	0.62
1:A:1502:A:H2	1:A:1505:G:H1	1.48	0.62
6:F:10:LEU:CD1	6:F:59:TYR:HB3	2.29	0.62
19:S:70:LYS:N	19:S:73:GLU:OE2	2.32	0.62
1:A:1342:C:O2'	9:I:124:GLN:HB2	1.99	0.62
2:B:82:ARG:O	2:B:86:GLU:HG3	2.00	0.62
2:B:91:PRO:HG2	2:B:155:LEU:CD2	2.30	0.62
3:C:5:ILE:CG2	10:J:51:ARG:HH12	2.12	0.62
3:C:35:GLU:OE1	3:C:95:THR:HB	2.00	0.62
3:C:167:TRP:HZ3	3:C:169:ALA:HB3	1.64	0.62
9:I:93:ARG:NH1	9:I:93:ARG:HB3	2.14	0.62
9:I:97:LYS:HA	9:I:102:LEU:HD11	1.82	0.62
12:L:10:LEU:HB3	17:Q:32:TYR:CE1	2.35	0.62
19:S:33:THR:HG22	19:S:35:SER:N	2.06	0.62
1:A:116:A:H2'	1:A:117:G:H8	1.65	0.61
11:K:57:THR:HG22	11:K:59:TYR:H	1.64	0.61
16:P:52:ASP:OD1	16:P:54:GLU:HG3	1.99	0.61
19:S:17:GLU:O	19:S:21:GLU:HB2	2.00	0.61
1:A:130:A:OP2	1:A:190(E):U:O2'	2.10	0.61
1:A:665:A:H2'	1:A:732:C:O2	2.00	0.61
2:B:128:GLU:HA	2:B:135:GLN:NE2	2.14	0.61
1:A:972:C:P	10:J:57:LYS:HD3	2.40	0.61
2:B:71:VAL:HG22	2:B:93:VAL:HB	1.83	0.61
1:A:667:G:H4'	15:O:51:HIS:CE1	2.34	0.61
1:A:913:A:H1'	1:A:914:A:OP2	2.00	0.61
1:A:974:A:P	14:N:41:ARG:HH12	2.24	0.61
1:A:1343:G:H2'	1:A:1344:C:C6	2.36	0.61
4:D:62:GLN:OE1	4:D:65:ARG:NH1	2.33	0.61
10:J:48:THR:HA	10:J:62:HIS:HB3	1.81	0.61
1:A:192:U:C1'	20:T:103:GLY:HA2	2.30	0.61
9:I:55:ALA:O	9:I:56:LEU:HD23	2.01	0.61
1:A:281:G:O2'	1:A:282:A:OP2	2.15	0.61
1:A:1402:4OC:HM22	1:A:1403:C:H5'	1.82	0.61
1:A:1518[B]:MA6:H102	1:A:1519[B]:MA6:H103	1.83	0.61
1:A:108:G:H2'	1:A:109:A:OP1	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1212:U:HO2'	1:A:1213:A:P	2.24	0.61
1:A:1406:U:H3'	1:A:1407:5MC:HM53	1.82	0.61
12:L:113:ARG:HH11	12:L:116:SER:H	1.48	0.61
1:A:262:A:C6	1:A:263:A:C6	2.89	0.61
10:J:46:ARG:HH11	10:J:46:ARG:HG3	1.66	0.61
1:A:706:A:O4'	11:K:29:ILE:HD11	2.00	0.60
1:A:938:A:N6	1:A:939:G:C6	2.69	0.60
14:N:8:GLU:O	14:N:11:LYS:HE3	2.00	0.60
1:A:1178:G:N7	9:I:97:LYS:NZ	2.47	0.60
1:A:1190:G:O2'	1:A:1191:A:OP2	2.19	0.60
3:C:188:LEU:HD11	3:C:195:VAL:HG22	1.83	0.60
7:G:78:ARG:HD2	7:G:156:TRP:HE3	1.65	0.60
1:A:1026:G:O2'	1:A:1027:C:OP1	2.18	0.60
1:A:1195:C:H5''	1:A:1196:U:OP2	2.01	0.60
2:B:80:ILE:HD11	2:B:208:ILE:HG22	1.83	0.60
2:B:219:VAL:O	2:B:223:ILE:HG12	2.00	0.60
4:D:24:GLU:O	4:D:25:ARG:HB3	2.01	0.60
7:G:12:LEU:HD12	7:G:12:LEU:N	2.16	0.60
13:M:65:LYS:C	13:M:66:LEU:HD23	2.25	0.60
1:A:109:A:H2'	1:A:326:G:N2	2.15	0.60
1:A:281:G:O2'	1:A:282:A:P	2.59	0.60
1:A:983:A:H1'	1:A:1049:U:O2	2.01	0.60
2:B:97:TRP:CH2	2:B:176:GLU:CD	2.77	0.60
3:C:30:ARG:HB3	14:N:36:PHE:O	2.01	0.60
4:D:170:VAL:CG1	4:D:174:LEU:HB2	2.31	0.60
8:H:27:PRO:HA	8:H:58:TYR:CD2	2.37	0.60
13:M:57:ARG:HG2	13:M:61:GLU:HG3	1.84	0.60
1:A:579:G:H5'	1:A:728:A:H1'	1.84	0.60
1:A:1391:U:H2'	1:A:1392:G:C8	2.36	0.60
2:B:130:ARG:HB3	2:B:131:PRO:CD	2.28	0.60
2:B:158:LEU:H	2:B:158:LEU:HD12	1.67	0.60
5:E:76:ILE:HG23	5:E:77:PRO:HD2	1.83	0.60
10:J:32:ALA:CB	10:J:76:ASN:HB2	2.31	0.60
1:A:631:G:O3'	1:A:632:A:H8	1.84	0.60
3:C:155:GLY:HA3	3:C:163:ALA:HB1	1.83	0.60
10:J:8:LEU:CD2	10:J:96:ILE:HG12	2.31	0.60
12:L:47:LYS:N	12:L:48:PRO:HD2	2.15	0.60
1:A:190(F):G:H4'	1:A:190(G):G:OP2	2.00	0.60
1:A:328:C:O2	1:A:328:C:C2'	2.44	0.60
1:A:524:G:H2'	1:A:525:C:C6	2.36	0.60
1:A:1349:A:OP1	9:I:118:LYS:HD2	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:74:LYS:HB3	20:T:74:LYS:HZ2	1.64	0.60
1:A:1097:C:H2'	1:A:1098:C:C6	2.37	0.60
1:A:1128:C:O2'	1:A:1130:A:C8	2.51	0.60
4:D:28:SER:O	4:D:30:LYS:N	2.33	0.60
5:E:24:ARG:HB3	5:E:24:ARG:HH11	1.66	0.60
1:A:633:G:H2'	1:A:634:C:C6	2.37	0.60
10:J:38:ILE:HB	10:J:71:LEU:HB3	1.83	0.60
10:J:50:ILE:HA	10:J:60:ARG:CA	2.30	0.60
17:Q:3:LYS:HD3	17:Q:61:GLU:O	2.02	0.60
1:A:337:C:H2'	1:A:338:A:C8	2.37	0.60
1:A:371:G:C2'	1:A:372:C:H5'	2.31	0.60
7:G:5:ARG:NE	7:G:7:ALA:HA	2.17	0.60
9:I:39:GLY:O	9:I:40:LEU:HD23	2.02	0.60
13:M:65:LYS:CG	13:M:69:GLU:HB3	2.31	0.60
1:A:889:A:H4'	1:A:890:G:OP1	2.00	0.59
16:P:34:GLU:OE2	16:P:55:ARG:HD2	2.02	0.59
20:T:39:LYS:HD3	20:T:55:ILE:HD13	1.83	0.59
1:A:1004:A:O2'	1:A:1005:A:OP1	2.15	0.59
1:A:1052:U:H2'	1:A:1055:A:OP1	2.02	0.59
1:A:1399:C:C2	1:A:1502:A:N6	2.71	0.59
5:E:12:LEU:HD13	5:E:31:LEU:HB2	1.85	0.59
6:F:33:TYR:CE2	6:F:74:ASP:HB3	2.36	0.59
1:A:284:G:H2'	1:A:285:G:H8	1.67	0.59
1:A:814:A:H2'	1:A:816:A:H5'	1.84	0.59
1:A:1540:PSU:H2'	1:A:1541:PSU:H5''	1.84	0.59
5:E:11:ILE:HG23	5:E:105:VAL:HG22	1.84	0.59
8:H:104:ARG:O	8:H:105:ARG:C	2.45	0.59
19:S:80:TYR:CE1	19:S:81:ARG:HD3	2.37	0.59
1:A:1498:UR3:C4'	1:A:1519[A]:MA6:H2	2.33	0.59
4:D:148:VAL:HG12	4:D:149:ALA:N	2.17	0.59
19:S:40:ILE:CG2	19:S:62:ILE:HD11	2.31	0.59
1:A:328:C:H1'	1:A:329:A:OP2	2.03	0.59
1:A:664:G:OP1	18:R:64:ARG:HD2	2.02	0.59
10:J:48:THR:HA	10:J:62:HIS:HB2	1.85	0.59
1:A:1381:U:C5	1:A:1382:C:C5	2.90	0.59
1:A:1405:G:HO2'	1:A:1518[B]:MA6:HO2'	1.48	0.59
1:A:631:G:H2'	27:A:2342:HOH:O	2.02	0.59
1:A:1249:C:O2'	9:I:73:GLN:NE2	2.35	0.59
1:A:110:C:H2'	1:A:111:G:O4'	2.03	0.59
1:A:501:C:H2'	1:A:502:G:C8	2.37	0.59
1:A:959:A:C2	1:A:1222:G:O4'	2.55	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1157:A:C2	1:A:1181:G:H1'	2.37	0.59
1:A:1356:G:H2'	1:A:1357:A:C8	2.37	0.59
1:A:1425:U:H3	1:A:1475:G:H1	1.49	0.59
19:S:15:LEU:O	19:S:19:VAL:HG12	2.03	0.59
1:A:1499:A:H1'	1:A:1520[A]:G:H5'	1.84	0.59
2:B:78:GLN:O	2:B:94:ASN:ND2	2.22	0.59
6:F:89:MET:HE2	18:R:76:LEU:HG	1.85	0.59
18:R:36:ASN:CG	18:R:39:VAL:HG12	2.28	0.59
3:C:150:LYS:HD3	3:C:152:ILE:HD11	1.84	0.59
4:D:64:LEU:HD12	4:D:75:PHE:CZ	2.38	0.59
1:A:600:C:OP1	8:H:97:VAL:HG12	2.03	0.58
1:A:689:C:P	11:K:46:GLY:HA3	2.43	0.58
1:A:914:A:OP1	25:A:1860:SRY:HI33	2.02	0.58
1:A:976:G:OP2	1:A:1358:U:O2'	2.20	0.58
1:A:1127:G:N2	1:A:1145:C:C2	2.71	0.58
2:B:63:MET:HB3	2:B:225:ALA:HB1	1.84	0.58
4:D:25:ARG:HA	4:D:28:SER:HB2	1.85	0.58
17:Q:31:LEU:HG	17:Q:32:TYR:CE2	2.37	0.58
1:A:474:G:O2'	1:A:475:G:H5'	2.04	0.58
1:A:991:U:O2'	1:A:992:U:O5'	2.17	0.58
1:A:1226:C:H4'	1:A:1227:A:OP1	2.01	0.58
1:A:1498:UR3:C2'	1:A:1499:A:OP2	2.51	0.58
5:E:79:GLU:HA	5:E:91:LEU:O	2.03	0.58
8:H:64:LYS:HG2	8:H:79:VAL:HG21	1.85	0.58
3:C:23:TYR:OH	10:J:9:ARG:HD3	2.03	0.58
1:A:179:A:H2'	1:A:180:U:C6	2.38	0.58
1:A:1320:C:H2'	1:A:1321:C:O4'	2.04	0.58
7:G:20:ASP:OD2	7:G:63:LYS:HE2	2.04	0.58
1:A:35:G:H2'	1:A:36:C:C6	2.39	0.58
1:A:1022:G:H2'	1:A:1023:G:C8	2.38	0.58
1:A:1305:G:N2	1:A:1331:G:O2'	2.36	0.58
4:D:63:LYS:HD2	4:D:198:VAL:HG22	1.85	0.58
7:G:5:ARG:HG3	7:G:7:ALA:H	1.67	0.58
1:A:1157:A:H4'	1:A:1158:C:O5'	2.03	0.58
2:B:22:LYS:HG3	2:B:23:ARG:N	2.19	0.58
2:B:27:LYS:HD2	2:B:193:ASP:OD1	2.04	0.58
4:D:24:GLU:HG2	4:D:25:ARG:N	2.17	0.58
6:F:91:VAL:HG12	6:F:92:LYS:O	2.04	0.58
7:G:69:VAL:HG12	7:G:100:ALA:HA	1.86	0.58
8:H:20:TYR:CE1	8:H:76:PRO:HG2	2.39	0.58
1:A:1057:G:H5''	3:C:154:SER:CB	2.25	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:150:GLU:OE2	4:D:150:GLU:N	2.28	0.58
8:H:102:ARG:H	8:H:102:ARG:CD	2.15	0.58
19:S:15:LEU:HA	19:S:18:LYS:HB2	1.85	0.58
1:A:117:G:OP2	27:A:1918:HOH:O	2.17	0.58
2:B:161:ALA:HB1	2:B:185:ILE:HD11	1.85	0.58
3:C:126:ARG:O	3:C:127:ARG:HB2	2.03	0.58
5:E:144:THR:HG22	5:E:146:ALA:N	2.19	0.58
12:L:69:TYR:CD1	12:L:90:VAL:HG21	2.39	0.58
15:O:3:ILE:HD13	15:O:34:LEU:HD13	1.85	0.58
19:S:27:GLU:HG2	19:S:28:LYS:H	1.69	0.58
1:A:1054:C:N4	23:W:34:G:C1'	2.59	0.58
2:B:106:LYS:O	2:B:109:SER:OG	2.21	0.58
10:J:62:HIS:O	10:J:62:HIS:ND1	2.32	0.58
19:S:41:VAL:HG23	19:S:43:GLU:HG2	1.85	0.58
20:T:10:LEU:CD1	20:T:12:ALA:H	2.17	0.58
1:A:975:A:H4'	1:A:976:G:C5'	2.30	0.58
2:B:17:PHE:O	2:B:204:ASN:HB2	2.04	0.58
9:I:79:LEU:HD22	9:I:83:ARG:HG3	1.86	0.58
13:M:16:ASP:N	13:M:16:ASP:OD2	2.37	0.57
13:M:88:ARG:HG2	13:M:98:VAL:HG12	1.86	0.57
17:Q:22:LEU:HD12	17:Q:23:VAL:N	2.18	0.57
1:A:945:G:C2	1:A:946:A:C8	2.92	0.57
1:A:1189:C:OP1	10:J:51:ARG:NH2	2.30	0.57
1:A:1513:A:H2'	1:A:1514:C:C6	2.39	0.57
4:D:150:GLU:CD	4:D:150:GLU:N	2.57	0.57
1:A:116:A:H2'	1:A:117:G:C8	2.39	0.57
2:B:130:ARG:HH21	3:C:207:VAL:HG21	1.69	0.57
15:O:56:LEU:HA	15:O:59:MET:HE2	1.86	0.57
1:A:200:G:H2'	1:A:201:C:O4'	2.04	0.57
1:A:337:C:H2'	1:A:338:A:H8	1.68	0.57
1:A:954:G:H21	1:A:1227:A:H62	1.52	0.57
5:E:24:ARG:HB3	5:E:24:ARG:NH1	2.19	0.57
5:E:95:ALA:O	5:E:98:THR:OG1	2.16	0.57
12:L:28:LYS:HB3	12:L:30:ALA:HB2	1.86	0.57
1:A:372:C:H1'	1:A:373:A:OP2	2.04	0.57
1:A:1208:C:H2'	1:A:1209:C:H6	1.69	0.57
13:M:23:TYR:HB3	13:M:67:GLU:H	1.69	0.57
17:Q:48:GLU:HB2	17:Q:50:LYS:HG3	1.85	0.57
20:T:56:MET:HE3	20:T:88:VAL:HG11	1.85	0.57
1:A:77:G:O2'	1:A:78:G:H5'	2.04	0.57
1:A:833:U:H2'	1:A:834:C:H6	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1069:C:O2'	1:A:1192:C:H1'	2.05	0.57
1:A:1208:C:H2'	1:A:1209:C:C6	2.39	0.57
2:B:167:PRO:HG2	2:B:192:SER:CB	2.34	0.57
6:F:69:GLU:H	6:F:69:GLU:CD	2.11	0.57
1:A:739:C:O2'	15:O:42:HIS:ND1	2.33	0.57
7:G:15:ASP:HB3	7:G:20:ASP:H	1.69	0.57
8:H:84:ARG:O	8:H:135:CYS:HB2	2.04	0.57
17:Q:18:THR:HG23	17:Q:69:LYS:HE3	1.86	0.57
1:A:376:G:H5''	16:P:5:ARG:HD2	1.86	0.57
1:A:393:A:C2'	1:A:394:G:H5'	2.35	0.57
1:A:811:C:H4'	1:A:900:A:N6	2.19	0.57
1:A:1026:G:O6	1:A:1027:C:N4	2.37	0.57
1:A:1091:U:O2	1:A:1093:A:C8	2.58	0.57
1:A:1197:G:OP1	27:A:2127:HOH:O	2.18	0.57
5:E:36:ASP:OD2	5:E:38:GLN:HB2	2.04	0.57
15:O:70:LEU:HD13	15:O:78:TYR:CA	2.35	0.57
1:A:1053:G:C4	1:A:1199:U:C5	2.93	0.57
2:B:126:GLU:O	2:B:129:GLU:HG2	2.05	0.57
3:C:11:ARG:O	3:C:14:ILE:O	2.22	0.57
1:A:982:U:H4'	1:A:983:A:O5'	2.05	0.57
1:A:1003(A):G:H2'	1:A:1004:A:H4'	1.85	0.57
1:A:1035:A:H2'	1:A:1036:G:C8	2.35	0.57
8:H:102:ARG:CD	8:H:102:ARG:N	2.67	0.57
12:L:27:LEU:C	12:L:29:GLY:N	2.63	0.57
13:M:96:LEU:O	13:M:110:ARG:NH1	2.38	0.57
17:Q:31:LEU:HG	17:Q:32:TYR:CD2	2.40	0.57
17:Q:83:ASP:OD1	17:Q:83:ASP:N	2.37	0.57
1:A:1114:C:H2'	1:A:1115:C:H6	1.70	0.56
2:B:170:GLU:OE2	2:B:170:GLU:HA	2.05	0.56
1:A:310:G:OP2	16:P:27:LYS:HE2	2.05	0.56
2:B:25:ASN:ND2	2:B:193:ASP:HB2	2.20	0.56
6:F:42:GLU:HG3	6:F:61:LEU:CD2	2.35	0.56
8:H:103:VAL:HG21	8:H:109:ILE:C	2.30	0.56
17:Q:27:PHE:CD1	17:Q:36:ILE:HD11	2.40	0.56
1:A:386:C:H1'	27:A:1902:HOH:O	2.06	0.56
1:A:559:A:H4'	1:A:560:U:O5'	2.04	0.56
1:A:1054:C:O2'	1:A:1055:A:O5'	2.22	0.56
8:H:54:ASP:CG	8:H:55:GLY:N	2.63	0.56
15:O:50:HIS:O	15:O:53:HIS:HB3	2.05	0.56
1:A:289:G:OP2	27:A:1917:HOH:O	2.17	0.56
1:A:1338:G:H2'	1:A:1339:A:C8	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1392:G:O2'	1:A:1393:U:H5'	2.06	0.56
9:I:39:GLY:C	9:I:40:LEU:HD23	2.30	0.56
20:T:8:ARG:N	20:T:8:ARG:HD2	2.21	0.56
1:A:559:A:OP1	5:E:126:ARG:NH2	2.29	0.56
1:A:794:A:OP1	27:A:2172:HOH:O	2.17	0.56
1:A:946:A:H2'	1:A:947:G:H8	1.70	0.56
1:A:1238:A:OP1	1:A:1336:C:H5	1.89	0.56
8:H:113:SER:HB2	8:H:134:ILE:HD11	1.88	0.56
9:I:48:GLU:CD	9:I:51:ARG:HH21	2.13	0.56
1:A:216:G:O2'	1:A:217:C:O4'	2.13	0.56
1:A:539:A:H2'	1:A:540:G:C8	2.40	0.56
1:A:807:A:H2'	1:A:808:C:C6	2.41	0.56
1:A:827:U:H5''	1:A:828:A:OP2	2.04	0.56
1:A:1505:G:H4'	1:A:1506:U:O5'	2.06	0.56
8:H:82:HIS:HD1	8:H:138:TRP:NE1	2.03	0.56
12:L:35:GLY:HA3	12:L:60:LEU:HD13	1.87	0.56
12:L:58:VAL:O	12:L:65:GLU:HA	2.05	0.56
17:Q:24:GLU:OE1	17:Q:37:LYS:HD3	2.05	0.56
1:A:714:G:H2'	1:A:715:A:C8	2.40	0.56
12:L:126:LYS:O	12:L:127:GLU:HG3	2.06	0.56
1:A:872:A:H4'	1:A:873:A:OP1	2.04	0.56
1:A:1211:U:H2'	1:A:1212:U:OP2	2.06	0.56
1:A:1402:4OC:O2	1:A:1500:A:N1	2.39	0.56
1:A:1427:U:H2'	1:A:1428:A:C8	2.41	0.56
1:A:384:G:H2'	1:A:385:C:C6	2.41	0.56
2:B:134:GLU:O	2:B:138:LEU:HG	2.06	0.56
4:D:20:TYR:CD2	4:D:26:CYS:HB3	2.39	0.56
4:D:146:ILE:N	4:D:146:ILE:HD12	2.21	0.56
4:D:175:SER:HB3	4:D:186:LEU:HD21	1.88	0.56
1:A:1086:U:H3	1:A:1099:G:N2	1.98	0.56
2:B:178:ARG:O	8:H:71:GLY:HA2	2.05	0.56
3:C:73:PRO:O	3:C:77:ILE:HG12	2.06	0.56
1:A:1006:C:H42	1:A:1024:G:N2	2.04	0.55
1:A:327:A:H4'	1:A:328:C:OP2	2.06	0.55
1:A:721:G:H4'	1:A:722:A:O4'	2.05	0.55
1:A:1157:A:H2	1:A:1181:G:H1'	1.72	0.55
13:M:22:ILE:HB	13:M:25:ILE:HD12	1.88	0.55
20:T:92:LEU:O	20:T:96:GLY:N	2.39	0.55
1:A:267:C:H2'	1:A:268:C:C6	2.41	0.55
1:A:838:G:H2'	1:A:839:U:H5''	1.87	0.55
4:D:18:LYS:HD3	4:D:20:TYR:CE2	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:45:THR:HB	16:P:46:PRO:HD2	1.88	0.55
1:A:426:G:OP1	4:D:36:ARG:NH2	2.38	0.55
1:A:1118:C:H1'	1:A:1179:A:C5	2.41	0.55
3:C:72:LYS:HD3	3:C:75:VAL:CG2	2.37	0.55
4:D:25:ARG:HG2	4:D:25:ARG:O	2.06	0.55
5:E:143:ARG:NH1	8:H:77:GLU:OE2	2.39	0.55
13:M:79:LYS:HE2	13:M:83:ASP:OD1	2.06	0.55
19:S:31:ILE:HG22	19:S:49:ILE:HA	1.89	0.55
1:A:267:C:H2'	1:A:268:C:H6	1.71	0.55
25:A:1860:SRY:O51	12:L:46:LYS:HE3	2.05	0.55
5:E:98:THR:HB	5:E:117:ASP:HB3	1.89	0.55
11:K:126:ARG:O	11:K:127:LYS:HB2	2.06	0.55
12:L:28:LYS:O	12:L:29:GLY:C	2.49	0.55
19:S:58:VAL:HG23	19:S:60:VAL:HG23	1.89	0.55
1:A:35:G:H2'	1:A:36:C:H6	1.72	0.55
1:A:1499:A:C1'	1:A:1520[A]:G:H5'	2.37	0.55
2:B:130:ARG:HH21	3:C:207:VAL:CG2	2.20	0.55
3:C:86:VAL:O	3:C:90:GLU:HG3	2.06	0.55
9:I:53:VAL:HG21	9:I:85:LEU:HD21	1.89	0.55
10:J:8:LEU:HD23	10:J:96:ILE:HG12	1.88	0.55
11:K:91:ARG:HG2	11:K:92:GLU:N	2.18	0.55
13:M:11:ARG:HG2	13:M:12:ASN:HB2	1.89	0.55
1:A:109:A:C6	1:A:326:G:C6	2.94	0.55
1:A:1330:U:OP1	13:M:23:TYR:O	2.24	0.55
1:A:1065:U:H1'	1:A:1066:C:OP2	2.06	0.55
1:A:1131:G:H2'	1:A:1132:C:C6	2.41	0.55
1:A:1319:A:H5'	19:S:5:LEU:CD2	2.37	0.55
2:B:187:LEU:HD23	2:B:205:ASP:HB3	1.89	0.55
4:D:19:LEU:HD23	4:D:19:LEU:H	1.72	0.55
20:T:10:LEU:HD12	20:T:10:LEU:O	2.07	0.55
1:A:1178:G:N2	1:A:1180:A:H3'	2.21	0.55
1:A:1329:A:C2'	1:A:1330:U:H5'	2.36	0.55
2:B:51:LEU:O	2:B:55:PHE:HB2	2.07	0.55
1:A:197:A:C6	1:A:221:C:H5'	2.42	0.55
1:A:247:G:OP2	17:Q:100:LYS:HB2	2.07	0.55
1:A:424:G:H2'	1:A:425:G:H8	1.71	0.55
1:A:1131:G:OP2	1:A:1131:G:H3'	2.06	0.55
1:A:1236:A:H4'	1:A:1304:G:H4'	1.88	0.55
1:A:1319:A:H5'	19:S:5:LEU:HD22	1.88	0.55
2:B:53:ARG:HA	2:B:56:ARG:HH12	1.70	0.55
2:B:167:PRO:HG2	2:B:192:SER:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:24:GLU:HG2	4:D:25:ARG:H	1.72	0.55
4:D:58:LEU:HD23	4:D:58:LEU:C	2.32	0.55
1:A:115:G:H4'	1:A:116:A:O5'	2.06	0.54
1:A:393:A:O2'	1:A:394:G:H5'	2.07	0.54
1:A:448:A:C4	1:A:487:A:C2	2.95	0.54
1:A:1145:C:H4'	1:A:1146:A:OP1	2.06	0.54
1:A:1180:A:OP1	9:I:103:THR:HG23	2.08	0.54
7:G:75:VAL:HG13	7:G:75:VAL:O	2.06	0.54
17:Q:53:LEU:HD21	17:Q:85:VAL:HG11	1.89	0.54
1:A:17:U:H2'	1:A:18:C:C6	2.42	0.54
1:A:243:A:C2	1:A:246:A:C8	2.94	0.54
1:A:328:C:C2'	1:A:329:A:OP2	2.55	0.54
1:A:972:C:O5'	10:J:57:LYS:HD3	2.07	0.54
2:B:181:PHE:CD2	8:H:70:GLN:HB3	2.42	0.54
3:C:41:GLY:O	3:C:45:LYS:HG3	2.08	0.54
13:M:3:ARG:HA	13:M:9:ILE:HG12	1.88	0.54
13:M:65:LYS:HG3	13:M:69:GLU:HB3	1.88	0.54
20:T:74:LYS:NZ	20:T:74:LYS:CB	2.70	0.54
1:A:37:U:O2'	1:A:500:G:H4'	2.07	0.54
1:A:239:U:O4	27:A:2450:HOH:O	2.17	0.54
1:A:728:A:C8	15:O:54:ARG:NH1	2.76	0.54
1:A:1236:A:H2'	1:A:1237:C:C6	2.43	0.54
9:I:65:VAL:HG11	9:I:73:GLN:HB3	1.90	0.54
11:K:59:TYR:CE2	11:K:63:LEU:HD11	2.42	0.54
13:M:59:TYR:O	13:M:63:THR:HG22	2.07	0.54
19:S:10:PHE:C	19:S:10:PHE:CD2	2.86	0.54
20:T:16:HIS:CE1	20:T:20:LEU:HD11	2.42	0.54
1:A:1004:A:O2'	1:A:1038:C:O2	2.26	0.54
1:A:1260:C:O5'	1:A:1284:C:H4'	2.07	0.54
1:A:1465:C:H2'	1:A:1466:C:O4'	2.07	0.54
2:B:84:GLU:OE1	2:B:216:SER:HA	2.07	0.54
3:C:134:ILE:HG22	3:C:151:VAL:HB	1.88	0.54
8:H:53:VAL:HB	8:H:58:TYR:CD1	2.41	0.54
18:R:53:ARG:HD3	18:R:63:GLN:HB2	1.88	0.54
1:A:235:C:C5'	17:Q:70:ARG:HG2	2.30	0.54
1:A:390:C:H2'	1:A:391:G:C8	2.42	0.54
1:A:1239:A:C4	1:A:1298:C:N4	2.76	0.54
13:M:88:ARG:HG3	19:S:3:ARG:NH2	2.22	0.54
15:O:4:THR:OG1	15:O:7:GLU:OE2	2.19	0.54
1:A:46:G:H2'	1:A:366:C:C5	2.42	0.54
1:A:355:C:H5'	1:A:389:A:OP2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:628:G:O2'	1:A:629:G:H5'	2.07	0.54
1:A:1005:A:C4	1:A:1026:G:N2	2.75	0.54
1:A:1220:G:H2'	1:A:1221:G:C8	2.43	0.54
1:A:1486:G:H2'	1:A:1487:G:O4'	2.07	0.54
7:G:75:VAL:CG2	7:G:86:GLN:HB3	2.36	0.54
1:A:275:G:H5'	17:Q:14:LYS:HB3	1.89	0.54
1:A:563:A:H2'	1:A:567:G:C8	2.43	0.54
1:A:1300:G:C2'	1:A:1301:U:OP2	2.55	0.54
2:B:165:VAL:O	2:B:187:LEU:O	2.26	0.54
7:G:122:HIS:HD2	7:G:125:MET:HE2	1.71	0.54
8:H:53:VAL:HB	8:H:58:TYR:CE1	2.43	0.54
8:H:102:ARG:H	8:H:102:ARG:HD2	1.71	0.54
9:I:69:GLY:O	9:I:73:GLN:HG3	2.08	0.54
11:K:13:GLN:HA	11:K:75:TYR:O	2.07	0.54
11:K:14:VAL:O	11:K:15:ALA:HB3	2.07	0.54
1:A:190(L):U:O2	20:T:105:SER:HB2	2.07	0.54
1:A:501:C:H2'	1:A:502:G:H8	1.72	0.54
1:A:685:G:O2'	1:A:686:U:H5'	2.08	0.54
1:A:1023:G:O6	1:A:1024:G:C2	2.61	0.54
1:A:1049:U:H4'	1:A:1050:G:O5'	2.08	0.54
2:B:74:LYS:O	2:B:75:LYS:HB2	2.06	0.54
4:D:201:GLN:NE2	5:E:116:THR:HG23	2.22	0.54
8:H:26:VAL:HG23	8:H:27:PRO:HD2	1.90	0.54
12:L:53:ARG:HG3	12:L:93:LEU:HD21	1.90	0.54
17:Q:34:LYS:HG3	17:Q:35:VAL:N	2.23	0.54
18:R:47:THR:HG22	18:R:48:GLY:N	2.21	0.54
20:T:45:GLN:HB2	20:T:91:LEU:HD13	1.90	0.54
1:A:229:U:H5''	16:P:33:ILE:HD13	1.89	0.54
3:C:95:THR:C	3:C:97:LYS:H	2.14	0.54
3:C:130:VAL:HG12	3:C:134:ILE:HD11	1.89	0.54
10:J:90:LEU:N	10:J:91:PRO:HD2	2.22	0.54
11:K:14:VAL:HG21	11:K:40:ILE:HD11	1.89	0.54
1:A:322:C:H4'	20:T:23:ARG:HD2	1.89	0.54
1:A:1053:G:O2'	1:A:1199:U:H5	1.91	0.54
1:A:1277:C:O2'	1:A:1279:A:H1'	2.08	0.54
7:G:78:ARG:HD2	7:G:156:TRP:CE3	2.43	0.54
1:A:262:A:N6	1:A:263:A:N6	2.56	0.53
1:A:737:A:H2'	1:A:738:C:C6	2.42	0.53
5:E:127:ASN:C	5:E:127:ASN:OD1	2.51	0.53
17:Q:84:LEU:N	17:Q:84:LEU:HD23	2.23	0.53
1:A:755:G:OP2	15:O:65:ARG:HD2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:951:G:OP2	13:M:102:ARG:NH2	2.41	0.53
1:A:1515[B]:C:H2'	1:A:1516[B]:G:H5'	1.91	0.53
2:B:75:LYS:HA	2:B:78:GLN:HB2	1.91	0.53
8:H:25:ASP:OD1	8:H:60:ARG:HD3	2.08	0.53
19:S:50:ALA:HA	19:S:58:VAL:O	2.09	0.53
1:A:532:A:H61	3:C:193:TYR:HA	1.74	0.53
1:A:958:A:N3	1:A:985:C:O2'	2.33	0.53
1:A:1124:G:N7	1:A:1145:C:O2'	2.34	0.53
1:A:1349:A:OP1	9:I:120:ARG:HB2	2.08	0.53
1:A:428:G:H4'	1:A:429:U:O5'	2.08	0.53
1:A:688:G:H2'	1:A:689:C:H6	1.72	0.53
1:A:984:C:H42	1:A:1221:G:H1	1.56	0.53
1:A:1064:G:H22	1:A:1190:G:C2'	2.21	0.53
1:A:1269:A:N1	1:A:1312:G:O2'	2.38	0.53
15:O:17:ARG:HG3	15:O:17:ARG:NH1	2.10	0.53
16:P:74:LEU:HB3	16:P:79:VAL:HG21	1.90	0.53
1:A:537:G:H2'	1:A:538:G:C8	2.43	0.53
1:A:556:C:C2'	1:A:557:G:H5'	2.38	0.53
1:A:1124:G:H4'	10:J:38:ILE:HD11	1.90	0.53
1:A:1399:C:C2	1:A:1401:G:C5	2.96	0.53
1:A:1516[A]:G:H2'	1:A:1518[A]:MA6:OP2	2.09	0.53
8:H:103:VAL:HG21	8:H:109:ILE:O	2.07	0.53
10:J:35:SER:HB3	10:J:73:ASP:O	2.09	0.53
17:Q:100:LYS:HB3	17:Q:101:ARG:CZ	2.38	0.53
1:A:701:C:H4'	1:A:702:A:O5'	2.08	0.53
1:A:1372:U:H2'	1:A:1373:G:O4'	2.08	0.53
3:C:113:ALA:N	3:C:114:PRO:HD2	2.23	0.53
3:C:115:LEU:HD23	3:C:118:GLN:OE1	2.09	0.53
5:E:76:ILE:HG22	5:E:78:HIS:H	1.74	0.53
7:G:38:LEU:HD11	7:G:42:ILE:HD11	1.90	0.53
8:H:111:ILE:O	8:H:134:ILE:HB	2.09	0.53
10:J:63:PHE:CZ	14:N:45:ARG:HA	2.43	0.53
1:A:302:G:H5''	12:L:17:LYS:HE2	1.91	0.53
1:A:836:G:C6	1:A:851:G:C6	2.96	0.53
1:A:1211:U:C2'	1:A:1212:U:OP2	2.56	0.53
3:C:148:GLY:HA3	3:C:172:ARG:O	2.09	0.53
8:H:21:LYS:O	8:H:65:TYR:OH	2.21	0.53
12:L:56:ALA:HB2	12:L:70:ILE:HD11	1.91	0.53
1:A:432:A:O2'	1:A:433:C:P	2.66	0.53
1:A:620:C:N1	4:D:135:LEU:HD13	2.23	0.53
1:A:853:G:C2'	1:A:854:G:H5'	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:61:LYS:HD2	4:D:61:LYS:C	2.33	0.53
15:O:4:THR:HB	15:O:6:GLU:HG2	1.90	0.53
1:A:797:C:OP1	11:K:124:LYS:HE2	2.09	0.53
1:A:1034:G:N2	1:A:1035:A:N6	2.57	0.53
1:A:1049:U:H4'	1:A:1050:G:C5'	2.39	0.53
4:D:31:CYS:C	4:D:33:MET:H	2.16	0.53
4:D:201:GLN:O	4:D:205:GLU:HG3	2.09	0.53
6:F:101:ALA:HB2	18:R:28:GLU:HB2	1.91	0.53
1:A:176:C:H2'	1:A:177:C:H6	1.73	0.53
1:A:1054:C:OP1	1:A:1197:G:OP2	2.26	0.53
1:A:1502:A:N1	1:A:1504:G:C2	2.76	0.53
2:B:121:LEU:HD23	2:B:121:LEU:C	2.34	0.53
3:C:50:ALA:HB1	3:C:70:VAL:HG11	1.89	0.53
5:E:39:GLY:O	5:E:69:VAL:N	2.33	0.53
8:H:4:ASP:OD2	8:H:89:PRO:HD3	2.08	0.53
9:I:24:GLY:CA	9:I:57:GLY:HA2	2.35	0.53
9:I:111:ARG:O	9:I:113:LYS:HD2	2.08	0.53
19:S:7:LYS:HD2	19:S:7:LYS:C	2.34	0.53
1:A:627:G:O2'	1:A:628:G:H5'	2.09	0.52
1:A:938:A:C6	1:A:939:G:C5	2.97	0.52
1:A:939:G:H2'	1:A:940:C:H6	1.68	0.52
1:A:993:G:H4'	1:A:994:A:OP2	2.10	0.52
1:A:1003:G:C6	1:A:1003(A):G:C6	2.97	0.52
1:A:1253:G:H1'	1:A:1355:G:O2'	2.10	0.52
1:A:1357:A:H5''	1:A:1358:U:OP2	2.10	0.52
3:C:6:HIS:HD2	3:C:7:PRO:CD	2.21	0.52
3:C:128:PHE:CD2	3:C:129:ALA:N	2.75	0.52
5:E:11:ILE:HB	5:E:31:LEU:HB3	1.90	0.52
10:J:71:LEU:HD13	10:J:72:VAL:N	2.25	0.52
13:M:102:ARG:HG3	13:M:102:ARG:O	2.09	0.52
18:R:53:ARG:NE	18:R:58:LEU:O	2.41	0.52
1:A:117:G:P	27:A:1918:HOH:O	2.67	0.52
1:A:658:G:OP1	15:O:8:LYS:NZ	2.43	0.52
1:A:1379:G:OP1	7:G:6:ARG:NH2	2.42	0.52
5:E:90:VAL:O	5:E:91:LEU:HD23	2.08	0.52
17:Q:20:THR:HG21	17:Q:41:LYS:HD2	1.91	0.52
1:A:961:U:H2'	1:A:962:C:H5'	1.90	0.52
1:A:1028:C:N3	1:A:1034:G:C2	2.76	0.52
1:A:1049:U:H1'	1:A:1050:G:OP2	2.09	0.52
1:A:1120:G:N2	1:A:1154:G:H1'	2.24	0.52
4:D:15:GLU:OE2	4:D:59:ARG:NE	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:90:VAL:O	5:E:120:THR:HA	2.09	0.52
12:L:76:ASN:O	12:L:77:LEU:HD23	2.09	0.52
18:R:52:PRO:O	18:R:56:THR:HG23	2.09	0.52
1:A:1104:G:O5'	2:B:111:ARG:HD2	2.08	0.52
19:S:14:HIS:O	19:S:18:LYS:HE3	2.09	0.52
19:S:44:MET:O	19:S:62:ILE:HG21	2.09	0.52
1:A:266:G:C5'	1:A:268:C:H41	2.19	0.52
1:A:478:A:O2'	1:A:479:C:H5'	2.10	0.52
1:A:1525:G:P	11:K:120:ARG:HH22	2.33	0.52
2:B:68:ILE:O	2:B:90:MET:HB3	2.09	0.52
2:B:187:LEU:CD1	2:B:214:ILE:HG13	2.40	0.52
5:E:12:LEU:HD22	5:E:12:LEU:C	2.35	0.52
6:F:53:ALA:C	6:F:54:LYS:HG2	2.35	0.52
19:S:53:ASN:OD1	19:S:56:GLN:N	2.39	0.52
20:T:13:LEU:C	20:T:13:LEU:CD1	2.82	0.52
1:A:192:U:H2'	1:A:193:C:H6	1.74	0.52
1:A:409:G:OP1	4:D:24:GLU:O	2.27	0.52
5:E:71:LEU:HD11	5:E:113:ALA:O	2.09	0.52
12:L:6:THR:O	12:L:9:GLN:HB2	2.10	0.52
12:L:55:VAL:HG12	12:L:56:ALA:N	2.24	0.52
1:A:204:U:O2	1:A:204:U:C2'	2.57	0.52
1:A:476:G:O2'	1:A:477:G:H5'	2.10	0.52
1:A:537:G:H2'	1:A:538:G:H8	1.74	0.52
1:A:1241:G:H2'	1:A:1242:C:C6	2.44	0.52
5:E:11:ILE:HG12	5:E:33:VAL:HG23	1.91	0.52
20:T:84:LEU:HD23	20:T:84:LEU:C	2.35	0.52
1:A:451:A:O2'	27:A:2407:HOH:O	1.83	0.52
1:A:1300:G:O2'	1:A:1301:U:OP2	2.28	0.52
10:J:24:VAL:O	10:J:28:ARG:HG3	2.10	0.52
17:Q:100:LYS:HD2	17:Q:101:ARG:NH2	2.25	0.52
1:A:109:A:H4'	1:A:110:C:OP2	2.09	0.52
1:A:129:U:O3'	1:A:129(A):G:H3'	2.09	0.52
1:A:289:G:P	27:A:1915:HOH:O	2.67	0.52
1:A:1397:C:C4'	1:A:1398:A:OP2	2.58	0.52
6:F:10:LEU:HD12	6:F:59:TYR:HB3	1.92	0.52
17:Q:4:LYS:HD2	17:Q:6:LEU:HD21	1.92	0.52
17:Q:59:ILE:HG23	17:Q:71:PHE:CD1	2.44	0.52
1:A:62:U:OP1	1:A:385:C:O2'	2.27	0.52
1:A:364:A:N6	12:L:28:LYS:HE2	2.25	0.52
19:S:31:ILE:HD13	19:S:32:LYS:H	1.74	0.52
20:T:61:SER:O	20:T:65:LYS:HG3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:500:G:H2'	1:A:501:C:C6	2.45	0.51
3:C:5:ILE:HD12	3:C:5:ILE:C	2.35	0.51
12:L:20:LYS:HD2	12:L:20:LYS:N	2.25	0.51
1:A:1054:C:O2	1:A:1054:C:C3'	2.55	0.51
25:A:1860:SRY:HH23	12:L:48:PRO:HG3	1.92	0.51
2:B:80:ILE:HD13	2:B:212:GLN:HB2	1.92	0.51
15:O:73:GLU:OE1	15:O:73:GLU:HA	2.10	0.51
1:A:421:U:H4'	1:A:422:C:OP2	2.08	0.51
1:A:1003:G:N2	1:A:1039:C:O2	2.43	0.51
1:A:1342:C:H2'	1:A:1343:G:C8	2.46	0.51
3:C:12:LEU:HD11	14:N:51:GLY:HA2	1.92	0.51
4:D:8:VAL:O	4:D:11:LEU:N	2.40	0.51
10:J:42:THR:HG23	10:J:67:THR:O	2.09	0.51
20:T:105:SER:O	20:T:106:ALA:C	2.53	0.51
1:A:631:G:H5'	1:A:632:A:P	2.51	0.51
1:A:633:G:H2'	1:A:634:C:H6	1.75	0.51
1:A:1104:G:P	2:B:111:ARG:HD2	2.51	0.51
1:A:1502:A:H2	1:A:1505:G:N1	2.09	0.51
4:D:191:ARG:HG3	4:D:192:GLU:OE2	2.10	0.51
12:L:28:LYS:O	12:L:28:LYS:HG3	2.09	0.51
1:A:325:A:H2'	1:A:326:G:O4'	2.10	0.51
1:A:1005:A:H8	1:A:1005:A:OP2	1.92	0.51
1:A:1368:G:H5''	9:I:112:LYS:HB3	1.92	0.51
5:E:76:ILE:O	5:E:93:PRO:HB3	2.11	0.51
7:G:26:PHE:O	7:G:30:ILE:HG13	2.10	0.51
11:K:34:ASP:HB2	11:K:35:PRO:CD	2.41	0.51
16:P:58:TYR:CE1	16:P:62:VAL:HG21	2.45	0.51
1:A:563:A:H5''	1:A:564:C:OP1	2.09	0.51
1:A:731:G:H5'	1:A:766:A:H4'	1.91	0.51
1:A:1035:A:C4	1:A:1036:G:C8	2.98	0.51
1:A:1095:U:H2'	1:A:1096:C:O4'	2.09	0.51
5:E:36:ASP:CG	5:E:38:GLN:HB2	2.35	0.51
11:K:48:ILE:HG22	11:K:49:GLY:H	1.75	0.51
12:L:28:LYS:O	12:L:30:ALA:N	2.43	0.51
17:Q:68:ARG:H	17:Q:70:ARG:NH1	2.08	0.51
1:A:62:U:H2'	1:A:63:C:C6	2.46	0.51
1:A:945:G:H2'	1:A:945:G:N3	2.25	0.51
2:B:53:ARG:HB3	2:B:53:ARG:HH11	1.75	0.51
5:E:96:PRO:HA	5:E:117:ASP:OD2	2.11	0.51
13:M:15:VAL:HG23	13:M:43:THR:O	2.11	0.51
17:Q:65:ILE:HD12	17:Q:65:ILE:H	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:213:LEU:O	2:B:217:ARG:HG2	2.11	0.51
4:D:138:TYR:C	4:D:138:TYR:CD2	2.88	0.51
9:I:126:SER:C	9:I:128:ARG:N	2.68	0.51
1:A:76:C:O2'	1:A:77:G:H5'	2.10	0.51
1:A:1054:C:H5	1:A:1196:U:C6	2.29	0.51
1:A:1190:G:HO2'	1:A:1191:A:P	2.34	0.51
1:A:1300:G:O2'	1:A:1301:U:H6	1.93	0.51
2:B:103:THR:HA	2:B:180:LEU:HD11	1.92	0.51
7:G:40:ALA:HB3	9:I:41:VAL:HG21	1.91	0.51
9:I:36:TYR:HD2	9:I:37:PHE:CE2	2.29	0.51
9:I:118:LYS:C	9:I:120:ARG:H	2.18	0.51
12:L:126:LYS:C	12:L:127:GLU:HG3	2.35	0.51
15:O:7:GLU:O	15:O:11:VAL:HG13	2.11	0.51
1:A:905:U:H2'	1:A:906:G:H5'	1.93	0.51
1:A:1068:G:OP2	1:A:1068:G:H8	1.93	0.51
4:D:61:LYS:HA	4:D:203:VAL:HG22	1.92	0.51
11:K:14:VAL:HG12	11:K:16:SER:H	1.75	0.51
20:T:70:SER:HA	20:T:73:HIS:CD2	2.46	0.51
1:A:327:A:O3'	1:A:328:C:C4'	2.59	0.50
1:A:456:C:H2'	1:A:457:C:C6	2.46	0.50
1:A:867:G:C2'	1:A:868:C:H5'	2.41	0.50
1:A:1024:G:N7	1:A:1025:U:C4	2.79	0.50
1:A:1030(B):C:H2'	1:A:1030(C):G:O4'	2.11	0.50
3:C:18:TRP:CD1	14:N:54:PRO:HA	2.46	0.50
9:I:95:LYS:HD2	9:I:95:LYS:N	2.25	0.50
16:P:81:ARG:HG3	16:P:83:GLU:HG2	1.92	0.50
19:S:31:ILE:CG2	19:S:49:ILE:HG23	2.41	0.50
20:T:56:MET:HG3	20:T:84:LEU:HD22	1.93	0.50
1:A:502:G:H2'	1:A:503:C:O4'	2.12	0.50
1:A:728:A:H2'	1:A:729:A:O4'	2.11	0.50
1:A:1026:G:C2'	1:A:1027:C:OP1	2.59	0.50
1:A:1368:G:OP2	9:I:112:LYS:HD3	2.10	0.50
2:B:33:TYR:C	2:B:33:TYR:CD2	2.87	0.50
9:I:46:ALA:HB2	9:I:74:ILE:HG23	1.92	0.50
12:L:50:SER:O	12:L:51:ALA:HB2	2.10	0.50
1:A:427:U:OP2	1:A:428:G:O2'	2.29	0.50
1:A:428:G:C1'	1:A:429:U:OP2	2.59	0.50
1:A:1298:C:H4'	1:A:1299:A:O4'	2.11	0.50
1:A:1327:C:H5	21:U:6:ARG:NH2	2.06	0.50
8:H:83:ILE:HG23	8:H:83:ILE:O	2.11	0.50
9:I:4:TYR:CE2	9:I:88:TYR:HD1	2.28	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:17:ARG:HH11	15:O:17:ARG:CG	2.13	0.50
1:A:895:G:H2'	1:A:896:C:C6	2.46	0.50
2:B:185:ILE:H	2:B:185:ILE:HD12	1.77	0.50
3:C:52:LEU:O	3:C:52:LEU:HD23	2.11	0.50
12:L:117:ARG:HH22	12:L:124:LYS:HD3	1.76	0.50
17:Q:100:LYS:HB3	17:Q:101:ARG:NH2	2.27	0.50
1:A:357:G:C2	1:A:358:U:C5	2.99	0.50
4:D:88:VAL:O	4:D:92:VAL:HG23	2.11	0.50
12:L:19:ARG:H	12:L:19:ARG:CD	2.14	0.50
15:O:17:ARG:NH1	15:O:77:ARG:NH1	2.58	0.50
23:W:28:G:H2'	23:W:28:G:N3	2.27	0.50
1:A:828:A:H4'	1:A:828:A:OP1	2.10	0.50
5:E:71:LEU:CD2	5:E:115:VAL:HG22	2.41	0.50
17:Q:67:LYS:O	17:Q:68:ARG:HB2	2.10	0.50
1:A:149:A:H2'	1:A:150:C:C6	2.47	0.50
1:A:181:G:C4'	1:A:182:U:OP2	2.60	0.50
1:A:509:A:HO2'	1:A:510:A:P	2.32	0.50
1:A:529:G:O6	12:L:49:ASN:OD1	2.30	0.50
1:A:922:G:C6	1:A:923:A:C6	3.00	0.50
1:A:1256:A:H4'	1:A:1257:U:OP2	2.10	0.50
5:E:43:LEU:O	5:E:62:ALA:HA	2.12	0.50
1:A:657:G:H4'	15:O:28:GLN:HG2	1.94	0.50
1:A:1385:G:H2'	1:A:1386:G:O4'	2.11	0.50
6:F:42:GLU:HG3	6:F:61:LEU:HD23	1.92	0.50
18:R:47:THR:HA	18:R:83:GLU:HB2	1.93	0.50
1:A:977:A:O2'	1:A:979:C:OP2	2.30	0.50
1:A:1300:G:C6	1:A:1335:C:C5	2.99	0.50
2:B:141:GLU:O	2:B:145:LEU:HG	2.12	0.50
4:D:8:VAL:HG12	4:D:21:LEU:HD13	1.93	0.50
10:J:48:THR:HG23	10:J:62:HIS:HB3	1.94	0.50
13:M:11:ARG:CG	13:M:12:ASN:N	2.74	0.50
14:N:42:ILE:O	14:N:46:GLU:HG3	2.11	0.50
17:Q:76:LEU:HD12	17:Q:77:VAL:N	2.27	0.50
1:A:281:G:H8	1:A:281:G:O5'	1.93	0.49
1:A:806:C:O2'	1:A:807:A:H5'	2.12	0.49
1:A:961:U:C2'	1:A:962:C:H5'	2.42	0.49
1:A:1106:G:H5''	3:C:172:ARG:HG2	1.94	0.49
1:A:1401:G:C2	1:A:1402:4OC:H1'	2.47	0.49
1:A:1511:G:H2'	1:A:1512:U:O4'	2.11	0.49
2:B:24:TRP:HA	2:B:190:THR:HG22	1.94	0.49
8:H:11:THR:O	8:H:12:ARG:C	2.55	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:A:H2'	1:A:89:C:O4'	2.12	0.49
1:A:192:U:H2'	1:A:193:C:C6	2.46	0.49
1:A:587:G:O2'	1:A:588:G:OP2	2.22	0.49
1:A:814:A:H2'	1:A:816:A:H5''	1.93	0.49
1:A:1162:C:H2'	1:A:1163:C:C6	2.47	0.49
1:A:1292:U:P	7:G:41:ARG:HH22	2.35	0.49
1:A:1515[B]:C:C2'	1:A:1516[B]:G:H5'	2.42	0.49
3:C:6:HIS:O	3:C:10:PHE:N	2.46	0.49
10:J:45:ARG:HG2	10:J:47:PHE:CZ	2.47	0.49
11:K:108:ILE:N	11:K:108:ILE:HD12	2.27	0.49
13:M:8:GLU:HG3	13:M:22:ILE:HG23	1.94	0.49
19:S:43:GLU:H	19:S:43:GLU:CD	2.19	0.49
21:U:10:ARG:CG	21:U:10:ARG:NH1	2.71	0.49
1:A:281:G:HO2'	1:A:282:A:P	2.31	0.49
1:A:645:C:O2'	1:A:646:U:H5'	2.13	0.49
1:A:771:G:O2'	1:A:772:U:H5'	2.12	0.49
1:A:1057:G:H2'	1:A:1058:G:O4'	2.11	0.49
1:A:1207:2MG:H2'	1:A:1208:C:H6	1.77	0.49
3:C:20:SER:HB3	3:C:40:ARG:HH22	1.77	0.49
4:D:10:ARG:HG2	4:D:11:LEU:HD23	1.93	0.49
4:D:52:SER:O	4:D:56:VAL:HG23	2.12	0.49
6:F:24:GLU:OE2	6:F:28:ARG:NH1	2.45	0.49
10:J:12:ASP:OD1	10:J:14:LYS:N	2.43	0.49
13:M:36:LYS:HB2	13:M:59:TYR:HE2	1.77	0.49
1:A:384:G:H2'	1:A:385:C:H6	1.77	0.49
1:A:484:G:H5'	1:A:486:U:O4'	2.13	0.49
1:A:742:G:C5'	15:O:58:MET:HE1	2.41	0.49
1:A:838:G:N2	1:A:849:C:C2	2.81	0.49
1:A:973:G:H3'	1:A:974:A:H5''	1.94	0.49
1:A:1062:U:H2'	1:A:1063:C:C6	2.47	0.49
1:A:1406:U:HO2'	1:A:1517[B]:G:N2	2.11	0.49
6:F:10:LEU:HD12	6:F:10:LEU:H	1.77	0.49
6:F:100:ASN:OD1	18:R:23:LYS:HE2	2.12	0.49
9:I:53:VAL:CG2	9:I:85:LEU:HD21	2.42	0.49
13:M:49:THR:HG22	13:M:52:GLU:N	2.19	0.49
16:P:38:TYR:HE2	16:P:50:LYS:HE2	1.77	0.49
19:S:22:LEU:O	19:S:26:GLY:O	2.30	0.49
1:A:295:C:H2'	1:A:296:U:O4'	2.12	0.49
1:A:477:G:H2'	1:A:478:A:H8	1.77	0.49
1:A:664:G:O2'	1:A:666:G:OP2	2.29	0.49
1:A:1203:C:H2'	1:A:1204:A:O4'	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1216:G:H2'	1:A:1217:C:H6	1.78	0.49
1:A:1423:G:H2'	1:A:1424:C:H6	1.77	0.49
2:B:8:LYS:O	2:B:12:GLU:HG3	2.12	0.49
2:B:69:LEU:HB3	2:B:162:ILE:HG22	1.94	0.49
4:D:54:TYR:CE2	4:D:58:LEU:HD12	2.48	0.49
10:J:19:SER:HB2	10:J:91:PRO:HG3	1.95	0.49
18:R:87:ARG:O	18:R:88:LYS:CB	2.60	0.49
1:A:370:C:H2'	1:A:371:G:H5'	1.93	0.49
1:A:421:U:H5'	1:A:422:C:C5	2.47	0.49
1:A:452:A:OP1	16:P:43:LYS:NZ	2.37	0.49
1:A:577:G:H1'	1:A:816:A:C4	2.48	0.49
1:A:1318:A:O2'	19:S:37:ARG:HD2	2.12	0.49
2:B:16:HIS:HB3	2:B:44:LEU:CD1	2.40	0.49
2:B:107:THR:O	2:B:110:GLN:HB2	2.13	0.49
3:C:20:SER:CB	3:C:40:ARG:HH22	2.24	0.49
4:D:12:CYS:HA	4:D:19:LEU:CD2	2.42	0.49
4:D:105:VAL:HG13	4:D:110:PHE:HB2	1.93	0.49
9:I:55:ALA:C	9:I:56:LEU:HD23	2.37	0.49
19:S:31:ILE:HG22	19:S:50:ALA:H	1.78	0.49
1:A:728:A:H8	1:A:728:A:O5'	1.96	0.49
1:A:1300:G:O2'	1:A:1301:U:O5'	2.31	0.49
1:A:1518[B]:MA6:H102	1:A:1519[B]:MA6:C10	2.43	0.49
4:D:150:GLU:HA	4:D:153:ARG:CZ	2.42	0.49
5:E:81:GLU:HG2	5:E:90:VAL:HG13	1.94	0.49
11:K:58:PRO:HA	11:K:90:GLY:HA3	1.93	0.49
16:P:55:ARG:O	16:P:58:TYR:HB3	2.13	0.49
23:W:37:A:N6	23:W:38:A:C2	2.81	0.49
1:A:78:G:C2'	1:A:79:G:O5'	2.60	0.49
1:A:328:C:HO2'	1:A:329:A:P	2.32	0.49
1:A:397:A:C6	1:A:548:G:N7	2.81	0.49
1:A:1220:G:H2'	1:A:1221:G:H8	1.77	0.49
7:G:23:VAL:O	7:G:27:ILE:HG12	2.12	0.49
1:A:16:A:O2'	5:E:16:THR:HB	2.13	0.49
1:A:114:U:H1'	1:A:353:A:H1'	1.95	0.49
1:A:269:C:H2'	1:A:270:A:C8	2.47	0.49
1:A:803:G:C5	1:A:804:U:C4	3.00	0.49
1:A:939:G:H5''	7:G:102:ARG:NH2	2.27	0.49
1:A:1275:A:H2'	1:A:1276:G:C8	2.48	0.49
1:A:1277:C:O2'	1:A:1279:A:H8	1.95	0.49
1:A:1292:U:P	7:G:41:ARG:NH2	2.85	0.49
1:A:1497:G:O2'	1:A:1518[A]:MA6:N1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:11:LYS:O	9:I:12:GLU:HB2	2.13	0.49
10:J:6:ILE:HD12	10:J:72:VAL:HG11	1.94	0.49
18:R:40:LEU:HB3	18:R:79:LEU:HD11	1.95	0.49
20:T:56:MET:HE2	20:T:85:MET:HA	1.94	0.49
1:A:80:G:C5'	1:A:81:U:OP2	2.61	0.49
1:A:129(A):G:H1'	1:A:190(E):U:H2'	1.94	0.49
1:A:539:A:H2'	1:A:540:G:H8	1.77	0.49
1:A:1308:U:C5	13:M:99:ARG:NH1	2.81	0.49
4:D:4:TYR:CE2	4:D:11:LEU:HD11	2.48	0.49
9:I:51:ARG:HG2	9:I:56:LEU:HD13	1.95	0.49
13:M:37:THR:HG22	13:M:39:ILE:HG13	1.95	0.49
20:T:53:LEU:HB2	20:T:100:ILE:CG2	2.43	0.49
1:A:386:C:C2'	1:A:387:U:H5'	2.43	0.48
1:A:723:U:O2	1:A:723:U:H2'	2.12	0.48
1:A:743:U:H2'	1:A:744:C:C6	2.48	0.48
1:A:1127:G:N2	1:A:1145:C:N3	2.55	0.48
1:A:1274:G:O5'	1:A:1274:G:H8	1.96	0.48
1:A:1516[A]:G:C6	1:A:1520[A]:G:C2	3.01	0.48
2:B:22:LYS:CG	2:B:23:ARG:N	2.76	0.48
3:C:79:ARG:O	3:C:82:GLU:HG3	2.12	0.48
19:S:51:VAL:O	19:S:58:VAL:HG22	2.13	0.48
1:A:432:A:O2'	1:A:433:C:OP1	2.30	0.48
1:A:857:C:H2'	1:A:858:G:O4'	2.14	0.48
1:A:1130:A:C2	1:A:1146:A:C4	3.00	0.48
1:A:1139:G:H4'	1:A:1140:C:OP1	2.13	0.48
4:D:148:VAL:HG12	4:D:149:ALA:H	1.78	0.48
8:H:11:THR:HG22	8:H:12:ARG:N	2.28	0.48
13:M:17:VAL:O	13:M:20:THR:HB	2.13	0.48
17:Q:75:ARG:HG3	17:Q:75:ARG:NH1	2.27	0.48
1:A:522:C:C2'	1:A:523:A:H5'	2.43	0.48
1:A:683:G:H2'	1:A:684:A:C8	2.49	0.48
1:A:1053:G:C3'	1:A:1054:C:H5'	2.43	0.48
1:A:1502:A:C2	1:A:1504:G:C2	3.01	0.48
2:B:38:GLY:C	2:B:39:ILE:HG13	2.38	0.48
7:G:54:THR:CG2	7:G:56:GLN:HB2	2.44	0.48
11:K:57:THR:CG2	11:K:58:PRO:HD2	2.44	0.48
13:M:107:ALA:O	13:M:111:LYS:HB2	2.13	0.48
17:Q:4:LYS:HD2	17:Q:6:LEU:CD2	2.42	0.48
19:S:80:TYR:CZ	19:S:81:ARG:HD3	2.48	0.48
20:T:43:LEU:HD12	20:T:52:ALA:HA	1.95	0.48
1:A:179:A:H2'	1:A:180:U:H6	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:738:C:OP1	6:F:2:ARG:NH1	2.47	0.48
1:A:923:A:O4'	1:A:1398:A:C2	2.67	0.48
1:A:1007:C:H42	1:A:1022:G:H1	1.60	0.48
13:M:91:ARG:NH1	13:M:96:LEU:HD13	2.29	0.48
19:S:31:ILE:HG21	19:S:49:ILE:HD12	1.94	0.48
1:A:182:U:OP2	1:A:182:U:H6	1.96	0.48
1:A:442:C:N4	1:A:492:G:H1	1.96	0.48
1:A:690:G:H2'	1:A:691:G:O4'	2.14	0.48
1:A:1316:G:H4'	14:N:18:VAL:CG1	2.43	0.48
1:A:1423:G:H2'	1:A:1424:C:C6	2.49	0.48
1:A:1427:U:H2'	1:A:1428:A:H8	1.78	0.48
4:D:28:SER:C	4:D:30:LYS:H	2.21	0.48
11:K:73:MET:O	11:K:76:GLY:N	2.40	0.48
1:A:353:A:H2'	1:A:354:G:OP2	2.14	0.48
1:A:542:G:H5'	4:D:41:GLY:HA3	1.95	0.48
1:A:905:U:C2'	1:A:906:G:H5'	2.43	0.48
1:A:1541:PSU:O4	1:A:1541:PSU:C2'	2.57	0.48
4:D:38:TYR:HB2	4:D:39:PRO:HD2	1.96	0.48
6:F:10:LEU:HD11	6:F:59:TYR:CD2	2.49	0.48
12:L:13:LYS:HE3	12:L:13:LYS:HB2	1.70	0.48
19:S:36:ARG:HH21	19:S:53:ASN:HA	1.78	0.48
20:T:53:LEU:HD13	20:T:100:ILE:HG22	1.94	0.48
1:A:547:A:OP2	4:D:2:GLY:HA3	2.14	0.48
1:A:1051:C:H2'	1:A:1052:U:C6	2.49	0.48
1:A:1092:A:H5''	7:G:4:ARG:NH1	2.28	0.48
3:C:123:GLN:O	3:C:128:PHE:HB2	2.14	0.48
4:D:9:CYS:O	4:D:12:CYS:HB2	2.14	0.48
4:D:112:VAL:HG22	4:D:116:GLN:OE1	2.13	0.48
4:D:112:VAL:N	4:D:116:GLN:OE1	2.42	0.48
16:P:20:VAL:HG11	16:P:32:TYR:CB	2.43	0.48
1:A:56:U:H2'	1:A:57:G:C8	2.48	0.48
1:A:353:A:H8	1:A:353:A:C5'	2.21	0.48
1:A:397:A:H3'	1:A:397:A:N3	2.29	0.48
1:A:793:U:O4	1:A:1517[A]:G:H5'	2.14	0.48
1:A:1002:G:H2'	1:A:1003:G:C8	2.48	0.48
1:A:1048:G:O3'	1:A:1049:U:H3'	2.14	0.48
1:A:1318:A:H4'	19:S:10:PHE:CE1	2.49	0.48
5:E:40:ARG:HG2	5:E:40:ARG:HH11	1.79	0.48
9:I:97:LYS:HB2	9:I:102:LEU:HD21	1.95	0.48
10:J:78:ASN:N	10:J:78:ASN:OD1	2.46	0.48
15:O:8:LYS:O	15:O:11:VAL:HG22	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:9:PHE:CE2	16:P:18:ARG:HD2	2.49	0.48
1:A:78:G:H2'	1:A:79:G:O5'	2.14	0.48
1:A:977:A:H2'	1:A:978:A:H5''	1.96	0.48
1:A:1308:U:OP2	13:M:99:ARG:HG3	2.14	0.48
1:A:1345:U:OP1	9:I:120:ARG:NH1	2.47	0.48
5:E:11:ILE:HD11	5:E:108:ALA:HB3	1.95	0.48
7:G:155:ARG:O	7:G:156:TRP:CG	2.67	0.48
8:H:86:ILE:HG21	8:H:133:LEU:HD13	1.96	0.48
9:I:118:LYS:O	9:I:120:ARG:N	2.42	0.48
10:J:50:ILE:HG22	10:J:60:ARG:CD	2.39	0.48
15:O:15:PHE:CE2	15:O:84:LYS:HD2	2.49	0.48
19:S:40:ILE:CG2	19:S:67:VAL:HA	2.43	0.48
1:A:19:C:O2'	1:A:20:U:H5'	2.13	0.48
1:A:108:G:C2'	1:A:109:A:OP1	2.62	0.48
1:A:716:A:H1'	11:K:117:ASN:O	2.13	0.48
8:H:36:LEU:HD12	8:H:59:LEU:HD22	1.96	0.48
17:Q:76:LEU:HD12	17:Q:76:LEU:C	2.39	0.48
1:A:376:G:P	16:P:67:THR:HG21	2.54	0.47
1:A:1091:U:O2	1:A:1093:A:H8	1.97	0.47
1:A:1149:C:OP1	9:I:9:ARG:NH1	2.47	0.47
1:A:1179:A:C2'	1:A:1180:A:O5'	2.62	0.47
1:A:1358:U:H3'	1:A:1359:C:H6	1.79	0.47
5:E:81:GLU:OE2	5:E:88:LYS:HE2	2.13	0.47
12:L:10:LEU:HB3	17:Q:32:TYR:CD1	2.49	0.47
15:O:26:GLU:HA	15:O:81:LEU:HD22	1.95	0.47
17:Q:35:VAL:O	17:Q:35:VAL:HG12	2.14	0.47
1:A:6:G:H4'	1:A:298:A:H4'	1.96	0.47
1:A:80:G:H5''	1:A:81:U:OP2	2.13	0.47
1:A:403:C:OP1	4:D:136:PRO:HD2	2.13	0.47
1:A:620:C:C1'	4:D:135:LEU:HD13	2.44	0.47
1:A:665:A:N3	1:A:732:C:H2'	2.28	0.47
1:A:817:C:H4'	1:A:818:G:OP1	2.14	0.47
1:A:818:G:HO2'	1:A:820:U:H6	1.62	0.47
1:A:1023:G:C6	1:A:1024:G:C2	3.02	0.47
1:A:1074:G:O6	27:A:2019:HOH:O	2.20	0.47
1:A:1408:A:H2'	1:A:1409:C:H6	1.79	0.47
1:A:1516[B]:G:N2	1:A:1519[B]:MA6:OP2	2.46	0.47
2:B:142:LEU:O	2:B:142:LEU:HD23	2.14	0.47
2:B:181:PHE:HD2	8:H:70:GLN:HB3	1.79	0.47
3:C:64:VAL:CB	3:C:99:VAL:HB	2.41	0.47
5:E:12:LEU:C	5:E:12:LEU:CD2	2.87	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:123:GLU:O	8:H:127:LEU:HB2	2.15	0.47
11:K:19:ALA:HB2	11:K:80:VAL:HG21	1.95	0.47
13:M:108:ARG:NH2	13:M:111:LYS:HE2	2.29	0.47
14:N:7:ILE:C	14:N:9:LYS:N	2.72	0.47
1:A:1216:G:H5''	14:N:5:ALA:CB	2.44	0.47
2:B:161:ALA:HB1	2:B:185:ILE:CD1	2.44	0.47
3:C:13:GLY:O	3:C:14:ILE:HD13	2.14	0.47
7:G:51:GLN:C	7:G:53:LYS:H	2.22	0.47
8:H:83:ILE:HG13	8:H:137:VAL:HG22	1.96	0.47
10:J:19:SER:O	10:J:22:LYS:HB2	2.15	0.47
13:M:65:LYS:O	13:M:70:LEU:HG	2.13	0.47
14:N:5:ALA:O	14:N:8:GLU:CG	2.62	0.47
1:A:664:G:N2	1:A:741:G:H1	1.95	0.47
1:A:1143:G:C6	1:A:1144:G:C6	3.02	0.47
1:A:1406:U:H4'	1:A:1518[B]:MA6:H1'	1.95	0.47
2:B:114:ARG:NH1	2:B:141:GLU:OE1	2.47	0.47
4:D:70:ILE:HD11	4:D:100:ARG:NE	2.29	0.47
4:D:142:PRO:HA	4:D:185:PHE:O	2.14	0.47
20:T:53:LEU:O	20:T:57:ARG:HD3	2.14	0.47
1:A:273:A:N6	1:A:274:A:C6	2.83	0.47
1:A:340:U:H2'	1:A:341:C:C6	2.49	0.47
1:A:913:A:C1'	1:A:914:A:OP2	2.63	0.47
1:A:983:A:H3'	1:A:983:A:N3	2.29	0.47
1:A:1114:C:H2'	1:A:1115:C:C6	2.50	0.47
1:A:1316:G:N1	1:A:1319:A:OP2	2.48	0.47
25:A:1860:SRV:OG2	12:L:91:LYS:NZ	2.33	0.47
2:B:61:LEU:HD21	2:B:160:ASP:CB	2.44	0.47
2:B:133:LYS:O	2:B:137:ARG:HG3	2.15	0.47
9:I:17:VAL:HG21	9:I:80:GLY:HA3	1.97	0.47
12:L:27:LEU:C	12:L:29:GLY:H	2.20	0.47
12:L:54:LYS:N	12:L:54:LYS:HD2	2.29	0.47
16:P:9:PHE:CD2	16:P:18:ARG:HG3	2.49	0.47
17:Q:100:LYS:O	17:Q:101:ARG:C	2.56	0.47
1:A:17:U:H4'	1:A:1080:A:O4'	2.14	0.47
1:A:1038:C:H2'	1:A:1039:C:H6	1.79	0.47
1:A:1440:C:H2'	1:A:1441:G:O4'	2.14	0.47
2:B:8:LYS:HA	2:B:11:LEU:HD13	1.95	0.47
7:G:41:ARG:O	7:G:42:ILE:C	2.58	0.47
7:G:122:HIS:CD2	7:G:125:MET:HE2	2.50	0.47
8:H:23:SER:HA	8:H:63:LEU:HD22	1.97	0.47
15:O:22:THR:O	15:O:27:VAL:HG11	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:A:H4'	1:A:345:C:OP2	2.14	0.47
1:A:1179:A:HO2'	1:A:1180:A:P	2.37	0.47
1:A:1201:A:H4'	1:A:1202:G:O5'	2.15	0.47
1:A:1468:A:H2'	1:A:1469:G:O4'	2.14	0.47
2:B:87:ARG:CZ	2:B:233:SER:HB2	2.45	0.47
4:D:31:CYS:O	4:D:32:ALA:HB3	2.15	0.47
7:G:145:ALA:O	7:G:146:GLU:CB	2.62	0.47
11:K:110:ASP:HB2	18:R:88:LYS:HG3	1.96	0.47
12:L:27:LEU:O	12:L:28:LYS:C	2.58	0.47
13:M:44:ARG:N	13:M:44:ARG:HD2	2.30	0.47
16:P:20:VAL:CG1	16:P:32:TYR:HB2	2.44	0.47
17:Q:54:GLY:O	17:Q:80:GLY:HA2	2.15	0.47
17:Q:63:ARG:HG2	17:Q:64:PRO:CD	2.45	0.47
18:R:59:SER:H	18:R:62:GLU:HB2	1.80	0.47
19:S:62:ILE:HG13	19:S:66:MET:HE2	1.96	0.47
1:A:17:U:H1'	1:A:1080:A:N3	2.30	0.47
1:A:103:C:P	20:T:17:ARG:HH12	2.37	0.47
1:A:325:A:OP2	20:T:70:SER:HB2	2.15	0.47
1:A:1412:C:H2'	1:A:1413:A:H8	1.69	0.47
2:B:6:THR:HA	2:B:9:GLU:OE1	2.14	0.47
8:H:48:TYR:HA	8:H:60:ARG:O	2.14	0.47
12:L:124:LYS:HD2	12:L:125:PRO:HD2	1.97	0.47
13:M:22:ILE:CB	13:M:25:ILE:HD12	2.45	0.47
1:A:31:G:O2'	1:A:48:C:N4	2.47	0.47
1:A:860:A:H2'	1:A:861:G:O4'	2.14	0.47
1:A:1124:G:H2'	1:A:1145:C:H5	1.79	0.47
1:A:1179:A:O2'	1:A:1180:A:P	2.72	0.47
19:S:22:LEU:HD23	19:S:25:LYS:NZ	2.29	0.47
20:T:35:THR:HA	20:T:38:LYS:HE3	1.96	0.47
1:A:1179:A:O2'	1:A:1180:A:OP1	2.29	0.47
1:A:1321:C:H4'	13:M:87:TYR:CE2	2.50	0.47
1:A:1400:5MC:H3'	1:A:1401:G:H5'	1.97	0.47
1:A:1411:C:H2'	1:A:1412:C:C6	2.50	0.47
2:B:100:GLY:N	2:B:176:GLU:OE2	2.44	0.47
3:C:36:ASP:O	3:C:39:ILE:HB	2.15	0.47
3:C:128:PHE:HD2	3:C:129:ALA:H	1.63	0.47
4:D:62:GLN:O	4:D:66:ARG:HB2	2.14	0.47
4:D:148:VAL:CG1	4:D:149:ALA:N	2.77	0.47
16:P:52:ASP:OD1	16:P:52:ASP:C	2.58	0.47
19:S:43:GLU:OE2	19:S:43:GLU:N	2.46	0.47
1:A:9:G:OP1	5:E:122:GLU:HG3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1304:G:H1'	1:A:1333:A:H61	1.80	0.46
1:A:1322:C:H4'	1:A:1323:G:OP1	2.14	0.46
1:A:1498:UR3:H4'	1:A:1519[A]:MA6:N1	2.29	0.46
7:G:113:GLU:CG	7:G:119:ARG:HG2	2.45	0.46
8:H:119:LEU:HA	8:H:123:GLU:OE1	2.15	0.46
17:Q:22:LEU:HD12	17:Q:23:VAL:H	1.80	0.46
18:R:59:SER:N	18:R:62:GLU:OE1	2.46	0.46
1:A:21:G:OP1	27:A:1942:HOH:O	2.19	0.46
1:A:253:U:OP1	17:Q:67:LYS:HE2	2.15	0.46
1:A:283:C:C2	1:A:284:G:C8	3.03	0.46
1:A:421:U:O2	1:A:421:U:H2'	2.15	0.46
1:A:854:G:H3'	1:A:871:U:O4	2.15	0.46
1:A:1001:A:H2'	1:A:1002:G:C8	2.50	0.46
1:A:1023:G:O6	1:A:1024:G:N2	2.47	0.46
1:A:1480:G:C6	1:A:1481:U:C4	3.04	0.46
1:A:1518[B]:MA6:O2'	1:A:1519[B]:MA6:O5'	2.34	0.46
2:B:97:TRP:CH2	2:B:176:GLU:OE2	2.68	0.46
5:E:33:VAL:HG11	5:E:109:ILE:HA	1.97	0.46
6:F:91:VAL:HG11	18:R:72:ARG:NH1	2.29	0.46
8:H:82:HIS:C	8:H:82:HIS:CD2	2.93	0.46
11:K:108:ILE:HG22	11:K:109:VAL:N	2.29	0.46
17:Q:5:VAL:O	17:Q:6:LEU:HD23	2.16	0.46
19:S:27:GLU:HG2	19:S:28:LYS:N	2.30	0.46
1:A:966:M2G:HM22	1:A:967:5MC:C2	2.50	0.46
1:A:1225:A:H2'	1:A:1225:A:N3	2.30	0.46
1:A:1450:U:H2'	1:A:1452:C:C5	2.50	0.46
4:D:191:ARG:O	4:D:191:ARG:HD2	2.15	0.46
7:G:113:GLU:HB2	7:G:119:ARG:HG2	1.97	0.46
8:H:104:ARG:CZ	8:H:138:TRP:CH2	2.98	0.46
1:A:28:G:O2'	1:A:296:U:OP1	2.32	0.46
1:A:60:A:H5'	27:A:1901:HOH:O	2.16	0.46
1:A:166:G:O2'	1:A:167:G:H5'	2.15	0.46
1:A:557:G:C6	1:A:558:G:C6	3.03	0.46
1:A:909:A:H2'	1:A:910:C:O4'	2.13	0.46
1:A:973:G:H2'	1:A:974:A:OP1	2.15	0.46
1:A:1072:G:H2'	1:A:1073:U:C6	2.49	0.46
1:A:1150:U:O2	10:J:39:PRO:HG2	2.16	0.46
1:A:1281:U:HO2'	1:A:1282:C:P	2.34	0.46
1:A:1339:A:H2'	1:A:1340:A:O4'	2.16	0.46
6:F:54:LYS:HE3	6:F:54:LYS:HA	1.97	0.46
13:M:59:TYR:CE1	13:M:63:THR:HG21	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:3:ILE:HG12	15:O:38:ARG:NH1	2.30	0.46
1:A:248:C:C2'	1:A:249:U:H5'	2.46	0.46
1:A:434:U:H2'	1:A:435:C:C6	2.50	0.46
1:A:437:U:C2'	1:A:438:G:H5'	2.45	0.46
1:A:594:G:C2'	1:A:595:G:H5'	2.45	0.46
1:A:1118:C:H1'	1:A:1179:A:C4	2.51	0.46
1:A:1158:C:O2	1:A:1158:C:C2'	2.64	0.46
3:C:64:VAL:HG12	3:C:66:VAL:HG23	1.96	0.46
6:F:8:ILE:HD11	6:F:79:LEU:HD13	1.97	0.46
7:G:51:GLN:C	7:G:53:LYS:N	2.71	0.46
1:A:157:G:H2'	1:A:158:G:H8	1.81	0.46
1:A:245:C:O2	1:A:283:C:N3	2.49	0.46
1:A:376:G:OP2	16:P:67:THR:HG21	2.15	0.46
1:A:452:A:HO2'	1:A:453:A:H8	1.60	0.46
1:A:491:G:C4	1:A:492:G:C8	3.03	0.46
1:A:559:A:H2'	1:A:559:A:N3	2.29	0.46
1:A:757:U:O2'	1:A:879:C:H1'	2.15	0.46
1:A:1332:A:C2	1:A:1333:A:C4	3.02	0.46
1:A:1531:A:O5'	1:A:1531:A:H8	1.98	0.46
9:I:71:SER:O	9:I:74:ILE:HB	2.16	0.46
10:J:60:ARG:H	10:J:60:ARG:HG2	1.32	0.46
11:K:21:ILE:HD13	11:K:94:ALA:CB	2.45	0.46
17:Q:19:VAL:HG23	17:Q:44:ALA:HB3	1.97	0.46
1:A:496:A:H4'	1:A:497:A:OP1	2.12	0.46
1:A:689:C:OP2	11:K:46:GLY:HA3	2.16	0.46
1:A:1149:C:H2'	1:A:1150:U:C6	2.51	0.46
1:A:1532:U:C2'	1:A:1533:C:H5''	2.44	0.46
2:B:164:VAL:HB	2:B:186:ALA:HB2	1.97	0.46
4:D:146:ILE:N	4:D:146:ILE:CD1	2.79	0.46
19:S:5:LEU:O	19:S:6:LYS:HB2	2.15	0.46
1:A:309:G:H1'	1:A:608:A:C2	2.51	0.46
1:A:437:U:H2'	1:A:438:G:H5'	1.96	0.46
1:A:487:A:H2'	1:A:488:C:O4'	2.15	0.46
1:A:739:C:HO2'	15:O:42:HIS:CE1	2.27	0.46
8:H:108:GLY:HA3	8:H:138:TRP:HB3	1.97	0.46
18:R:55:ARG:NH1	18:R:55:ARG:HB3	2.31	0.46
1:A:321:A:C2	1:A:333:G:C2	3.03	0.46
1:A:766:A:C8	1:A:814:A:C6	3.04	0.46
1:A:926:G:H3'	1:A:1505:G:H21	1.80	0.46
1:A:1038:C:H2'	1:A:1039:C:C6	2.51	0.46
1:A:1238:A:H5'	1:A:1336:C:H41	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1331:G:C2'	1:A:1332:A:OP2	2.64	0.46
1:A:1413:A:H2'	1:A:1414:U:O4'	2.16	0.46
7:G:15:ASP:O	7:G:19:GLY:HA2	2.15	0.46
16:P:4:ILE:O	16:P:66:PRO:HA	2.16	0.46
17:Q:59:ILE:HG23	17:Q:71:PHE:HD1	1.80	0.46
20:T:33:ILE:HD12	20:T:63:ILE:HG12	1.97	0.46
1:A:114:U:O2'	1:A:115:G:H5'	2.16	0.46
1:A:197:A:N6	1:A:221:C:H5'	2.31	0.46
1:A:328:C:H4'	1:A:329:A:H5''	1.98	0.46
1:A:376:G:H2'	1:A:377:G:C8	2.47	0.46
1:A:390:C:H6	1:A:390:C:O5'	1.98	0.46
1:A:474:G:H4'	16:P:81:ARG:NH2	2.30	0.46
1:A:497:A:H4'	1:A:498:U:OP2	2.15	0.46
1:A:820:U:H4'	1:A:821:G:OP2	2.16	0.46
1:A:1007:C:H2'	1:A:1008:C:C6	2.51	0.46
1:A:1223:C:P	19:S:78:ARG:HH12	2.39	0.46
12:L:69:TYR:HE2	12:L:71:PRO:HA	1.81	0.46
15:O:78:TYR:CZ	15:O:82:ILE:CD1	2.98	0.46
20:T:10:LEU:HD13	20:T:12:ALA:H	1.81	0.46
1:A:237:C:OP2	17:Q:40:LYS:NZ	2.45	0.45
1:A:390:C:H2'	1:A:391:G:H8	1.80	0.45
1:A:646:U:H2'	1:A:647:C:H6	1.80	0.45
1:A:797:C:O2'	1:A:798:G:H5'	2.16	0.45
1:A:815:A:O2'	1:A:1527:C:H1'	2.15	0.45
1:A:979:C:OP2	1:A:980:C:H5	1.99	0.45
1:A:1165:C:C2'	1:A:1166:G:H5'	2.47	0.45
1:A:1251:A:H2'	1:A:1252:A:O4'	2.16	0.45
1:A:1518[B]:MA6:C2'	1:A:1519[B]:MA6:O5'	2.64	0.45
25:A:1860:SRY:C22	25:A:1860:SRY:HI32	2.46	0.45
2:B:46:LYS:CA	2:B:46:LYS:HE3	2.45	0.45
6:F:33:TYR:HE2	6:F:74:ASP:HB3	1.78	0.45
8:H:11:THR:O	8:H:14:ARG:N	2.49	0.45
8:H:94:TYR:HE2	8:H:132:GLU:OE1	1.99	0.45
10:J:38:ILE:O	10:J:71:LEU:N	2.39	0.45
11:K:33:THR:HG22	11:K:39:PRO:HA	1.98	0.45
13:M:45:VAL:HG13	13:M:48:LEU:HD12	1.98	0.45
13:M:54:VAL:O	13:M:58:GLU:HB2	2.16	0.45
14:N:50:LYS:HE3	14:N:50:LYS:HB3	1.65	0.45
1:A:407:G:C2	1:A:436:C:C2	3.04	0.45
1:A:556:C:H2'	1:A:557:G:O4'	2.16	0.45
1:A:737:A:H2'	1:A:738:C:H6	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:975:A:N6	1:A:1366:C:O2'	2.47	0.45
1:A:1127:G:N2	1:A:1145:C:O2	2.50	0.45
1:A:1191:A:H5''	3:C:4:LYS:HZ3	1.81	0.45
1:A:1281:U:O3'	1:A:1282:C:H6	1.99	0.45
1:A:1292:U:OP1	7:G:41:ARG:NH2	2.40	0.45
6:F:4:TYR:CZ	6:F:72:VAL:HG21	2.52	0.45
1:A:126:G:H4'	1:A:634:C:O2	2.17	0.45
1:A:695:A:H2'	1:A:696:A:C8	2.51	0.45
1:A:1122:U:C2'	1:A:1123:A:H5'	2.47	0.45
4:D:79:PHE:HA	4:D:93:PHE:CD2	2.52	0.45
4:D:148:VAL:CG1	4:D:149:ALA:H	2.29	0.45
5:E:57:LYS:HG2	5:E:61:TYR:CE2	2.51	0.45
6:F:4:TYR:HE1	6:F:92:LYS:HG2	1.80	0.45
9:I:16:ARG:HD2	9:I:64:THR:HB	1.97	0.45
9:I:105:ASP:OD1	9:I:107:ARG:HG3	2.16	0.45
12:L:76:ASN:O	12:L:76:ASN:CG	2.59	0.45
17:Q:68:ARG:N	17:Q:70:ARG:NH1	2.64	0.45
1:A:666:G:H5'	1:A:726:C:H1'	1.97	0.45
1:A:911:U:H2'	1:A:912:C:C6	2.51	0.45
1:A:1366:C:O2'	1:A:1367:C:H5'	2.16	0.45
3:C:15:THR:HG21	3:C:179:ARG:HA	1.99	0.45
3:C:64:VAL:HB	3:C:99:VAL:CB	2.38	0.45
3:C:154:SER:CB	3:C:197:GLY:H	2.30	0.45
7:G:8:GLU:H	7:G:8:GLU:HG3	1.61	0.45
11:K:43:SER:O	11:K:44:SER:HB3	2.16	0.45
16:P:7:ALA:O	16:P:17:TYR:HA	2.17	0.45
20:T:10:LEU:C	20:T:10:LEU:CD1	2.89	0.45
20:T:33:ILE:HD13	20:T:62:LEU:HB3	1.98	0.45
1:A:281:G:C2'	1:A:282:A:OP2	2.64	0.45
1:A:782:A:H4'	1:A:1514:C:O2'	2.15	0.45
1:A:1120:G:C2	1:A:1154:G:N3	2.84	0.45
1:A:1256:A:H5'	1:A:1258:G:C1'	2.43	0.45
2:B:215:LEU:HD23	2:B:215:LEU:HA	1.69	0.45
9:I:10:ARG:O	9:I:11:LYS:C	2.60	0.45
9:I:42:ARG:NH1	9:I:42:ARG:HB2	2.32	0.45
9:I:99:LEU:HD22	9:I:99:LEU:N	2.30	0.45
19:S:13:ASP:O	19:S:17:GLU:HG2	2.17	0.45
1:A:52:G:O2'	1:A:53:A:H5'	2.16	0.45
1:A:757:U:H2'	1:A:758:G:O4'	2.16	0.45
1:A:897:C:H5'	17:Q:101:ARG:O	2.16	0.45
1:A:1285:A:O4'	1:A:1286:A:N7	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1327:C:OP2	21:U:12:LYS:NZ	2.50	0.45
5:E:51:VAL:N	5:E:52:PRO:HD2	2.32	0.45
11:K:51:LYS:O	11:K:55:LYS:HE2	2.17	0.45
1:A:328:C:C1'	1:A:329:A:OP2	2.64	0.45
1:A:382:A:H2'	1:A:383:A:C8	2.51	0.45
1:A:403:C:O2'	1:A:404:U:H5'	2.17	0.45
1:A:629:G:H2'	1:A:630:G:O4'	2.16	0.45
1:A:949:A:C2	1:A:1233:G:N3	2.85	0.45
1:A:1024:G:N7	1:A:1025:U:C5	2.85	0.45
1:A:1067:A:H4'	1:A:1068:G:O5'	2.17	0.45
1:A:1072:G:C5	1:A:1073:U:C4	3.04	0.45
1:A:1287:A:H2'	1:A:1288:A:C8	2.52	0.45
1:A:1337:G:H5''	1:A:1338:G:OP1	2.17	0.45
5:E:96:PRO:HA	5:E:117:ASP:CG	2.41	0.45
7:G:43:PHE:O	7:G:46:ALA:HB3	2.16	0.45
14:N:11:LYS:HD3	14:N:11:LYS:HA	1.72	0.45
15:O:26:GLU:OE2	15:O:77:ARG:NH1	2.50	0.45
20:T:14:LYS:O	20:T:18:GLN:HG3	2.16	0.45
20:T:74:LYS:HZ3	20:T:74:LYS:CA	2.27	0.45
1:A:389:A:C6	1:A:390:C:H1'	2.52	0.45
1:A:446:G:H2'	1:A:447:G:O4'	2.16	0.45
3:C:34:LEU:HD21	3:C:38:ARG:HH22	1.79	0.45
5:E:28:PHE:O	5:E:47:LYS:HA	2.16	0.45
6:F:2:ARG:CD	6:F:69:GLU:HG2	2.46	0.45
8:H:88:LYS:O	8:H:92:ARG:HG2	2.15	0.45
9:I:125:TYR:H	9:I:125:TYR:HD2	1.64	0.45
12:L:100:ILE:N	12:L:100:ILE:HD12	2.32	0.45
13:M:37:THR:HG23	13:M:55:ARG:CG	2.47	0.45
1:A:68:G:C2'	1:A:69:G:O5'	2.65	0.45
1:A:577:G:H1'	1:A:816:A:N3	2.32	0.45
1:A:1371:G:OP1	9:I:11:LYS:O	2.34	0.45
1:A:1375:A:H2'	1:A:1376:U:O4'	2.16	0.45
25:A:1860:SRV:HI32	25:A:1860:SRV:O13	2.15	0.45
2:B:103:THR:N	2:B:176:GLU:OE1	2.30	0.45
3:C:135:LYS:HE3	5:E:50:GLU:HG2	1.99	0.45
13:M:37:THR:HG22	13:M:37:THR:O	2.15	0.45
13:M:96:LEU:C	13:M:110:ARG:HG2	2.42	0.45
20:T:32:ALA:O	20:T:33:ILE:C	2.59	0.45
20:T:85:MET:HE2	20:T:104:LEU:CD2	2.44	0.45
1:A:376:G:H5''	16:P:5:ARG:CD	2.47	0.45
1:A:477:G:H2'	1:A:478:A:C8	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:778:G:O2'	1:A:779:C:H5'	2.17	0.45
4:D:57:ARG:HB3	4:D:206:PHE:HB2	1.99	0.45
9:I:8:GLY:HA2	9:I:79:LEU:HD13	1.99	0.45
9:I:48:GLU:N	9:I:49:PRO:CD	2.79	0.45
12:L:34:ARG:O	12:L:61:THR:HG23	2.17	0.45
17:Q:56:VAL:HG21	17:Q:81:ARG:HD3	1.98	0.45
1:A:519:C:H2'	1:A:520:A:C8	2.52	0.44
1:A:688:G:H5'	11:K:46:GLY:C	2.42	0.44
1:A:862:C:O2'	1:A:863:U:H5'	2.17	0.44
1:A:1152:A:OP1	10:J:68:HIS:ND1	2.50	0.44
1:A:1240:U:H3'	1:A:1241:G:H5'	1.99	0.44
1:A:1323:G:H2'	1:A:1324:A:C8	2.52	0.44
3:C:95:THR:C	3:C:97:LYS:N	2.75	0.44
5:E:80:ILE:HD11	5:E:138:ALA:HB1	1.98	0.44
9:I:127:LYS:O	9:I:128:ARG:HB2	2.16	0.44
1:A:224:C:O2'	1:A:225:C:H5'	2.17	0.44
1:A:369:C:O2	1:A:369:C:H2'	2.17	0.44
1:A:527:7MG:C2'	1:A:528:C:H5'	2.47	0.44
1:A:660:G:C2	1:A:746:A:C2	3.06	0.44
1:A:1104:G:OP1	2:B:111:ARG:HD2	2.18	0.44
1:A:1428:A:H2'	1:A:1429:C:C6	2.52	0.44
1:A:1508:G:H2'	1:A:1509:C:O4'	2.17	0.44
2:B:92:TYR:O	2:B:151:GLY:HA3	2.17	0.44
7:G:5:ARG:CZ	7:G:7:ALA:HA	2.48	0.44
8:H:127:LEU:HD22	8:H:127:LEU:HA	1.70	0.44
10:J:90:LEU:N	10:J:91:PRO:CD	2.80	0.44
11:K:84:VAL:HG21	11:K:95:ILE:HD11	1.98	0.44
11:K:111:ASP:O	11:K:111:ASP:OD2	2.35	0.44
12:L:39:VAL:HG23	12:L:57:LYS:HB2	1.98	0.44
18:R:42:ARG:NH1	18:R:42:ARG:HB3	2.32	0.44
1:A:19:C:H2'	1:A:20:U:H6	1.83	0.44
1:A:357:G:O2'	1:A:358:U:H5'	2.16	0.44
1:A:526:C:OP1	1:A:913:A:H3'	2.16	0.44
1:A:782:A:O3'	1:A:1515[A]:C:H4'	2.18	0.44
1:A:1320:C:N3	19:S:36:ARG:HD3	2.32	0.44
1:A:1358:U:H3'	1:A:1359:C:C6	2.51	0.44
1:A:1443:G:N3	1:A:1443:G:H5''	2.33	0.44
3:C:91:LEU:HD23	3:C:92:ALA:N	2.31	0.44
5:E:43:LEU:HD11	5:E:132:ALA:HB1	1.99	0.44
7:G:38:LEU:O	7:G:38:LEU:HD12	2.17	0.44
7:G:102:ARG:O	7:G:106:GLN:HG3	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:78:ASN:C	10:J:80:LYS:N	2.73	0.44
11:K:111:ASP:O	11:K:112:THR:C	2.61	0.44
12:L:92:0TD:C	12:L:92:0TD:OD1	2.65	0.44
13:M:37:THR:HG23	13:M:55:ARG:CD	2.46	0.44
15:O:76:GLU:HA	15:O:76:GLU:OE1	2.16	0.44
1:A:190(D):U:O2'	1:A:190(E):U:H5'	2.18	0.44
1:A:342:C:H2'	1:A:343:U:H5'	1.99	0.44
1:A:509:A:C8	1:A:509:A:H3'	2.52	0.44
1:A:631:G:O3'	1:A:632:A:C8	2.69	0.44
1:A:1064:G:N2	1:A:1190:G:C2'	2.81	0.44
1:A:1077:G:C6	1:A:1081:G:C6	3.05	0.44
1:A:1477:C:H2'	1:A:1478:C:H6	1.82	0.44
1:A:1505:G:C8	1:A:1505:G:H3'	2.52	0.44
3:C:50:ALA:HB1	3:C:70:VAL:CG1	2.47	0.44
6:F:100:ASN:HD21	18:R:23:LYS:HG2	1.82	0.44
7:G:12:LEU:H	7:G:12:LEU:CD1	2.26	0.44
12:L:28:LYS:HG2	12:L:33:ARG:HH12	1.82	0.44
15:O:29:VAL:HG12	15:O:85:LEU:CD1	2.48	0.44
16:P:43:LYS:HA	16:P:48:TRP:HB3	1.99	0.44
20:T:31:SER:O	20:T:32:ALA:C	2.61	0.44
1:A:22:G:H2'	1:A:23:C:H6	1.82	0.44
1:A:81:U:H3'	1:A:81:U:H6	1.83	0.44
1:A:287:U:O2'	1:A:288:A:H5'	2.17	0.44
1:A:401:C:H2'	1:A:402:G:H8	1.82	0.44
1:A:484:G:H1'	1:A:485:G:OP2	2.16	0.44
1:A:505:G:C6	1:A:535:A:C2	3.06	0.44
1:A:551:U:H2'	1:A:552:U:C6	2.52	0.44
1:A:558:G:H3'	1:A:559:A:H3'	1.99	0.44
1:A:651:C:H2'	1:A:652:U:C6	2.52	0.44
1:A:984:C:N4	1:A:1221:G:H1	2.15	0.44
1:A:1054:C:C5	1:A:1196:U:C6	3.06	0.44
1:A:1532:U:H2'	1:A:1533:C:C5'	2.46	0.44
4:D:78:LEU:HA	4:D:78:LEU:HD23	1.45	0.44
6:F:67:MET:HB2	6:F:68:PRO:HD2	2.00	0.44
12:L:46:LYS:C	12:L:48:PRO:HD2	2.42	0.44
12:L:69:TYR:CE2	12:L:71:PRO:HA	2.53	0.44
13:M:79:LYS:HA	13:M:82:MET:CE	2.46	0.44
14:N:9:LYS:O	14:N:10:ALA:C	2.60	0.44
17:Q:45:HIS:CD2	17:Q:47:PRO:HG3	2.53	0.44
17:Q:48:GLU:OE1	17:Q:50:LYS:HD2	2.18	0.44
1:A:168:G:C2	1:A:169:C:C5	3.06	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:G:H2'	1:A:285:G:C8	2.50	0.44
1:A:452:A:N3	16:P:72:ARG:NH1	2.66	0.44
1:A:575:G:O2'	1:A:821:G:OP2	2.30	0.44
1:A:594:G:H2'	1:A:595:G:H5'	1.98	0.44
1:A:1030(C):G:C6	1:A:1030(D):A:C6	3.06	0.44
1:A:1379:G:C6	1:A:1380:U:C4	3.06	0.44
1:A:1540:PSU:H6	1:A:1540:PSU:C3'	2.06	0.44
2:B:239:VAL:O	2:B:240:GLN:CB	2.64	0.44
3:C:20:SER:HB3	3:C:57:ILE:HB	1.99	0.44
3:C:73:PRO:O	3:C:76:VAL:HG22	2.17	0.44
4:D:149:ALA:HB3	4:D:152:SER:HB2	1.99	0.44
5:E:31:LEU:HD23	5:E:31:LEU:HA	1.49	0.44
5:E:80:ILE:HD11	5:E:138:ALA:CA	2.47	0.44
7:G:15:ASP:OD1	7:G:18:TYR:N	2.40	0.44
11:K:34:ASP:HB2	11:K:35:PRO:HD2	2.00	0.44
11:K:126:ARG:C	11:K:128:ALA:H	2.26	0.44
20:T:53:LEU:O	20:T:54:LYS:C	2.61	0.44
1:A:221:C:O2'	1:A:222:U:H5'	2.17	0.44
1:A:243:A:H4'	1:A:244:U:H5''	2.00	0.44
1:A:316:G:H4'	27:A:2121:HOH:O	2.18	0.44
1:A:328:C:O2'	1:A:329:A:P	2.75	0.44
1:A:403:C:H2'	1:A:404:U:H6	1.83	0.44
1:A:485:G:O2'	1:A:486:U:OP2	2.32	0.44
1:A:1028:C:C5	1:A:1029:C:C5	3.06	0.44
1:A:1426:C:H2'	1:A:1427:U:H6	1.83	0.44
2:B:61:LEU:HD13	2:B:61:LEU:C	2.43	0.44
2:B:91:PRO:HG3	2:B:154:LEU:HB2	1.99	0.44
3:C:56:ASP:O	3:C:66:VAL:HA	2.17	0.44
3:C:70:VAL:HG12	3:C:72:LYS:H	1.83	0.44
3:C:187:ALA:HB3	3:C:198:VAL:HB	2.00	0.44
5:E:76:ILE:CG2	5:E:77:PRO:HD2	2.47	0.44
7:G:137:LYS:O	7:G:141:VAL:HG23	2.18	0.44
11:K:124:LYS:HD2	11:K:125:PHE:CE2	2.53	0.44
15:O:41:GLU:OE1	15:O:44:LYS:HD2	2.17	0.44
17:Q:60:ILE:HD13	17:Q:61:GLU:O	2.17	0.44
18:R:45:SER:O	18:R:47:THR:O	2.36	0.44
1:A:401:C:O2'	1:A:621:A:N3	2.49	0.44
1:A:429:U:H1'	1:A:430:A:H5''	1.99	0.44
1:A:564:C:H2'	1:A:565:U:O4'	2.18	0.44
1:A:948:C:O2'	1:A:949:A:H5'	2.17	0.44
1:A:1496:C:H2'	1:A:1497:G:O4'	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:22:LYS:C	2:B:24:TRP:H	2.25	0.44
2:B:125:PRO:HG2	2:B:126:GLU:OE1	2.17	0.44
3:C:134:ILE:CG2	3:C:151:VAL:HB	2.48	0.44
5:E:116:THR:HG22	5:E:117:ASP:OD2	2.17	0.44
7:G:78:ARG:NH1	7:G:156:TRP:HB3	2.33	0.44
12:L:68:ALA:HB3	12:L:100:ILE:HD11	1.99	0.44
13:M:8:GLU:OE1	13:M:23:TYR:N	2.48	0.44
19:S:13:ASP:HA	19:S:16:LEU:HB3	1.99	0.44
1:A:564:C:C5	17:Q:31:LEU:HD11	2.53	0.44
1:A:1271:G:H5'	1:A:1314:C:OP1	2.18	0.44
1:A:1347:G:H2'	1:A:1373:G:H1	1.82	0.44
5:E:73:ASN:CG	5:E:73:ASN:O	2.61	0.44
7:G:21:VAL:HG23	7:G:22:LEU:N	2.33	0.44
8:H:10:LEU:HD22	8:H:83:ILE:HD11	1.99	0.44
9:I:10:ARG:CZ	9:I:105:ASP:OD2	2.66	0.44
10:J:4:ILE:HD12	10:J:4:ILE:O	2.18	0.44
10:J:89:ASP:OD2	10:J:91:PRO:HG2	2.17	0.44
16:P:9:PHE:N	16:P:16:HIS:O	2.49	0.44
1:A:79:G:C2	1:A:91:C:C2	3.06	0.43
1:A:342:C:C2'	1:A:343:U:H5'	2.47	0.43
1:A:417:C:H2'	1:A:418:C:H6	1.82	0.43
1:A:522:C:OP2	12:L:69:TYR:OH	2.24	0.43
1:A:789:U:H2'	1:A:791:G:OP2	2.18	0.43
1:A:1519[B]:MA6:H5'	1:A:1520[B]:G:OP2	2.17	0.43
5:E:12:LEU:HD13	5:E:31:LEU:CB	2.48	0.43
5:E:144:THR:H	5:E:147:ASP:HB2	1.83	0.43
10:J:74:ILE:O	10:J:74:ILE:HG13	2.17	0.43
11:K:21:ILE:HD13	11:K:94:ALA:HB1	2.00	0.43
13:M:70:LEU:HA	13:M:70:LEU:HD23	1.73	0.43
15:O:85:LEU:HB2	15:O:87:ILE:HG13	1.99	0.43
16:P:38:TYR:CE2	16:P:50:LYS:HB3	2.53	0.43
1:A:317:G:C6	1:A:318:G:N7	2.86	0.43
1:A:854:G:C6	1:A:855:G:N7	2.86	0.43
1:A:1402:4OC:H2'	1:A:1403:C:O4'	2.18	0.43
2:B:239:VAL:O	2:B:240:GLN:HB3	2.17	0.43
3:C:152:ILE:HB	3:C:199:LYS:HB2	1.99	0.43
4:D:188:LEU:HD23	4:D:188:LEU:HA	1.90	0.43
7:G:104:LEU:HD23	7:G:104:LEU:HA	1.81	0.43
8:H:59:LEU:HD12	8:H:59:LEU:N	2.33	0.43
12:L:60:LEU:HB3	12:L:62:SER:HB3	2.00	0.43
1:A:298:A:H2'	1:A:299:G:O4'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1308:U:P	13:M:99:ARG:HG3	2.58	0.43
1:A:1450:U:H2'	1:A:1452:C:C4	2.54	0.43
14:N:7:ILE:C	14:N:9:LYS:H	2.26	0.43
20:T:87:LYS:HE2	20:T:87:LYS:HB2	1.80	0.43
1:A:327:A:O2'	1:A:328:C:H6	2.02	0.43
1:A:420:U:H1'	1:A:424:G:N2	2.34	0.43
1:A:644:G:C5	1:A:645:C:C5	3.06	0.43
1:A:803:G:C6	1:A:804:U:C4	3.06	0.43
1:A:838:G:C2'	1:A:839:U:H5''	2.48	0.43
1:A:1030(A):G:N2	1:A:1030(C):G:O5'	2.51	0.43
1:A:1190:G:C2'	1:A:1191:A:OP2	2.66	0.43
1:A:1426:C:C2	1:A:1427:U:C5	3.06	0.43
2:B:73:THR:O	2:B:73:THR:HG22	2.19	0.43
3:C:6:HIS:HE2	3:C:8:ILE:HD12	1.84	0.43
4:D:80:GLU:O	4:D:84:LYS:HG3	2.18	0.43
8:H:29:SER:OG	8:H:32:LYS:HG3	2.18	0.43
13:M:31:LYS:O	13:M:35:GLU:HG3	2.18	0.43
16:P:58:TYR:O	16:P:61:SER:N	2.51	0.43
19:S:12:ASP:H	19:S:38:SER:HB3	1.83	0.43
1:A:532:A:N6	3:C:193:TYR:HA	2.33	0.43
1:A:781:A:C5	1:A:802:A:C2	3.07	0.43
1:A:836:G:OP1	18:R:61:LYS:NZ	2.40	0.43
1:A:1229:A:P	13:M:114:ARG:HD3	2.59	0.43
2:B:208:ILE:HD13	2:B:208:ILE:N	2.33	0.43
3:C:34:LEU:HD21	3:C:38:ARG:CZ	2.49	0.43
6:F:14:LEU:HD21	6:F:84:ASN:OD1	2.18	0.43
10:J:24:VAL:HG13	10:J:34:VAL:HG11	2.00	0.43
1:A:181:G:H4'	1:A:182:U:OP2	2.17	0.43
1:A:185:A:N3	20:T:81:LYS:NZ	2.59	0.43
1:A:321:A:H2'	1:A:322:C:C6	2.53	0.43
1:A:977:A:C2'	1:A:978:A:H5''	2.49	0.43
1:A:1106:G:O2'	1:A:1107:C:H5'	2.18	0.43
1:A:1190:G:OP1	3:C:4:LYS:HA	2.17	0.43
4:D:199:ASN:OD1	4:D:199:ASN:C	2.60	0.43
13:M:74:VAL:O	13:M:77:ASN:N	2.52	0.43
15:O:17:ARG:NH1	15:O:17:ARG:CG	2.77	0.43
1:A:191:G:O2'	20:T:102:GLY:O	2.29	0.43
1:A:1262:C:H2'	1:A:1263:C:C6	2.53	0.43
1:A:1347:G:C6	9:I:107:ARG:NH2	2.87	0.43
1:A:1406:U:C4'	1:A:1518[B]:MA6:H1'	2.48	0.43
13:M:34:LEU:HD13	13:M:41:PRO:CA	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:75:ARG:HG3	17:Q:75:ARG:HH11	1.84	0.43
1:A:190(C):C:H2'	1:A:190(D):U:O4'	2.19	0.43
1:A:353:A:C2'	1:A:354:G:OP2	2.67	0.43
1:A:373:A:C2'	1:A:374:A:O5'	2.66	0.43
1:A:377:G:C2	1:A:387:U:O2	2.72	0.43
1:A:1004:A:N7	1:A:1036:G:O6	2.52	0.43
1:A:1221:G:C4	1:A:1222:G:C8	3.06	0.43
1:A:1223:C:P	19:S:78:ARG:NH1	2.92	0.43
2:B:135:GLN:O	2:B:139:LYS:HB2	2.19	0.43
9:I:102:LEU:H	9:I:102:LEU:HD12	1.84	0.43
13:M:10:PRO:CB	13:M:18:ALA:HB1	2.42	0.43
17:Q:95:TYR:O	17:Q:96:GLN:C	2.62	0.43
19:S:27:GLU:N	19:S:27:GLU:OE1	2.52	0.43
1:A:427:U:H3'	1:A:428:G:H2'	2.00	0.43
1:A:600:C:H2'	1:A:601:C:H6	1.83	0.43
1:A:659:U:O2'	1:A:660:G:H5'	2.18	0.43
1:A:895:G:H2'	1:A:896:C:H6	1.84	0.43
1:A:1055:A:N7	1:A:1200:C:N4	2.66	0.43
1:A:1127:G:O2'	9:I:16:ARG:NH2	2.44	0.43
1:A:1347:G:H1'	1:A:1348:U:H5	1.82	0.43
1:A:1497:G:HO2'	1:A:1518[A]:MA6:C2	2.31	0.43
8:H:116:LYS:HA	8:H:116:LYS:HD3	1.88	0.43
10:J:39:PRO:HB3	10:J:70:ARG:HH11	1.79	0.43
11:K:33:THR:HB	11:K:38:ASN:C	2.44	0.43
12:L:126:LYS:N	12:L:126:LYS:HD2	2.34	0.43
16:P:1:MET:HE2	16:P:1:MET:HB3	1.83	0.43
19:S:19:VAL:HG13	19:S:20:LEU:N	2.34	0.43
1:A:201:C:H42	1:A:216:G:H1	1.67	0.43
1:A:1206:G:C4	1:A:1207:2MG:C8	3.07	0.43
1:A:1347:G:HO2'	1:A:1348:U:H6	1.61	0.43
2:B:28:PHE:CD2	2:B:190:THR:HA	2.54	0.43
2:B:33:TYR:C	2:B:33:TYR:HD2	2.27	0.43
2:B:92:TYR:CD1	2:B:151:GLY:HA3	2.54	0.43
2:B:100:GLY:O	2:B:104:ASN:N	2.51	0.43
2:B:187:LEU:HA	2:B:201:ILE:HB	2.01	0.43
7:G:114:ARG:O	7:G:119:ARG:NH1	2.51	0.43
12:L:60:LEU:HB3	12:L:62:SER:H	1.83	0.43
16:P:2:VAL:HG13	16:P:64:ALA:HA	2.01	0.43
16:P:41:PRO:O	16:P:43:LYS:HD2	2.19	0.43
16:P:42:ARG:O	16:P:43:LYS:C	2.61	0.43
20:T:91:LEU:HD23	20:T:91:LEU:HA	1.70	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:G:C6	1:A:23:C:C4	3.07	0.42
1:A:101:A:O2'	1:A:102:G:H5'	2.18	0.42
1:A:123:C:OP1	1:A:312:C:H5'	2.19	0.42
1:A:181:G:H4'	1:A:182:U:H5'	2.01	0.42
1:A:327:A:HO2'	1:A:328:C:H6	1.66	0.42
1:A:530:G:N7	23:W:34:G:N2	2.66	0.42
1:A:622:A:C8	1:A:623:C:C6	3.07	0.42
1:A:1299:A:C5	1:A:1301:U:O2	2.72	0.42
1:A:1346:A:C4	7:G:10:ARG:NH2	2.87	0.42
1:A:1497:G:C3'	1:A:1498:UR3:H5'	2.48	0.42
2:B:132:LYS:HD3	2:B:135:GLN:HB2	2.01	0.42
4:D:142:PRO:HA	4:D:185:PHE:HD2	1.84	0.42
9:I:112:LYS:NZ	9:I:113:LYS:O	2.52	0.42
12:L:27:LEU:HG	12:L:28:LYS:H	1.84	0.42
1:A:12:U:O2'	1:A:914:A:OP1	2.31	0.42
1:A:285:G:O2'	1:A:286:G:H5'	2.19	0.42
1:A:392:G:C2	1:A:393:A:C4	3.06	0.42
1:A:436:C:H2'	1:A:437:U:C6	2.54	0.42
1:A:779:C:H2'	1:A:780:A:O4'	2.19	0.42
1:A:1054:C:HO2'	1:A:1055:A:P	2.40	0.42
1:A:1080:A:H5''	5:E:16:THR:HG21	2.01	0.42
1:A:1300:G:C5	1:A:1335:C:C5	3.07	0.42
1:A:1389:C:H2'	1:A:1390:U:O4'	2.18	0.42
2:B:47:THR:HG23	2:B:202:PRO:O	2.19	0.42
3:C:84:ILE:HG13	3:C:88:ARG:NH1	2.35	0.42
6:F:97:PHE:HB2	18:R:32:ARG:HH11	1.75	0.42
8:H:104:ARG:O	8:H:106:GLY:N	2.51	0.42
16:P:57:ARG:O	16:P:58:TYR:C	2.62	0.42
19:S:36:ARG:NH2	19:S:53:ASN:HA	2.34	0.42
1:A:67:C:O2'	1:A:171:A:H1'	2.19	0.42
1:A:321:A:H2'	1:A:322:C:H6	1.83	0.42
1:A:1189:C:H5''	3:C:5:ILE:HG12	2.00	0.42
1:A:1321:C:C5'	13:M:87:TYR:HE2	2.31	0.42
1:A:1368:G:OP2	9:I:114:TYR:N	2.52	0.42
3:C:154:SER:OG	3:C:197:GLY:N	2.42	0.42
7:G:135:VAL:O	7:G:139:GLU:HG3	2.19	0.42
9:I:8:GLY:HA3	9:I:79:LEU:HB3	2.01	0.42
9:I:48:GLU:OE1	9:I:48:GLU:HA	2.19	0.42
1:A:260:G:H2'	1:A:261:U:C6	2.54	0.42
1:A:273:A:N6	1:A:274:A:N6	2.68	0.42
1:A:338:A:C6	1:A:339:C:C4	3.07	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:625:G:H2'	1:A:626:U:C6	2.55	0.42
1:A:693:G:C6	1:A:694:A:C5	3.07	0.42
1:A:767:A:H2'	1:A:768:A:O4'	2.19	0.42
1:A:890:G:O2'	1:A:906:G:O6	2.30	0.42
1:A:993:G:H2'	1:A:993:G:N3	2.35	0.42
1:A:1400:5MC:H3'	1:A:1401:G:C5'	2.48	0.42
1:A:1417:G:H1'	1:A:1483:A:N6	2.34	0.42
2:B:69:LEU:HD12	2:B:155:LEU:HD11	2.01	0.42
2:B:93:VAL:HG11	2:B:97:TRP:HD1	1.84	0.42
3:C:127:ARG:HH22	3:C:191:THR:HB	1.83	0.42
3:C:189:ALA:HB3	3:C:196:LEU:HB2	2.00	0.42
4:D:153:ARG:HG2	4:D:181:MET:SD	2.60	0.42
4:D:187:ARG:HH21	4:D:193:ASP:CG	2.27	0.42
6:F:91:VAL:HG13	18:R:72:ARG:NH2	2.33	0.42
17:Q:27:PHE:O	17:Q:36:ILE:HD13	2.18	0.42
1:A:919:A:O2'	1:A:920:U:H5'	2.20	0.42
1:A:1003(A):G:C6	1:A:1004:A:N3	2.87	0.42
1:A:1015:A:H2'	1:A:1016:A:O4'	2.18	0.42
1:A:1060:C:C5	3:C:2:GLY:HA2	2.54	0.42
1:A:1500:A:OP1	27:A:1927:HOH:O	2.22	0.42
3:C:39:ILE:O	3:C:43:LEU:HD23	2.19	0.42
5:E:43:LEU:HD23	5:E:43:LEU:HA	1.82	0.42
5:E:144:THR:O	5:E:145:LYS:C	2.62	0.42
6:F:76:ALA:O	6:F:77:ARG:C	2.61	0.42
7:G:40:ALA:O	7:G:41:ARG:C	2.63	0.42
9:I:17:VAL:HG11	9:I:81:ILE:HA	2.00	0.42
10:J:82:ILE:O	10:J:82:ILE:HG22	2.18	0.42
13:M:49:THR:HB	13:M:52:GLU:OE1	2.18	0.42
20:T:33:ILE:O	20:T:34:LYS:C	2.60	0.42
1:A:232:G:H1'	1:A:262:A:N1	2.35	0.42
1:A:1090:U:O2'	1:A:1091:U:H5'	2.20	0.42
2:B:100:GLY:HA3	2:B:104:ASN:HB2	2.01	0.42
3:C:40:ARG:O	3:C:44:GLU:HG3	2.19	0.42
4:D:200:GLU:CD	4:D:200:GLU:H	2.27	0.42
5:E:24:ARG:HH11	5:E:24:ARG:CB	2.31	0.42
5:E:112:LEU:HD23	5:E:112:LEU:HA	1.76	0.42
9:I:100:GLY:O	9:I:103:THR:HB	2.20	0.42
9:I:102:LEU:HD12	9:I:102:LEU:N	2.34	0.42
10:J:54:PHE:HD2	10:J:55:LYS:HG2	1.84	0.42
11:K:57:THR:HG23	11:K:58:PRO:HD2	2.02	0.42
14:N:14:PRO:O	14:N:15:LYS:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:27:VAL:O	15:O:31:LEU:HD13	2.19	0.42
1:A:575:G:O2'	1:A:821:G:H5'	2.20	0.42
1:A:948:C:OP2	13:M:108:ARG:HB2	2.19	0.42
1:A:1094:G:O5'	1:A:1095:U:H5	2.03	0.42
1:A:1216:G:H5''	14:N:5:ALA:HB2	2.00	0.42
2:B:158:LEU:HD12	2:B:158:LEU:N	2.33	0.42
6:F:10:LEU:HD11	6:F:59:TYR:HD2	1.83	0.42
10:J:62:HIS:O	14:N:59:ALA:HB3	2.20	0.42
11:K:69:ALA:HB1	11:K:103:LEU:HD12	2.02	0.42
19:S:22:LEU:HD23	19:S:22:LEU:HA	1.90	0.42
1:A:1498:UR3:OP2	1:A:1542:U:O2'	2.32	0.42
25:A:1860:SRV:HI32	25:A:1860:SRV:H22	2.01	0.42
5:E:11:ILE:HG22	5:E:12:LEU:N	2.35	0.42
5:E:43:LEU:HD22	5:E:44:GLY:N	2.35	0.42
7:G:54:THR:C	7:G:56:GLN:H	2.28	0.42
8:H:13:ILE:O	8:H:17:THR:HG23	2.19	0.42
11:K:114:VAL:HG22	11:K:115:PRO:O	2.20	0.42
13:M:64:TRP:HB2	13:M:66:LEU:HD21	2.02	0.42
15:O:45:VAL:HB	15:O:46:HIS:CD2	2.55	0.42
17:Q:59:ILE:HD12	17:Q:73:VAL:HA	2.02	0.42
18:R:31:LEU:HD23	18:R:31:LEU:HA	1.91	0.42
1:A:28:G:H2'	1:A:29:G:O4'	2.20	0.42
1:A:190(L):U:C2	20:T:105:SER:HB2	2.54	0.42
1:A:1077:G:N2	1:A:1080:A:OP2	2.51	0.42
1:A:1240:U:H3'	1:A:1241:G:C5'	2.50	0.42
1:A:1488:G:H2'	1:A:1489:G:H8	1.83	0.42
3:C:114:PRO:O	3:C:118:GLN:HG3	2.20	0.42
5:E:105:VAL:N	5:E:106:PRO:HD2	2.35	0.42
5:E:145:LYS:HE3	8:H:107:LEU:HD23	2.01	0.42
8:H:1:MET:HG3	8:H:2:LEU:O	2.19	0.42
16:P:38:TYR:CE2	16:P:50:LYS:HE2	2.55	0.42
17:Q:34:LYS:CG	17:Q:35:VAL:N	2.83	0.42
17:Q:86:GLU:O	17:Q:87:LYS:C	2.59	0.42
1:A:327:A:O2'	1:A:328:C:O4'	2.38	0.42
1:A:552:U:O2'	1:A:553:A:H5'	2.19	0.42
1:A:981:U:H2'	1:A:982:U:C5	2.55	0.42
1:A:1516[B]:G:C4	1:A:1518[B]:MA6:OP2	2.72	0.42
3:C:58:GLU:HB2	3:C:65:ALA:HB2	2.02	0.42
4:D:140:VAL:CG1	4:D:146:ILE:HD11	2.50	0.42
8:H:31:PHE:O	8:H:32:LYS:C	2.62	0.42
10:J:28:ARG:HA	10:J:34:VAL:HG21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:79:LYS:HA	13:M:82:MET:HE2	2.02	0.42
14:N:4:LYS:HD2	14:N:4:LYS:N	2.34	0.42
15:O:21:ASP:OD2	15:O:24:SER:HB3	2.20	0.42
1:A:130:A:C8	17:Q:63:ARG:HG3	2.55	0.41
1:A:243:A:N6	1:A:281:G:H1'	2.35	0.41
1:A:581:G:O3'	15:O:64:ARG:NH2	2.53	0.41
1:A:815:A:N7	1:A:1509:C:O2'	2.44	0.41
1:A:922:G:H4'	5:E:19:MET:O	2.19	0.41
1:A:944:G:H5''	1:A:945:G:OP2	2.20	0.41
1:A:967:5MC:H5''	1:A:968:A:OP2	2.19	0.41
1:A:1167:A:C6	1:A:1168:A:C6	3.07	0.41
2:B:73:THR:HG23	2:B:95:GLN:O	2.20	0.41
8:H:104:ARG:C	8:H:106:GLY:N	2.76	0.41
1:A:22:G:H2'	1:A:23:C:C6	2.55	0.41
1:A:364:A:H61	12:L:28:LYS:HE2	1.84	0.41
1:A:413:G:O2'	1:A:428:G:N2	2.53	0.41
1:A:510:A:H5''	1:A:511:C:P	2.60	0.41
1:A:542:G:O2'	1:A:543:C:H5'	2.20	0.41
1:A:556:C:H2'	1:A:557:G:C5'	2.49	0.41
1:A:688:G:H2'	1:A:689:C:C6	2.53	0.41
1:A:991:U:HO2'	1:A:992:U:P	2.43	0.41
1:A:991:U:O4	1:A:1212:U:H1'	2.19	0.41
1:A:1228:C:O2'	13:M:117:VAL:HG22	2.19	0.41
1:A:1281:U:H5''	1:A:1282:C:H5	1.85	0.41
3:C:15:THR:O	3:C:16:ARG:HB2	2.19	0.41
10:J:7:LYS:HE3	10:J:40:LEU:CD1	2.50	0.41
17:Q:29:HIS:HE1	17:Q:31:LEU:HB3	1.85	0.41
1:A:302:G:O2'	1:A:556:C:H5''	2.21	0.41
1:A:597:G:H2'	1:A:598:U:H5'	2.03	0.41
1:A:645:C:H2'	1:A:646:U:C6	2.55	0.41
1:A:781:A:H5'	1:A:782:A:OP2	2.21	0.41
1:A:926:G:C6	1:A:1505:G:C5	3.09	0.41
1:A:1315:U:H2'	1:A:1316:G:O4'	2.21	0.41
1:A:1432:G:O5'	1:A:1432:G:H8	2.02	0.41
1:A:1539:C:OP1	1:A:1540:PSU:OP2	2.38	0.41
2:B:61:LEU:HD21	2:B:160:ASP:HB3	2.02	0.41
3:C:115:LEU:HD23	3:C:115:LEU:HA	1.82	0.41
6:F:44:GLY:HA2	6:F:59:TYR:CZ	2.55	0.41
7:G:26:PHE:CE2	7:G:30:ILE:HD11	2.55	0.41
8:H:104:ARG:NH2	8:H:138:TRP:CH2	2.88	0.41
13:M:36:LYS:HD2	13:M:59:TYR:OH	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:24:CYS:O	14:N:28:GLY:HA2	2.20	0.41
15:O:36:ILE:HA	15:O:59:MET:HE1	2.02	0.41
20:T:10:LEU:HD12	20:T:12:ALA:H	1.83	0.41
1:A:115:G:H1'	1:A:116:A:N7	2.35	0.41
1:A:462:G:C6	1:A:463:A:C5	3.08	0.41
1:A:636:U:H2'	1:A:637:G:C8	2.56	0.41
1:A:1124:G:H2'	1:A:1145:C:C5	2.55	0.41
1:A:1130:A:OP1	1:A:1131:G:P	2.78	0.41
1:A:1502:A:N3	1:A:1502:A:C2'	2.83	0.41
2:B:83:MET:HA	2:B:86:GLU:HB2	2.03	0.41
3:C:180:ALA:HB1	3:C:182:ILE:CG1	2.48	0.41
6:F:11:ASN:OD1	6:F:13:ASN:N	2.45	0.41
9:I:44:VAL:HG12	9:I:51:ARG:HH22	1.86	0.41
16:P:15:PRO:HG2	16:P:41:PRO:HG2	2.03	0.41
19:S:22:LEU:HD23	19:S:25:LYS:HZ3	1.86	0.41
20:T:50:GLU:CB	20:T:99:LEU:HD12	2.41	0.41
1:A:397:A:C6	1:A:548:G:C8	3.08	0.41
1:A:662:G:H2'	1:A:663:A:C8	2.55	0.41
1:A:867:G:O2'	1:A:868:C:H5'	2.20	0.41
1:A:1026:G:C6	1:A:1027:C:N4	2.89	0.41
1:A:1107:C:C4	1:A:1108:G:C8	3.08	0.41
1:A:1494:G:O2'	1:A:1495:U:H5'	2.20	0.41
5:E:69:VAL:HA	5:E:70:PRO:HD3	1.77	0.41
8:H:30:ARG:O	8:H:33:GLU:HB3	2.21	0.41
9:I:17:VAL:CG2	9:I:80:GLY:HA3	2.50	0.41
13:M:67:GLU:HB3	13:M:68:GLY:H	1.52	0.41
15:O:32:LEU:HA	15:O:32:LEU:HD23	1.76	0.41
17:Q:98:LEU:H	17:Q:98:LEU:HG	1.79	0.41
1:A:556:C:H2'	1:A:557:G:H5'	2.02	0.41
1:A:1035:A:C4	1:A:1036:G:N7	2.88	0.41
1:A:1287:A:C6	1:A:1288:A:C6	3.09	0.41
1:A:1288:A:C6	1:A:1289:A:C5	3.09	0.41
1:A:1288:A:C6	1:A:1289:A:C6	3.09	0.41
1:A:1347:G:O2'	1:A:1348:U:O5'	2.37	0.41
2:B:43:ASP:OD1	2:B:43:ASP:C	2.64	0.41
2:B:191:ASP:OD1	2:B:191:ASP:N	2.52	0.41
2:B:230:VAL:HG12	2:B:231:GLU:O	2.20	0.41
5:E:11:ILE:HA	5:E:11:ILE:HD13	1.69	0.41
7:G:32:ARG:O	7:G:33:ASP:C	2.63	0.41
11:K:33:THR:HB	11:K:38:ASN:O	2.20	0.41
13:M:4:ILE:O	13:M:5:ALA:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:70:ALA:O	16:P:74:LEU:HG	2.20	0.41
19:S:18:LYS:HB2	19:S:18:LYS:HE3	1.87	0.41
1:A:415:A:H2'	1:A:416:G:C8	2.56	0.41
1:A:575:G:C8	1:A:881:G:N2	2.88	0.41
1:A:939:G:C6	1:A:940:C:N4	2.88	0.41
1:A:973:G:C2'	1:A:974:A:OP1	2.69	0.41
1:A:1064:G:N2	1:A:1190:G:H2'	2.36	0.41
1:A:1090:U:H2'	1:A:1091:U:H6	1.85	0.41
1:A:1342:C:H2'	1:A:1343:G:H8	1.84	0.41
1:A:1426:C:H2'	1:A:1427:U:C6	2.55	0.41
1:A:1494:G:C2'	1:A:1495:U:H5'	2.51	0.41
2:B:236:TYR:O	2:B:239:VAL:HG23	2.20	0.41
4:D:61:LYS:NZ	4:D:72:GLU:OE2	2.53	0.41
5:E:78:HIS:CE1	8:H:104:ARG:HH21	2.37	0.41
6:F:9:VAL:HG22	6:F:60:PHE:CE2	2.56	0.41
13:M:59:TYR:CD1	13:M:63:THR:HG21	2.56	0.41
15:O:2:PRO:HB2	15:O:3:ILE:H	1.76	0.41
16:P:65:GLN:HA	16:P:66:PRO:HD3	1.80	0.41
16:P:74:LEU:HD22	16:P:79:VAL:HG21	2.02	0.41
20:T:22:ARG:O	20:T:23:ARG:C	2.62	0.41
1:A:190(J):U:H2'	1:A:190(K):G:C8	2.56	0.41
1:A:246:A:N1	1:A:278:G:O2'	2.44	0.41
1:A:564:C:C6	17:Q:31:LEU:HD11	2.56	0.41
1:A:825:G:N2	8:H:11:THR:HG21	2.33	0.41
1:A:904:C:C2'	1:A:905:U:H5'	2.51	0.41
1:A:978:A:C6	1:A:1318:A:C6	3.09	0.41
1:A:1028:C:C6	1:A:1029:C:C5	3.09	0.41
1:A:1179:A:H2'	1:A:1180:A:O5'	2.20	0.41
1:A:1218:C:H2'	1:A:1219:U:C6	2.55	0.41
2:B:90:MET:HA	2:B:91:PRO:HD3	1.85	0.41
2:B:130:ARG:HD3	2:B:130:ARG:HA	1.63	0.41
2:B:149:LEU:O	2:B:153:ARG:HB3	2.20	0.41
4:D:140:VAL:HG11	4:D:146:ILE:HD11	2.01	0.41
6:F:27:GLN:O	6:F:31:GLU:HG3	2.20	0.41
6:F:40:VAL:HG23	6:F:62:TRP:O	2.21	0.41
8:H:82:HIS:ND1	8:H:138:TRP:CE2	2.88	0.41
9:I:55:ALA:O	9:I:56:LEU:C	2.63	0.41
1:A:37:U:H2'	1:A:38:G:O4'	2.20	0.41
1:A:98:U:O2'	1:A:99:C:H5'	2.21	0.41
1:A:149:A:O2'	1:A:150:C:H5'	2.21	0.41
1:A:192:U:O4'	20:T:103:GLY:HA2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:G:C6	1:A:393:A:C5	3.09	0.41
1:A:504:C:C2	1:A:542:G:N2	2.89	0.41
1:A:692:U:H2'	1:A:694:A:OP2	2.20	0.41
1:A:738:C:OP1	6:F:92:LYS:HD3	2.21	0.41
1:A:791:G:C6	1:A:792:A:N7	2.89	0.41
1:A:812:C:H1'	1:A:813:U:OP2	2.21	0.41
1:A:1002:G:C6	1:A:1003:G:C6	3.09	0.41
1:A:1004:A:C6	1:A:1037:C:N4	2.88	0.41
1:A:1241:G:H2'	1:A:1242:C:H6	1.85	0.41
1:A:1399:C:O2	1:A:1401:G:N7	2.54	0.41
2:B:124:SER:HB2	2:B:125:PRO:CD	2.45	0.41
2:B:167:PRO:HG2	2:B:192:SER:HB3	2.03	0.41
2:B:180:LEU:HD23	2:B:180:LEU:HA	1.91	0.41
2:B:231:GLU:HB3	2:B:232:PRO:HD2	2.02	0.41
2:B:238:LEU:HD23	2:B:238:LEU:HA	1.89	0.41
3:C:150:LYS:CG	3:C:169:ALA:HB2	2.40	0.41
3:C:152:ILE:N	3:C:152:ILE:HD12	2.36	0.41
4:D:50:ARG:HA	4:D:51:PRO:HD3	1.81	0.41
4:D:52:SER:O	4:D:55:ALA:HB3	2.21	0.41
4:D:63:LYS:O	4:D:67:ILE:HG13	2.21	0.41
5:E:80:ILE:HD11	5:E:138:ALA:HA	2.02	0.41
8:H:114:THR:OG1	8:H:116:LYS:N	2.51	0.41
16:P:21:VAL:HG11	16:P:59:TRP:CD2	2.56	0.41
17:Q:59:ILE:CG2	17:Q:71:PHE:CD1	3.03	0.41
18:R:45:SER:HB2	18:R:46:GLU:OE2	2.21	0.41
19:S:31:ILE:HG23	19:S:32:LYS:N	2.35	0.41
21:U:23:PRO:C	21:U:25:LYS:H	2.27	0.41
1:A:166:G:H2'	1:A:167:G:H8	1.86	0.41
1:A:216:G:O2'	1:A:217:C:C5'	2.68	0.41
1:A:514:C:H2'	1:A:515:G:H8	1.85	0.41
1:A:567:G:H2'	1:A:568:G:O4'	2.21	0.41
1:A:645:C:H2'	1:A:646:U:O4'	2.21	0.41
1:A:658:G:H2'	1:A:659:U:C6	2.56	0.41
1:A:1137:C:OP2	1:A:1137:C:H6	2.04	0.41
1:A:1408:A:H2'	1:A:1409:C:C6	2.55	0.41
2:B:102:LEU:HA	2:B:102:LEU:HD12	1.81	0.41
2:B:115:LEU:HD21	2:B:153:ARG:HH21	1.85	0.41
3:C:50:ALA:HB2	3:C:75:VAL:HB	2.02	0.41
5:E:100:VAL:HG13	5:E:118:ILE:HG22	2.02	0.41
8:H:6:ILE:HB	8:H:85:ARG:NH2	2.36	0.41
8:H:40:ALA:O	8:H:41:ARG:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:8:GLY:CA	9:I:79:LEU:HB3	2.51	0.41
13:M:59:TYR:CD1	13:M:59:TYR:C	2.99	0.41
16:P:20:VAL:CG1	16:P:32:TYR:CB	2.99	0.41
20:T:8:ARG:N	20:T:8:ARG:CD	2.82	0.41
21:U:10:ARG:HA	21:U:10:ARG:HD3	1.69	0.41
1:A:538:G:C2	1:A:539:A:C4	3.09	0.40
1:A:663:A:O2'	1:A:664:G:H5'	2.20	0.40
1:A:1124:G:O5'	10:J:35:SER:O	2.39	0.40
1:A:1125:U:O2'	1:A:1126:U:P	2.79	0.40
1:A:1133:G:C2	1:A:1134:G:C8	3.09	0.40
1:A:1165:C:H2'	1:A:1166:G:H5'	2.03	0.40
1:A:1403:C:O2	1:A:1403:C:H2'	2.20	0.40
1:A:1518[B]:MA6:H102	1:A:1519[B]:MA6:N6	2.36	0.40
2:B:130:ARG:CB	2:B:131:PRO:HD2	2.37	0.40
5:E:139:LEU:HD23	5:E:139:LEU:HA	1.87	0.40
7:G:31:MET:CG	7:G:32:ARG:N	2.84	0.40
7:G:120:ILE:HD12	7:G:120:ILE:N	2.36	0.40
9:I:46:ALA:O	9:I:81:ILE:HD12	2.20	0.40
9:I:93:ARG:HB3	9:I:93:ARG:CZ	2.51	0.40
14:N:12:ARG:NH1	14:N:12:ARG:N	2.69	0.40
16:P:69:THR:O	16:P:72:ARG:HB3	2.20	0.40
17:Q:29:HIS:CE1	17:Q:32:TYR:H	2.39	0.40
20:T:50:GLU:HB2	20:T:99:LEU:CD1	2.43	0.40
1:A:173:U:H4'	1:A:174:C:OP2	2.21	0.40
1:A:384:G:O2'	1:A:385:C:H5'	2.21	0.40
1:A:665:A:H1'	1:A:733:A:O4'	2.22	0.40
1:A:695:A:OP1	11:K:52:GLY:HA3	2.20	0.40
1:A:1277:C:O2'	1:A:1279:A:C8	2.74	0.40
1:A:1300:G:H1'	1:A:1301:U:H5	1.87	0.40
1:A:1453:G:N2	1:A:1454:G:N7	2.70	0.40
3:C:11:ARG:NH1	3:C:177:THR:O	2.54	0.40
3:C:159:GLY:HA2	3:C:193:TYR:CD1	2.55	0.40
6:F:62:TRP:CH2	6:F:64:GLN:HB2	2.56	0.40
7:G:110:GLN:OE1	7:G:110:GLN:HA	2.21	0.40
9:I:125:TYR:N	9:I:125:TYR:CD2	2.89	0.40
10:J:63:PHE:HA	14:N:59:ALA:N	2.30	0.40
13:M:63:THR:HG23	13:M:64:TRP:N	2.32	0.40
13:M:86:CYS:SG	13:M:87:TYR:N	2.94	0.40
14:N:44:LEU:HD12	14:N:44:LEU:C	2.46	0.40
15:O:36:ILE:HG12	15:O:59:MET:HE3	2.02	0.40
16:P:82:GLN:O	16:P:83:GLU:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:24:GLU:HG2	17:Q:39:SER:HB3	2.03	0.40
18:R:36:ASN:O	18:R:40:LEU:HG	2.21	0.40
20:T:50:GLU:H	20:T:99:LEU:HD12	1.85	0.40
20:T:73:HIS:HB3	20:T:74:LYS:H	1.62	0.40
1:A:247:G:C6	1:A:278:G:C2	3.09	0.40
1:A:501:C:H1'	1:A:549:C:H1'	2.03	0.40
1:A:519:C:H2'	1:A:520:A:O4'	2.20	0.40
1:A:556:C:O2'	1:A:557:G:H5'	2.20	0.40
1:A:1029:C:O2'	1:A:1030:C:H5'	2.21	0.40
1:A:1035:A:C5	1:A:1036:G:N7	2.89	0.40
1:A:1069:C:HO2'	1:A:1192:C:H1'	1.87	0.40
1:A:1098:C:H2'	1:A:1099:G:O4'	2.22	0.40
1:A:1276:G:O5'	1:A:1276:G:H8	2.05	0.40
1:A:1488:G:H2'	1:A:1489:G:C8	2.57	0.40
2:B:108:ILE:O	2:B:111:ARG:HB2	2.21	0.40
3:C:177:THR:O	3:C:180:ALA:HB2	2.21	0.40
6:F:80:ARG:NH1	6:F:88:VAL:HB	2.35	0.40
7:G:136:LYS:NZ	7:G:140:ASP:OD2	2.38	0.40
11:K:34:ASP:O	11:K:37:GLY:N	2.41	0.40
11:K:43:SER:OG	11:K:44:SER:N	2.54	0.40
12:L:53:ARG:NH1	12:L:92:OTD:OD1	2.54	0.40
13:M:99:ARG:HB2	13:M:101:GLN:OE1	2.22	0.40
20:T:53:LEU:HB2	20:T:100:ILE:HG22	2.03	0.40
1:A:522:C:O2'	1:A:523:A:H5'	2.21	0.40
1:A:613:C:H2'	1:A:614:A:H8	1.87	0.40
1:A:664:G:H2'	1:A:666:G:OP1	2.22	0.40
1:A:735:C:H2'	1:A:736:C:H6	1.86	0.40
1:A:749:C:H2'	1:A:750:G:H8	1.87	0.40
1:A:756:C:H2'	1:A:757:U:O4'	2.20	0.40
1:A:771:G:C2'	1:A:772:U:H5'	2.51	0.40
1:A:1073:U:OP2	5:E:57:LYS:NZ	2.29	0.40
1:A:1160:G:N3	1:A:1160:G:H2'	2.36	0.40
1:A:1211:U:H2'	1:A:1211:U:O2	2.21	0.40
1:A:1316:G:N2	1:A:1319:A:OP2	2.54	0.40
7:G:54:THR:HB	7:G:56:GLN:H	1.86	0.40
7:G:120:ILE:N	7:G:120:ILE:CD1	2.85	0.40
10:J:62:HIS:CE1	14:N:61:TRP:CH2	3.09	0.40
15:O:67:LEU:HD23	15:O:67:LEU:HA	1.91	0.40
17:Q:43:LEU:HG	17:Q:68:ARG:HH12	1.86	0.40
19:S:9:VAL:HG12	19:S:10:PHE:N	2.36	0.40
1:A:375:U:C4	1:A:376:G:N7	2.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:A:H2'	1:A:394:G:H5'	2.03	0.40
1:A:401:C:H2'	1:A:402:G:C8	2.55	0.40
1:A:428:G:O4'	1:A:430:A:C8	2.74	0.40
1:A:429:U:H4'	1:A:430:A:O5'	2.22	0.40
1:A:884:U:H4'	1:A:885:G:H5''	2.03	0.40
1:A:953:G:H2'	1:A:954:G:O4'	2.21	0.40
1:A:1053:G:C3'	1:A:1054:C:C5'	3.00	0.40
1:A:1092:A:C6	1:A:1093:A:C6	3.09	0.40
1:A:1447:G:H2'	1:A:1448:C:H6	1.86	0.40
1:A:1447:G:H2'	1:A:1448:C:C6	2.56	0.40
1:A:1509:C:H2'	1:A:1510:U:O4'	2.22	0.40
1:A:1525:G:OP1	11:K:120:ARG:NH2	2.55	0.40
5:E:116:THR:HG22	5:E:117:ASP:CG	2.47	0.40
5:E:152:ARG:HB3	8:H:43:GLY:HA3	2.03	0.40
9:I:63:ILE:HD13	9:I:77:ILE:HG23	2.03	0.40
10:J:62:HIS:HE1	14:N:61:TRP:CZ3	2.38	0.40
11:K:58:PRO:O	11:K:61:ALA:HB3	2.21	0.40
20:T:53:LEU:HB2	20:T:100:ILE:HG21	2.03	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:702:A:N6	1:A:1447:G:OP1[4_554]	2.18	0.02

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	234/256 (91%)	209 (89%)	24 (10%)	1 (0%)	30 62
3	C	205/239 (86%)	183 (89%)	22 (11%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	206/209 (99%)	197 (96%)	9 (4%)	0	100	100
5	E	149/162 (92%)	141 (95%)	8 (5%)	0	100	100
6	F	99/101 (98%)	96 (97%)	3 (3%)	0	100	100
7	G	153/156 (98%)	139 (91%)	14 (9%)	0	100	100
8	H	136/138 (99%)	130 (96%)	6 (4%)	0	100	100
9	I	125/128 (98%)	113 (90%)	11 (9%)	1 (1%)	16	49
10	J	97/105 (92%)	80 (82%)	16 (16%)	1 (1%)	12	44
11	K	117/129 (91%)	102 (87%)	14 (12%)	1 (1%)	14	46
12	L	122/135 (90%)	109 (89%)	12 (10%)	1 (1%)	16	49
13	M	116/126 (92%)	105 (90%)	11 (10%)	0	100	100
14	N	58/61 (95%)	54 (93%)	4 (7%)	0	100	100
15	O	86/89 (97%)	80 (93%)	6 (7%)	0	100	100
16	P	82/88 (93%)	78 (95%)	4 (5%)	0	100	100
17	Q	98/105 (93%)	93 (95%)	5 (5%)	0	100	100
18	R	71/88 (81%)	68 (96%)	3 (4%)	0	100	100
19	S	79/93 (85%)	69 (87%)	8 (10%)	2 (2%)	4	28
20	T	97/106 (92%)	84 (87%)	13 (13%)	0	100	100
21	U	23/27 (85%)	22 (96%)	1 (4%)	0	100	100
All	All	2353/2541 (93%)	2152 (92%)	194 (8%)	7 (0%)	36	67

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	L	28	LYS
19	S	31	ILE
19	S	6	LYS
11	K	117	ASN
9	I	119	ALA
2	B	229	VAL
10	J	34	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	201/220 (91%)	183 (91%)	18 (9%)	9	33
3	C	160/188 (85%)	135 (84%)	25 (16%)	2	15
4	D	180/181 (99%)	161 (89%)	19 (11%)	6	27
5	E	115/123 (94%)	96 (84%)	19 (16%)	2	14
6	F	90/90 (100%)	77 (86%)	13 (14%)	3	18
7	G	126/127 (99%)	115 (91%)	11 (9%)	9	34
8	H	119/119 (100%)	103 (87%)	16 (13%)	4	20
9	I	98/99 (99%)	80 (82%)	18 (18%)	1	9
10	J	87/92 (95%)	74 (85%)	13 (15%)	3	17
11	K	90/99 (91%)	78 (87%)	12 (13%)	4	21
12	L	103/110 (94%)	88 (85%)	15 (15%)	3	17
13	M	94/101 (93%)	85 (90%)	9 (10%)	8	31
14	N	49/50 (98%)	44 (90%)	5 (10%)	7	28
15	O	79/80 (99%)	71 (90%)	8 (10%)	7	29
16	P	72/74 (97%)	67 (93%)	5 (7%)	14	41
17	Q	95/97 (98%)	83 (87%)	12 (13%)	4	22
18	R	64/77 (83%)	59 (92%)	5 (8%)	11	37
19	S	71/80 (89%)	61 (86%)	10 (14%)	3	19
20	T	76/82 (93%)	63 (83%)	13 (17%)	2	12
21	U	19/22 (86%)	17 (90%)	2 (10%)	6	28
All	All	1988/2111 (94%)	1740 (88%)	248 (12%)	4	22

All (248) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	42	ILE
2	B	46	LYS
2	B	53	ARG
2	B	64	ARG
2	B	82	ARG
2	B	102	LEU
2	B	114	ARG

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Mol	Chain	Res	Type
2	B	127	ILE
2	B	132	LYS
2	B	139	LYS
2	B	144	ARG
2	B	178	ARG
2	B	187	LEU
2	B	197	VAL
2	B	208	ILE
2	B	221	LEU
2	B	223	ILE
2	B	240	GLN
3	C	3	ASN
3	C	17	ASP
3	C	27	LYS
3	C	34	LEU
3	C	37	GLN
3	C	52	LEU
3	C	72	LYS
3	C	91	LEU
3	C	95	THR
3	C	99	VAL
3	C	107	GLN
3	C	111	LEU
3	C	126	ARG
3	C	127	ARG
3	C	134	ILE
3	C	138	VAL
3	C	144	SER
3	C	167	TRP
3	C	172	ARG
3	C	175	LEU
3	C	178	LEU
3	C	188	LEU
3	C	195	VAL
3	C	196	LEU
3	C	204	LEU
4	D	3	ARG
4	D	8	VAL
4	D	10	ARG
4	D	15	GLU
4	D	19	LEU
4	D	26	CYS

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Mol	Chain	Res	Type
4	D	35	ARG
4	D	70	ILE
4	D	78	LEU
4	D	97	LEU
4	D	122	ARG
4	D	127	THR
4	D	150	GLU
4	D	162	LEU
4	D	170	VAL
4	D	178	VAL
4	D	192	GLU
4	D	201	GLN
4	D	202	LEU
5	E	6	PHE
5	E	8	GLU
5	E	10	MET
5	E	12	LEU
5	E	15	ARG
5	E	31	LEU
5	E	34	VAL
5	E	41	VAL
5	E	43	LEU
5	E	50	GLU
5	E	53	LEU
5	E	55	VAL
5	E	64	ARG
5	E	79	GLU
5	E	80	ILE
5	E	82	VAL
5	E	120	THR
5	E	125	SER
5	E	137	GLU
6	F	3	ARG
6	F	10	LEU
6	F	15	ASP
6	F	25	ILE
6	F	43	LEU
6	F	54	LYS
6	F	55	ASP
6	F	69	GLU
6	F	72	VAL
6	F	73	ASN

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Mol	Chain	Res	Type
6	F	74	ASP
6	F	77	ARG
6	F	82	ARG
7	G	8	GLU
7	G	11	GLN
7	G	12	LEU
7	G	38	LEU
7	G	48	LYS
7	G	54	THR
7	G	63	LYS
7	G	113	GLU
7	G	114	ARG
7	G	124	LEU
7	G	137	LYS
8	H	11	THR
8	H	25	ASP
8	H	26	VAL
8	H	39	LEU
8	H	63	LEU
8	H	85	ARG
8	H	91	ARG
8	H	92	ARG
8	H	93	VAL
8	H	97	VAL
8	H	102	ARG
8	H	114	THR
8	H	120	THR
8	H	127	LEU
8	H	129	VAL
8	H	133	LEU
9	I	14	VAL
9	I	27	THR
9	I	41	VAL
9	I	44	VAL
9	I	66	ARG
9	I	79	LEU
9	I	86	VAL
9	I	87	GLN
9	I	96	LEU
9	I	102	LEU
9	I	109	VAL
9	I	111	ARG

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Mol	Chain	Res	Type
9	I	113	LYS
9	I	118	LYS
9	I	121	ARG
9	I	124	GLN
9	I	125	TYR
9	I	127	LYS
10	J	6	ILE
10	J	16	LEU
10	J	22	LYS
10	J	60	ARG
10	J	62	HIS
10	J	63	PHE
10	J	65	LEU
10	J	66	ARG
10	J	67	THR
10	J	71	LEU
10	J	78	ASN
10	J	83	GLU
10	J	88	LEU
11	K	11	LYS
11	K	13	GLN
11	K	16	SER
11	K	18	ARG
11	K	29	ILE
11	K	47	VAL
11	K	48	ILE
11	K	91	ARG
11	K	96	ARG
11	K	98	LEU
11	K	103	LEU
11	K	122	LYS
12	L	10	LEU
12	L	11	VAL
12	L	13	LYS
12	L	18	VAL
12	L	19	ARG
12	L	20	LYS
12	L	39	VAL
12	L	44	THR
12	L	46	LYS
12	L	60	LEU
12	L	67	THR

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Mol	Chain	Res	Type
12	L	82	VAL
12	L	83	VAL
12	L	96	VAL
12	L	111	LYS
13	M	44	ARG
13	M	49	THR
13	M	56	LEU
13	M	58	GLU
13	M	62	ASN
13	M	63	THR
13	M	66	LEU
13	M	99	ARG
13	M	109	THR
14	N	7	ILE
14	N	8	GLU
14	N	12	ARG
14	N	22	THR
14	N	44	LEU
15	O	6	GLU
15	O	11	VAL
15	O	17	ARG
15	O	34	LEU
15	O	39	LEU
15	O	45	VAL
15	O	70	LEU
15	O	83	GLU
16	P	1	MET
16	P	53	VAL
16	P	54	GLU
16	P	62	VAL
16	P	82	GLN
17	Q	9	VAL
17	Q	19	VAL
17	Q	22	LEU
17	Q	29	HIS
17	Q	34	LYS
17	Q	36	ILE
17	Q	38	ARG
17	Q	59	ILE
17	Q	60	ILE
17	Q	68	ARG
17	Q	84	LEU

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Mol	Chain	Res	Type
17	Q	98	LEU
18	R	38	GLU
18	R	46	GLU
18	R	82	THR
18	R	86	VAL
18	R	88	LYS
19	S	6	LYS
19	S	7	LYS
19	S	13	ASP
19	S	14	HIS
19	S	15	LEU
19	S	30	LEU
19	S	31	ILE
19	S	43	GLU
19	S	70	LYS
19	S	81	ARG
20	T	8	ARG
20	T	9	ASN
20	T	10	LEU
20	T	17	ARG
20	T	19	SER
20	T	35	THR
20	T	54	LYS
20	T	57	ARG
20	T	62	LEU
20	T	72	LEU
20	T	74	LYS
20	T	75	ASN
20	T	87	LYS
21	U	10	ARG
21	U	15	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	76	GLN
2	B	113	HIS
2	B	135	GLN
2	B	240	GLN
3	C	108	ASN
3	C	139	GLN
3	C	170	GLN

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Mol	Chain	Res	Type
7	G	56	GLN
9	I	23	ASN
9	I	73	GLN
15	O	9	GLN
20	T	18	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1504/1522 (98%)	251 (16%)	43 (2%)
22	V	2/3 (66%)	0	0
23	W	14/15 (93%)	3 (21%)	0
All	All	1520/1540 (98%)	254 (16%)	43 (2%)

All (254) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	7	G
1	A	9	G
1	A	32	A
1	A	39	G
1	A	44	G
1	A	47	C
1	A	48	C
1	A	51	A
1	A	60	A
1	A	61	G
1	A	80	G
1	A	81	U
1	A	101	A
1	A	115	G
1	A	116	A
1	A	117	G
1	A	121	C
1	A	129(A)	G
1	A	130	A
1	A	131	C
1	A	145	G
1	A	163	C
1	A	182	U
1	A	195	A

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Mol	Chain	Res	Type
1	A	197	A
1	A	202	U
1	A	204	U
1	A	216	G
1	A	217	C
1	A	226	G
1	A	231	G
1	A	247	G
1	A	251	G
1	A	266	G
1	A	267	C
1	A	282	A
1	A	289	G
1	A	319	G
1	A	321	A
1	A	328	C
1	A	329	A
1	A	332	G
1	A	344	A
1	A	345	C
1	A	351	G
1	A	352	C
1	A	353	A
1	A	354	G
1	A	367	U
1	A	372	C
1	A	373	A
1	A	374	A
1	A	384	G
1	A	397	A
1	A	398	C
1	A	406	G
1	A	411	A
1	A	412	A
1	A	413	G
1	A	419	C
1	A	421	U
1	A	423	G
1	A	428	G
1	A	429	U
1	A	430	A
1	A	433	C

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Mol	Chain	Res	Type
1	A	439	A
1	A	442	C
1	A	444	C
1	A	452	A
1	A	461	C
1	A	485	G
1	A	495	U
1	A	497	A
1	A	498	U
1	A	509	A
1	A	510	A
1	A	511	C
1	A	518	C
1	A	521	G
1	A	527	7MG
1	A	531	U
1	A	532	A
1	A	533	A
1	A	547	A
1	A	559	A
1	A	560	U
1	A	562	C
1	A	563	A
1	A	564	C
1	A	572	A
1	A	573	A
1	A	576	G
1	A	577	G
1	A	579	G
1	A	588	G
1	A	607	A
1	A	631	G
1	A	632	A
1	A	653	A
1	A	665	A
1	A	671	G
1	A	687	A
1	A	688	G
1	A	701	C
1	A	702	A
1	A	723	U
1	A	724	G

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Mol	Chain	Res	Type
1	A	731	G
1	A	755	G
1	A	766	A
1	A	774	G
1	A	777	A
1	A	792	A
1	A	793	U
1	A	794	A
1	A	813	U
1	A	815	A
1	A	816	A
1	A	817	C
1	A	828	A
1	A	839	U
1	A	840	C
1	A	841	U
1	A	848	C
1	A	859	A
1	A	873	A
1	A	874	G
1	A	876	G
1	A	887	G
1	A	902	G
1	A	914	A
1	A	922	G
1	A	926	G
1	A	927	G
1	A	934	C
1	A	935	A
1	A	960	U
1	A	964	A
1	A	966	M2G
1	A	968	A
1	A	969	A
1	A	971	G
1	A	972	C
1	A	974	A
1	A	975	A
1	A	976	G
1	A	977	A
1	A	983	A
1	A	991	U

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Mol	Chain	Res	Type
1	A	992	U
1	A	993	G
1	A	1004	A
1	A	1005	A
1	A	1023	G
1	A	1025	U
1	A	1026	G
1	A	1027	C
1	A	1031	G
1	A	1050	G
1	A	1053	G
1	A	1054	C
1	A	1055	A
1	A	1065	U
1	A	1066	C
1	A	1068	G
1	A	1094	G
1	A	1095	U
1	A	1101	A
1	A	1125	U
1	A	1126	U
1	A	1127	G
1	A	1129	C
1	A	1130	A
1	A	1131	G
1	A	1136	U
1	A	1137	C
1	A	1138	G
1	A	1139	G
1	A	1140	C
1	A	1159	U
1	A	1160	G
1	A	1171	G
1	A	1180	A
1	A	1181	G
1	A	1183	A
1	A	1184	G
1	A	1191	A
1	A	1196	U
1	A	1197	G
1	A	1200	C
1	A	1201	A

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Mol	Chain	Res	Type
1	A	1202	G
1	A	1211	U
1	A	1212	U
1	A	1213	A
1	A	1215	G
1	A	1225	A
1	A	1238	A
1	A	1250	A
1	A	1251	A
1	A	1256	A
1	A	1257	U
1	A	1258	G
1	A	1270	C
1	A	1280	A
1	A	1281	U
1	A	1282	C
1	A	1287	A
1	A	1288	A
1	A	1289	A
1	A	1300	G
1	A	1301	U
1	A	1302	U
1	A	1303	C
1	A	1319	A
1	A	1320	C
1	A	1322	C
1	A	1332	A
1	A	1338	G
1	A	1348	U
1	A	1353	G
1	A	1362	C
1	A	1363	A
1	A	1364	U
1	A	1370	G
1	A	1379	G
1	A	1381	U
1	A	1397	C
1	A	1398	A
1	A	1400	5MC
1	A	1401	G
1	A	1402	4OC
1	A	1442	G

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Mol	Chain	Res	Type
1	A	1443	G
1	A	1446	A
1	A	1469	G
1	A	1487	G
1	A	1492	A
1	A	1494	G
1	A	1498	UR3
1	A	1499	A
1	A	1502	A
1	A	1504	G
1	A	1505	G
1	A	1506	U
1	A	1507	A
1	A	1528	U
1	A	1529	G
1	A	1530	G
1	A	1531	A
23	W	30	G
23	W	33	U
23	W	34	G

All (43) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	60	A
1	A	115	G
1	A	129(A)	G
1	A	181	G
1	A	216	G
1	A	250	A
1	A	266	G
1	A	281	G
1	A	328	C
1	A	372	C
1	A	428	G
1	A	429	U
1	A	432	A
1	A	484	G
1	A	496	A
1	A	509	A
1	A	559	A
1	A	575	G

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Mol	Chain	Res	Type
1	A	687	A
1	A	701	C
1	A	812	C
1	A	913	A
1	A	991	U
1	A	1004	A
1	A	1026	G
1	A	1049	U
1	A	1065	U
1	A	1067	A
1	A	1129	C
1	A	1179	A
1	A	1182	G
1	A	1190	G
1	A	1201	A
1	A	1211	U
1	A	1212	U
1	A	1281	U
1	A	1300	G
1	A	1331	G
1	A	1347	G
1	A	1397	C
1	A	1443	G
1	A	1505	G
1	A	1528	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	A	1541	1	18,21,22	1.16	1 (5%)	21,30,33	1.78	2 (9%)
1	5MC	A	967	1	19,22,23	1.01	0	26,32,35	1.00	3 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	5MC	A	1400	1	19,22,23	1.16	3 (15%)	26,32,35	0.92	1 (3%)
1	7MG	A	527	1	23,26,27	4.17	4 (17%)	27,39,42	2.29	9 (33%)
1	4OC	A	1402	1	20,23,24	0.92	1 (5%)	25,32,35	0.73	0
1	5MC	A	1407	1	19,22,23	1.23	3 (15%)	26,32,35	1.09	3 (11%)
1	MA6	A	1518[A]	1	23,26,27	1.26	3 (13%)	33,38,41	0.80	1 (3%)
1	5MC	A	1404	1	19,22,23	1.66	3 (15%)	26,32,35	1.32	4 (15%)
1	MA6	A	1518[B]	1	23,26,27	1.32	4 (17%)	33,38,41	0.90	0
1	UR3	A	1498	1	19,22,23	1.13	1 (5%)	26,32,35	1.00	1 (3%)
1	MA6	A	1519[A]	1	23,26,27	1.00	2 (8%)	33,38,41	0.90	1 (3%)
1	M2G	A	966	1	24,27,28	1.00	2 (8%)	33,40,43	1.00	2 (6%)
1	PSU	A	516	24,1	18,21,22	1.09	1 (5%)	21,30,33	1.72	5 (23%)
1	MA6	A	1519[B]	1	23,26,27	1.31	3 (13%)	33,38,41	0.90	1 (3%)
1	2MG	A	1207	1	23,26,27	1.30	3 (13%)	33,38,41	1.15	4 (12%)
1	PSU	A	1540	1	18,21,22	1.36	1 (5%)	21,30,33	1.92	5 (23%)
12	0TD	L	92	12	8,9,10	1.15	0	6,11,13	2.34	1 (16%)

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
1	PSU	A	1541	1	-	1/7/25/26	0/2/2/2
1	5MC	A	967	1	-	0/7/25/26	0/2/2/2
1	5MC	A	1400	1	-	2/7/25/26	0/2/2/2
1	7MG	A	527	1	-	2/7/37/38	0/3/3/3
1	4OC	A	1402	1	-	4/9/29/30	0/2/2/2
1	5MC	A	1407	1	-	0/7/25/26	0/2/2/2
1	MA6	A	1518[A]	1	-	0/11/29/30	0/3/3/3
1	5MC	A	1404	1	-	2/7/25/26	0/2/2/2
1	MA6	A	1518[B]	1	-	0/11/29/30	0/3/3/3
1	UR3	A	1498	1	-	2/7/25/26	0/2/2/2
1	MA6	A	1519[A]	1	-	3/11/29/30	0/3/3/3
1	M2G	A	966	1	-	1/11/29/30	0/3/3/3
1	PSU	A	516	24,1	-	0/7/25/26	0/2/2/2
1	MA6	A	1519[B]	1	-	5/11/29/30	0/3/3/3
1	2MG	A	1207	1	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	A	1540	1	-	1/7/25/26	0/2/2/2
12	0TD	L	92	12	-	2/7/12/14	-

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	527	7MG	C8-N9	-18.69	1.33	1.45
1	A	1404	5MC	C5-C4	5.57	1.48	1.44
1	A	1540	PSU	C6-C5	4.86	1.40	1.35
1	A	527	7MG	C2-N2	4.29	1.44	1.34
1	A	1541	PSU	C6-C5	4.21	1.39	1.35
1	A	527	7MG	C5-N7	3.97	1.40	1.35
1	A	516	PSU	C6-C5	3.67	1.39	1.35
1	A	1498	UR3	C2-N1	3.34	1.43	1.38
1	A	1207	2MG	C2-N2	3.17	1.40	1.33
1	A	1407	5MC	C5-C4	3.09	1.46	1.44
1	A	1519[B]	MA6	C5-C4	3.08	1.44	1.39
1	A	1518[A]	MA6	C5-C4	3.06	1.44	1.39
1	A	1518[B]	MA6	C5-C4	2.95	1.44	1.39
1	A	1518[A]	MA6	C8-N9	2.79	1.42	1.37
1	A	1404	5MC	C2-N3	2.78	1.41	1.36
1	A	1519[B]	MA6	C2-N1	2.72	1.38	1.33
1	A	1400	5MC	C2-N1	2.68	1.45	1.40
1	A	1518[B]	MA6	C8-N9	2.66	1.42	1.37
1	A	1402	4OC	C2-N3	2.57	1.41	1.36
1	A	1207	2MG	C4-N3	2.54	1.40	1.34
1	A	1207	2MG	C2-N1	2.47	1.40	1.36
1	A	1400	5MC	C2-N3	2.46	1.41	1.36
1	A	1518[B]	MA6	C2-N1	2.46	1.38	1.33
1	A	1407	5MC	C2-N1	2.45	1.45	1.40
1	A	1404	5MC	C2-N1	2.43	1.45	1.40
1	A	1519[A]	MA6	C8-N9	2.41	1.41	1.37
1	A	1519[A]	MA6	C5-C4	2.40	1.43	1.39
1	A	966	M2G	C4-N3	2.39	1.39	1.34
1	A	1518[A]	MA6	C2-N1	2.38	1.38	1.33
1	A	527	7MG	C4-N3	2.36	1.39	1.34
1	A	1519[B]	MA6	C8-N9	2.35	1.41	1.37
1	A	1407	5MC	C2-N3	2.27	1.40	1.36
1	A	966	M2G	C2-N2	2.03	1.38	1.35
1	A	1518[B]	MA6	C8-N7	2.03	1.35	1.31
1	A	1400	5MC	C6-C5	2.01	1.37	1.34

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	527	7MG	C5-C6-N1	5.10	119.92	110.94
1	A	527	7MG	C2-N3-C4	4.86	120.68	112.30
1	A	1541	PSU	C4-N3-C2	-4.75	119.83	126.37
12	L	92	0TD	CSB-SB-CB	-4.74	93.84	102.36
1	A	527	7MG	N9-C4-N3	4.63	132.24	125.46
1	A	1541	PSU	N1-C2-N3	4.41	119.82	115.17
1	A	516	PSU	C4-N3-C2	-4.37	120.35	126.37
1	A	516	PSU	N1-C2-N3	4.25	119.65	115.17
1	A	527	7MG	C5-C4-N3	-4.19	120.26	128.13
1	A	1540	PSU	N1-C2-N3	4.06	119.45	115.17
1	A	1540	PSU	C6-N1-C2	-3.79	119.18	122.69
1	A	1540	PSU	C4-N3-C2	-3.77	121.18	126.37
1	A	1540	PSU	O2-C2-N1	-3.67	119.01	122.79
1	A	527	7MG	N9-C8-N7	3.54	108.38	103.37
1	A	1404	5MC	N4-C4-N3	-3.20	112.71	118.51
1	A	527	7MG	C2-N1-C6	-2.95	119.77	125.11
1	A	1407	5MC	N4-C4-N3	-2.88	113.29	118.51
1	A	1498	UR3	C6-N1-C2	-2.88	119.44	121.80
1	A	527	7MG	C6-C5-C4	-2.82	117.44	122.40
1	A	966	M2G	C5-C4-N3	-2.80	123.93	128.39
1	A	1404	5MC	C1'-N1-C6	-2.80	116.55	121.15
1	A	527	7MG	O6-C6-C5	-2.72	120.93	127.62
1	A	527	7MG	C6-C5-N7	2.71	136.13	131.93
1	A	1207	2MG	C5-C4-N3	-2.70	124.10	128.39
1	A	1207	2MG	N9-C4-N3	2.61	131.16	125.95
1	A	967	5MC	N4-C4-N3	-2.58	113.83	118.51
1	A	1207	2MG	O6-C6-N1	-2.52	115.38	120.11
1	A	1404	5MC	C5-C4-N3	2.37	124.19	121.75
1	A	1404	5MC	C4-N3-C2	-2.37	117.52	120.81
1	A	1519[B]	MA6	C4-C5-C6	2.29	118.28	115.91
1	A	516	PSU	O2-C2-N1	-2.27	120.44	122.79
1	A	1407	5MC	C5-C4-N3	2.25	124.06	121.75
1	A	967	5MC	C4-N3-C2	-2.24	117.70	120.81
1	A	1400	5MC	N4-C4-N3	-2.23	114.48	118.51
1	A	1518[A]	MA6	C2-N1-C6	2.21	117.22	111.83
1	A	516	PSU	C6-N1-C2	-2.20	120.65	122.69
1	A	1407	5MC	C4-N3-C2	-2.19	117.77	120.81
1	A	516	PSU	O4'-C1'-C2'	2.14	108.11	105.15
1	A	1519[A]	MA6	C2-N1-C6	2.10	116.96	111.83
1	A	966	M2G	O6-C6-N1	-2.08	116.21	120.11
1	A	967	5MC	C5-C4-N3	2.05	123.86	121.75
1	A	1540	PSU	C3'-C2'-C1'	-2.05	99.27	101.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1207	2MG	C2-N1-C6	-2.03	122.09	124.55

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	527	7MG	O4'-C4'-C5'-O5'
1	A	1400	5MC	O4'-C4'-C5'-O5'
1	A	1402	4OC	O4'-C4'-C5'-O5'
1	A	1519[B]	MA6	C5-C6-N6-C9
1	A	1541	PSU	C2'-C1'-C5-C4
12	L	92	0TD	SB-CB-CG-OD2
1	A	527	7MG	C3'-C4'-C5'-O5'
1	A	1519[A]	MA6	O4'-C4'-C5'-O5'
1	A	1402	4OC	C3'-C4'-C5'-O5'
1	A	1498	UR3	O4'-C4'-C5'-O5'
1	A	1498	UR3	C3'-C4'-C5'-O5'
1	A	1519[B]	MA6	N1-C6-N6-C9
1	A	1400	5MC	C3'-C4'-C5'-O5'
1	A	1404	5MC	O4'-C4'-C5'-O5'
1	A	1519[A]	MA6	C3'-C4'-C5'-O5'
1	A	1404	5MC	C3'-C4'-C5'-O5'
1	A	1519[B]	MA6	C3'-C4'-C5'-O5'
1	A	1519[A]	MA6	C5-C6-N6-C9
12	L	92	0TD	CG-CB-SB-CSB
1	A	966	M2G	C4'-C5'-O5'-P
1	A	1519[B]	MA6	C5-C6-N6-C10
1	A	1402	4OC	C3'-C2'-O2'-CM2
1	A	1519[B]	MA6	O4'-C4'-C5'-O5'
1	A	1402	4OC	C1'-C2'-O2'-CM2
1	A	1540	PSU	O4'-C1'-C5-C6

There are no ring outliers.

15 monomers are involved in 51 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1541	PSU	3	0
1	A	967	5MC	3	0
1	A	1400	5MC	3	0
1	A	527	7MG	2	0
1	A	1402	4OC	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1407	5MC	1	0
1	A	1518[A]	MA6	3	0
1	A	1518[B]	MA6	9	0
1	A	1498	UR3	9	0
1	A	1519[A]	MA6	3	0
1	A	966	M2G	3	0
1	A	1519[B]	MA6	7	0
1	A	1207	2MG	3	0
1	A	1540	PSU	6	0
12	L	92	0TD	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 275 ligands modelled in this entry, 274 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
25	SRY	A	1860	-	40,42,42	2.41	10 (25%)	49,63,63	2.03	10 (20%)

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
25	SRY	A	1860	-	-	3/20/87/87	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	1860	SRV	CD1-N31	9.19	1.49	1.33
25	A	1860	SRV	CA1-N11	7.21	1.45	1.33
25	A	1860	SRV	O53-C53	-3.47	1.35	1.44
25	A	1860	SRV	C23-N23	-2.99	1.42	1.47
25	A	1860	SRV	CA1-NB1	2.99	1.45	1.34
25	A	1860	SRV	C32-CG2	-2.87	1.47	1.52
25	A	1860	SRV	O32-C32	-2.73	1.40	1.44
25	A	1860	SRV	CD1-NE1	2.69	1.44	1.34
25	A	1860	SRV	C21-C11	-2.46	1.48	1.53
25	A	1860	SRV	O51-C51	-2.36	1.37	1.43

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	1860	SRV	C13-O13-C22	-7.67	103.22	116.26
25	A	1860	SRV	CI3-N23-C23	-5.27	107.43	114.23
25	A	1860	SRV	C12-O42-C42	-4.62	101.02	108.48
25	A	1860	SRV	C61-C11-N11	-4.08	103.10	110.62
25	A	1860	SRV	O13-C13-C23	3.66	114.01	108.07
25	A	1860	SRV	C43-C33-C23	-3.56	105.21	110.40
25	A	1860	SRV	O41-C41-C51	2.71	114.11	107.23
25	A	1860	SRV	O53-C53-C43	2.65	114.47	109.70
25	A	1860	SRV	OG2-CG2-C32	-2.63	118.12	124.17
25	A	1860	SRV	C63-C53-C43	-2.40	107.12	113.02

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	A	1860	SRV	C13-C23-N23-CI3
25	A	1860	SRV	C43-C53-C63-O63
25	A	1860	SRV	O42-C12-O41-C41

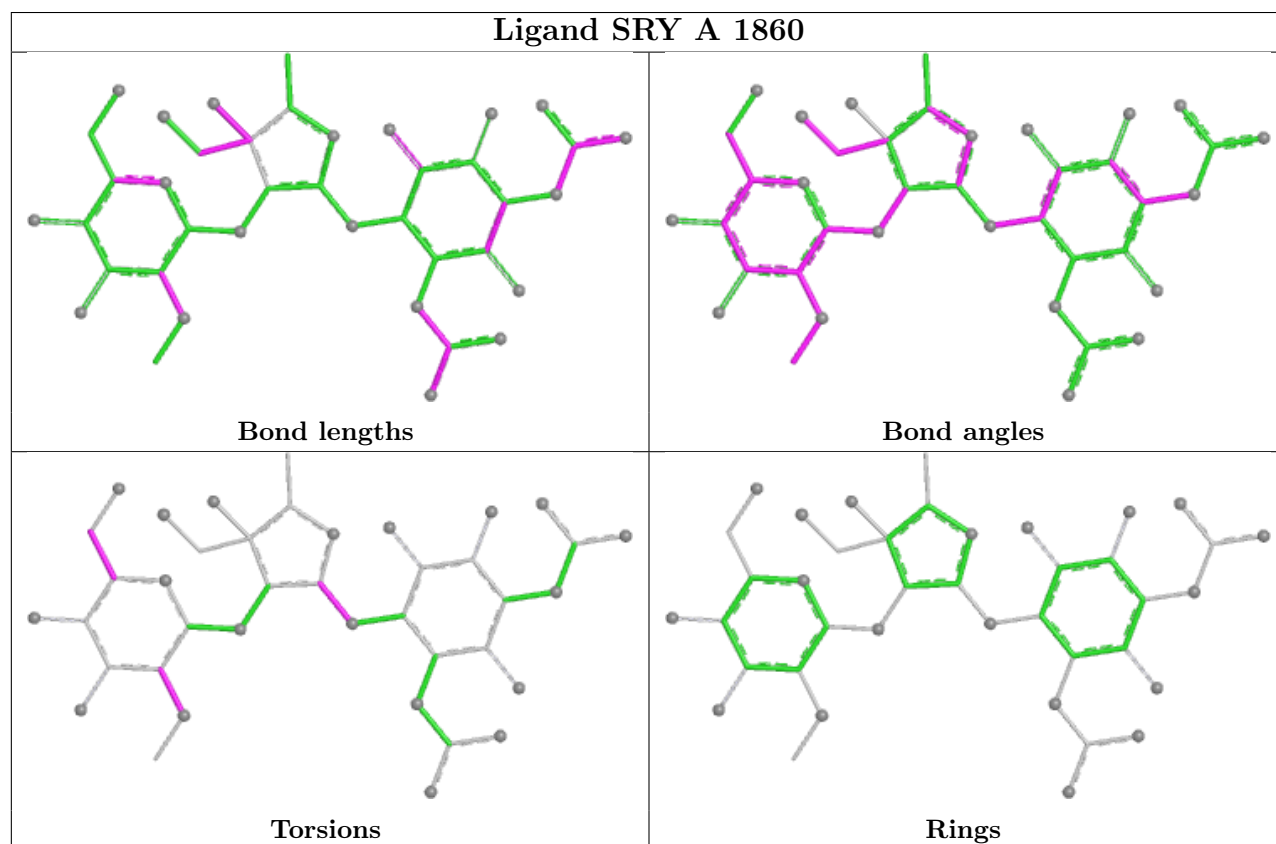
There are no ring outliers.

1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	A	1860	SRV	9	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1498/1522 (98%)	-0.82	3 (0%) 91 83	41, 101, 189, 333	4 (0%)
2	B	236/256 (92%)	-0.50	0 100 100	93, 136, 194, 231	0
3	C	207/239 (86%)	-0.42	1 (0%) 87 70	106, 142, 183, 216	0
4	D	208/209 (99%)	-0.39	9 (4%) 40 23	77, 113, 175, 202	0
5	E	151/162 (93%)	-0.63	0 100 100	68, 95, 131, 177	0
6	F	101/101 (100%)	-0.57	0 100 100	93, 133, 164, 185	0
7	G	155/156 (99%)	-0.50	0 100 100	90, 120, 183, 219	0
8	H	138/138 (100%)	-0.77	0 100 100	62, 85, 115, 146	0
9	I	127/128 (99%)	-0.24	2 (1%) 70 46	95, 144, 180, 216	0
10	J	99/105 (94%)	-0.01	1 (1%) 79 56	105, 165, 237, 271	0
11	K	119/129 (92%)	-0.46	2 (1%) 69 44	72, 101, 148, 212	0
12	L	124/135 (91%)	-0.41	0 100 100	64, 110, 146, 220	0
13	M	118/126 (93%)	-0.44	2 (1%) 69 44	92, 124, 162, 204	0
14	N	60/61 (98%)	-0.18	1 (1%) 69 44	107, 133, 172, 248	0
15	O	88/89 (98%)	-0.63	0 100 100	68, 102, 144, 210	0
16	P	84/88 (95%)	-0.57	0 100 100	75, 96, 122, 171	0
17	Q	100/105 (95%)	-0.54	0 100 100	63, 89, 126, 182	0
18	R	73/88 (82%)	-0.42	0 100 100	86, 109, 197, 245	0
19	S	81/93 (87%)	0.05	3 (3%) 45 27	120, 154, 199, 254	0
20	T	99/106 (93%)	-0.56	1 (1%) 79 56	73, 96, 140, 176	0
21	U	25/27 (92%)	-0.42	0 100 100	101, 121, 153, 171	0
22	V	3/3 (100%)	0.48	0 100 100	166, 166, 170, 185	3 (100%)
23	W	15/15 (100%)	-0.05	0 100 100	163, 202, 273, 301	8 (53%)
All	All	3909/4081 (95%)	-0.59	25 (0%) 85 66	41, 112, 187, 333	15 (0%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1129	C	8.2
19	S	3	ARG	7.7
4	D	2	GLY	7.0
19	S	2	PRO	5.4
11	K	129	SER	3.8
4	D	31	CYS	3.8
4	D	9	CYS	3.3
4	D	26	CYS	3.3
9	I	127	LYS	3.0
13	M	7	VAL	3.0
13	M	8	GLU	3.0
20	T	12	ALA	2.8
19	S	5	LEU	2.7
9	I	126	SER	2.7
14	N	2	ALA	2.6
4	D	3	ARG	2.5
4	D	23	GLY	2.5
4	D	22	LYS	2.4
10	J	90	LEU	2.4
1	A	266	G	2.3
4	D	30	LYS	2.2
11	K	128	ALA	2.1
1	A	1539	C	2.1
4	D	21	LEU	2.1
3	C	2	GLY	2.1

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	PSU	A	1540	20/21	0.73	0.23	193,205,213,214	0
1	PSU	A	1541	20/21	0.76	0.23	188,196,202,203	0
1	5MC	A	1407	21/22	0.94	0.11	107,119,130,134	0
1	PSU	A	516	20/21	0.96	0.08	120,125,133,136	0
1	UR3	A	1498	21/22	0.96	0.10	87,96,109,112	0
1	M2G	A	966	25/26	0.96	0.07	88,105,117,123	0
1	5MC	A	1404	21/22	0.96	0.07	84,88,103,117	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
12	0TD	L	92	10/11	0.96	0.10	83,93,97,207	0
1	2MG	A	1207	24/25	0.97	0.06	120,123,131,135	0
1	5MC	A	1400	21/22	0.97	0.07	71,102,119,121	0
1	MA6	A	1518[B]	24/25	0.98	0.09	79,88,110,112	24
1	5MC	A	967	21/22	0.98	0.06	90,98,107,115	0
1	7MG	A	527	24/25	0.98	0.07	66,86,94,104	0
1	MA6	A	1518[A]	24/25	0.98	0.09	81,85,92,101	24
1	4OC	A	1402	22/23	0.99	0.08	89,101,107,111	0
1	MA6	A	1519[A]	24/25	0.99	0.08	77,81,91,95	24
1	MA6	A	1519[B]	24/25	0.99	0.08	76,83,90,91	24

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	MG	G	201	1/1	0.53	0.28	116,116,116,116	0
24	MG	A	1808	1/1	0.63	0.15	377,377,377,377	0
24	MG	A	1732	1/1	0.64	0.55	97,97,97,97	0
24	MG	A	1710	1/1	0.70	0.34	177,177,177,177	0
24	MG	A	1746	1/1	0.71	0.48	99,99,99,99	0
24	MG	A	1680	1/1	0.72	0.22	250,250,250,250	0
24	MG	A	1717	1/1	0.74	0.50	125,125,125,125	0
24	MG	A	1615	1/1	0.75	0.19	72,72,72,72	0
24	MG	A	1812	1/1	0.76	0.10	290,290,290,290	0
24	MG	A	1766	1/1	0.77	0.59	95,95,95,95	0
24	MG	A	1825	1/1	0.77	0.11	401,401,401,401	0
24	MG	A	1833	1/1	0.77	0.16	335,335,335,335	0
24	MG	A	1729	1/1	0.77	0.46	111,111,111,111	0
24	MG	A	1728	1/1	0.78	0.08	95,95,95,95	0
24	MG	A	1674	1/1	0.78	0.27	125,125,125,125	0
24	MG	A	1679	1/1	0.79	0.15	168,168,168,168	0
24	MG	A	1851	1/1	0.79	0.66	92,92,92,92	0
24	MG	A	1666	1/1	0.79	0.26	103,103,103,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	MG	A	1796	1/1	0.80	0.29	98,98,98,98	0
24	MG	A	1771	1/1	0.81	0.57	82,82,82,82	0
24	MG	A	1841	1/1	0.81	0.10	266,266,266,266	0
24	MG	A	1789	1/1	0.81	0.31	92,92,92,92	0
24	MG	A	1859	1/1	0.81	0.32	94,94,94,94	0
24	MG	A	1830	1/1	0.81	0.11	273,273,273,273	0
24	MG	A	1850	1/1	0.82	0.33	117,117,117,117	0
24	MG	A	1764	1/1	0.82	0.26	104,104,104,104	0
24	MG	A	1819	1/1	0.82	0.25	371,371,371,371	0
24	MG	A	1749	1/1	0.82	0.63	98,98,98,98	0
24	MG	A	1656	1/1	0.83	0.15	177,177,177,177	0
24	MG	A	1853	1/1	0.83	0.46	96,96,96,96	0
24	MG	A	1845	1/1	0.83	0.08	293,293,293,293	0
24	MG	A	1681	1/1	0.83	0.12	160,160,160,160	0
24	MG	A	1695	1/1	0.84	0.40	88,88,88,88	0
24	MG	A	1809	1/1	0.84	0.09	355,355,355,355	0
24	MG	A	1770	1/1	0.84	0.31	98,98,98,98	0
24	MG	A	1658	1/1	0.84	0.15	102,102,102,102	0
24	MG	A	1778	1/1	0.84	0.24	78,78,78,78	0
24	MG	A	1753	1/1	0.84	0.70	110,110,110,110	0
24	MG	A	1740	1/1	0.84	0.20	89,89,89,89	0
24	MG	A	1794	1/1	0.85	0.13	120,120,120,120	0
24	MG	A	1667	1/1	0.85	0.58	168,168,168,168	0
24	MG	A	1687	1/1	0.85	0.28	116,116,116,116	0
24	MG	A	1739	1/1	0.85	0.69	103,103,103,103	0
24	MG	A	1785	1/1	0.85	0.21	92,92,92,92	0
24	MG	A	1768	1/1	0.85	0.56	99,99,99,99	0
24	MG	A	1857	1/1	0.85	0.24	89,89,89,89	0
24	MG	A	1790	1/1	0.85	0.25	88,88,88,88	0
24	MG	A	1791	1/1	0.85	0.47	109,109,109,109	0
24	MG	A	1801	1/1	0.86	0.09	248,248,248,248	0
24	MG	A	1826	1/1	0.86	0.32	354,354,354,354	0
24	MG	A	1777	1/1	0.86	0.17	100,100,100,100	0
24	MG	A	1769	1/1	0.86	0.15	92,92,92,92	0
24	MG	A	1724	1/1	0.86	0.26	99,99,99,99	0
24	MG	A	1706	1/1	0.86	0.14	174,174,174,174	0
24	MG	A	1723	1/1	0.87	0.44	117,117,117,117	0
24	MG	A	1803	1/1	0.87	0.19	324,324,324,324	0
24	MG	A	1815	1/1	0.87	0.08	309,309,309,309	0
24	MG	A	1633	1/1	0.87	0.22	85,85,85,85	0
24	MG	A	1683	1/1	0.88	0.27	110,110,110,110	0
24	MG	A	1646	1/1	0.88	0.15	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	MG	A	1714	1/1	0.88	0.30	99,99,99,99	0
24	MG	A	1795	1/1	0.88	0.31	85,85,85,85	0
24	MG	A	1818	1/1	0.88	0.11	249,249,249,249	0
24	MG	A	1688	1/1	0.88	0.15	120,120,120,120	0
24	MG	A	1659	1/1	0.88	0.41	121,121,121,121	0
24	MG	A	1697	1/1	0.88	0.44	102,102,102,102	0
24	MG	A	1805	1/1	0.88	0.23	280,280,280,280	0
24	MG	Q	201	1/1	0.88	0.10	84,84,84,84	0
24	MG	A	1745	1/1	0.89	0.31	82,82,82,82	0
24	MG	A	1719	1/1	0.89	0.17	88,88,88,88	0
24	MG	A	1747	1/1	0.89	0.44	111,111,111,111	0
24	MG	A	1603	1/1	0.89	0.16	97,97,97,97	0
24	MG	A	1606	1/1	0.89	0.23	87,87,87,87	0
24	MG	A	1755	1/1	0.89	0.43	131,131,131,131	0
24	MG	A	1821	1/1	0.89	0.13	178,178,178,178	0
24	MG	A	1761	1/1	0.89	0.25	107,107,107,107	0
24	MG	D	303	1/1	0.89	0.20	97,97,97,97	0
24	MG	A	1663	1/1	0.89	0.16	94,94,94,94	0
24	MG	N	102	1/1	0.89	0.23	99,99,99,99	0
24	MG	A	1788	1/1	0.89	0.19	84,84,84,84	0
24	MG	A	1638	1/1	0.90	0.18	87,87,87,87	0
24	MG	A	1707	1/1	0.90	0.20	163,163,163,163	0
24	MG	A	1844	1/1	0.90	0.17	310,310,310,310	0
24	MG	A	1742	1/1	0.90	0.35	89,89,89,89	0
24	MG	A	1849	1/1	0.90	0.15	74,74,74,74	0
24	MG	A	1669	1/1	0.90	0.19	134,134,134,134	0
24	MG	A	1813	1/1	0.90	0.09	181,181,181,181	0
24	MG	A	1672	1/1	0.90	0.52	92,92,92,92	0
24	MG	A	1793	1/1	0.90	0.17	80,80,80,80	0
24	MG	A	1641	1/1	0.90	0.19	92,92,92,92	0
24	MG	A	1718	1/1	0.90	0.16	220,220,220,220	0
24	MG	A	1750	1/1	0.90	0.62	92,92,92,92	0
24	MG	A	1738	1/1	0.90	0.21	58,58,58,58	0
24	MG	A	1754	1/1	0.90	0.31	105,105,105,105	0
24	MG	A	1684	1/1	0.91	0.16	90,90,90,90	0
24	MG	A	1722	1/1	0.91	0.25	118,118,118,118	0
24	MG	A	1804	1/1	0.91	0.13	304,304,304,304	0
24	MG	A	1757	1/1	0.91	0.33	83,83,83,83	0
24	MG	A	1620	1/1	0.91	0.27	141,141,141,141	0
24	MG	A	1762	1/1	0.91	0.43	83,83,83,83	0
24	MG	A	1848	1/1	0.91	0.60	87,87,87,87	0
24	MG	A	1810	1/1	0.91	0.13	295,295,295,295	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	MG	A	1709	1/1	0.91	0.19	250,250,250,250	0
24	MG	A	1644	1/1	0.91	0.28	95,95,95,95	0
24	MG	A	1792	1/1	0.91	0.14	91,91,91,91	0
24	MG	A	1817	1/1	0.91	0.23	180,180,180,180	0
24	MG	A	1634	1/1	0.91	0.15	243,243,243,243	0
24	MG	A	1731	1/1	0.91	0.33	114,114,114,114	0
24	MG	A	1621	1/1	0.91	0.20	131,131,131,131	0
24	MG	A	1823	1/1	0.91	0.20	281,281,281,281	0
24	MG	A	1699	1/1	0.91	0.22	100,100,100,100	0
24	MG	A	1686	1/1	0.92	0.17	194,194,194,194	0
24	MG	A	1827	1/1	0.92	0.07	244,244,244,244	0
24	MG	A	1612	1/1	0.92	0.12	97,97,97,97	0
24	MG	A	1650	1/1	0.92	0.16	107,107,107,107	0
24	MG	A	1856	1/1	0.92	0.15	104,104,104,104	0
24	MG	A	1836	1/1	0.92	0.09	300,300,300,300	0
24	MG	A	1784	1/1	0.92	0.21	92,92,92,92	0
24	MG	A	1822	1/1	0.92	0.16	209,209,209,209	0
24	MG	A	1700	1/1	0.92	0.15	272,272,272,272	0
24	MG	A	1847	1/1	0.92	0.07	334,334,334,334	0
24	MG	P	102	1/1	0.92	0.19	96,96,96,96	0
24	MG	A	1705	1/1	0.92	0.33	69,69,69,69	0
24	MG	A	1773	1/1	0.93	0.57	88,88,88,88	0
24	MG	A	1614	1/1	0.93	0.12	79,79,79,79	0
24	MG	A	1765	1/1	0.93	0.16	93,93,93,93	0
24	MG	A	1828	1/1	0.93	0.14	284,284,284,284	0
24	MG	A	1855	1/1	0.93	0.09	115,115,115,115	0
24	MG	A	1639	1/1	0.93	0.14	73,73,73,73	0
24	MG	A	1767	1/1	0.93	0.14	64,64,64,64	0
24	MG	A	1800	1/1	0.93	0.16	203,203,203,203	0
24	MG	A	1786	1/1	0.93	0.14	96,96,96,96	0
24	MG	A	1604	1/1	0.93	0.13	153,153,153,153	0
24	MG	A	1758	1/1	0.93	0.16	70,70,70,70	0
24	MG	A	1643	1/1	0.93	0.15	99,99,99,99	0
24	MG	A	1689	1/1	0.93	0.21	132,132,132,132	0
24	MG	A	1691	1/1	0.94	0.10	139,139,139,139	0
24	MG	A	1673	1/1	0.94	0.14	102,102,102,102	0
24	MG	A	1748	1/1	0.94	0.13	77,77,77,77	0
24	MG	A	1653	1/1	0.94	0.30	89,89,89,89	0
24	MG	A	1806	1/1	0.94	0.14	211,211,211,211	0
24	MG	A	1698	1/1	0.94	0.10	218,218,218,218	0
24	MG	A	1783	1/1	0.94	0.12	89,89,89,89	0
24	MG	A	1611	1/1	0.94	0.10	120,120,120,120	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	MG	A	1726	1/1	0.94	0.12	86,86,86,86	0
24	MG	A	1727	1/1	0.94	0.19	79,79,79,79	0
24	MG	A	1609	1/1	0.94	0.08	74,74,74,74	0
24	MG	A	1702	1/1	0.94	0.10	163,163,163,163	0
24	MG	A	1616	1/1	0.94	0.11	93,93,93,93	0
24	MG	A	1618	1/1	0.94	0.17	85,85,85,85	0
24	MG	A	1734	1/1	0.94	0.17	99,99,99,99	0
24	MG	A	1858	1/1	0.94	0.25	98,98,98,98	0
24	MG	A	1645	1/1	0.94	0.14	108,108,108,108	0
24	MG	A	1637	1/1	0.94	0.21	86,86,86,86	0
24	MG	A	1619	1/1	0.94	0.08	72,72,72,72	0
24	MG	L	201	1/1	0.94	0.06	81,81,81,81	0
24	MG	A	1671	1/1	0.94	0.13	99,99,99,99	0
24	MG	A	1798	1/1	0.94	0.11	115,115,115,115	0
24	MG	A	1652	1/1	0.94	0.12	96,96,96,96	0
24	MG	A	1832	1/1	0.95	0.08	112,112,112,112	0
24	MG	A	1677	1/1	0.95	0.10	113,113,113,113	0
24	MG	A	1733	1/1	0.95	0.24	68,68,68,68	0
24	MG	A	1725	1/1	0.95	0.31	109,109,109,109	0
24	MG	A	1842	1/1	0.95	0.17	334,334,334,334	0
24	MG	A	1787	1/1	0.95	0.15	78,78,78,78	0
24	MG	A	1735	1/1	0.95	0.35	96,96,96,96	0
24	MG	A	1846	1/1	0.95	0.10	225,225,225,225	0
24	MG	A	1811	1/1	0.95	0.09	121,121,121,121	0
24	MG	A	1737	1/1	0.95	0.14	81,81,81,81	0
24	MG	A	1685	1/1	0.95	0.23	134,134,134,134	0
24	MG	A	1613	1/1	0.95	0.13	88,88,88,88	0
24	MG	A	1662	1/1	0.95	0.10	145,145,145,145	0
24	MG	A	1756	1/1	0.95	0.23	101,101,101,101	0
24	MG	A	1772	1/1	0.95	0.39	78,78,78,78	0
24	MG	A	1668	1/1	0.95	0.18	138,138,138,138	0
24	MG	A	1774	1/1	0.95	0.15	61,61,61,61	0
24	MG	A	1797	1/1	0.95	0.14	94,94,94,94	0
24	MG	A	1824	1/1	0.95	0.08	202,202,202,202	0
24	MG	D	302	1/1	0.95	0.12	86,86,86,86	0
24	MG	A	1744	1/1	0.95	0.35	109,109,109,109	0
24	MG	F	201	1/1	0.95	0.26	79,79,79,79	0
24	MG	A	1760	1/1	0.95	0.12	101,101,101,101	0
24	MG	H	201	1/1	0.95	0.07	63,63,63,63	0
24	MG	A	1779	1/1	0.95	0.61	94,94,94,94	0
24	MG	A	1782	1/1	0.95	0.09	65,65,65,65	0
24	MG	A	1829	1/1	0.95	0.13	267,267,267,267	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	MG	A	1655	1/1	0.95	0.65	210,210,210,210	0
24	MG	S	101	1/1	0.95	0.25	80,80,80,80	0
24	MG	A	1682	1/1	0.96	0.30	228,228,228,228	0
24	MG	A	1692	1/1	0.96	0.10	119,119,119,119	0
24	MG	A	1780	1/1	0.96	0.41	80,80,80,80	0
24	MG	A	1781	1/1	0.96	0.36	75,75,75,75	0
24	MG	A	1610	1/1	0.96	0.14	71,71,71,71	0
24	MG	A	1711	1/1	0.96	0.15	109,109,109,109	0
24	MG	A	1617	1/1	0.96	0.13	81,81,81,81	0
24	MG	A	1854	1/1	0.96	0.28	89,89,89,89	0
24	MG	A	1675	1/1	0.96	0.08	223,223,223,223	0
24	MG	A	1626	1/1	0.96	0.11	103,103,103,103	0
24	MG	A	1654	1/1	0.96	0.06	97,97,97,97	0
24	MG	A	1752	1/1	0.96	0.09	90,90,90,90	0
24	MG	A	1721	1/1	0.96	0.47	95,95,95,95	0
24	MG	A	1642	1/1	0.96	0.07	112,112,112,112	0
24	MG	A	1834	1/1	0.96	0.16	231,231,231,231	0
24	MG	E	201	1/1	0.96	0.19	87,87,87,87	0
24	MG	A	1704	1/1	0.96	0.14	116,116,116,116	0
24	MG	A	1837	1/1	0.96	0.07	244,244,244,244	0
24	MG	A	1839	1/1	0.96	0.16	205,205,205,205	1
24	MG	A	1840	1/1	0.96	0.14	289,289,289,289	0
24	MG	A	1664	1/1	0.96	0.31	131,131,131,131	0
24	MG	A	1690	1/1	0.96	0.16	193,193,193,193	0
24	MG	P	103	1/1	0.96	0.07	93,93,93,93	0
24	MG	A	1776	1/1	0.96	0.25	96,96,96,96	0
24	MG	A	1741	1/1	0.96	0.19	101,101,101,101	0
26	ZN	D	301	1/1	0.96	0.18	114,114,114,114	0
24	MG	A	1799	1/1	0.97	0.08	277,277,277,277	0
24	MG	A	1608	1/1	0.97	0.23	84,84,84,84	0
24	MG	A	1763	1/1	0.97	0.18	72,72,72,72	0
24	MG	A	1852	1/1	0.97	0.26	84,84,84,84	0
24	MG	A	1802	1/1	0.97	0.10	206,206,206,206	0
24	MG	A	1602	1/1	0.97	0.06	108,108,108,108	0
24	MG	A	1730	1/1	0.97	0.34	90,90,90,90	0
24	MG	A	1713	1/1	0.97	0.06	112,112,112,112	0
24	MG	A	1661	1/1	0.97	0.13	121,121,121,121	0
24	MG	A	1807	1/1	0.97	0.13	397,397,397,397	0
24	MG	A	1678	1/1	0.97	0.08	133,133,133,133	0
24	MG	A	1751	1/1	0.97	0.14	83,83,83,83	0
24	MG	A	1622	1/1	0.97	0.31	75,75,75,75	0
24	MG	A	1701	1/1	0.97	0.14	73,73,73,73	0

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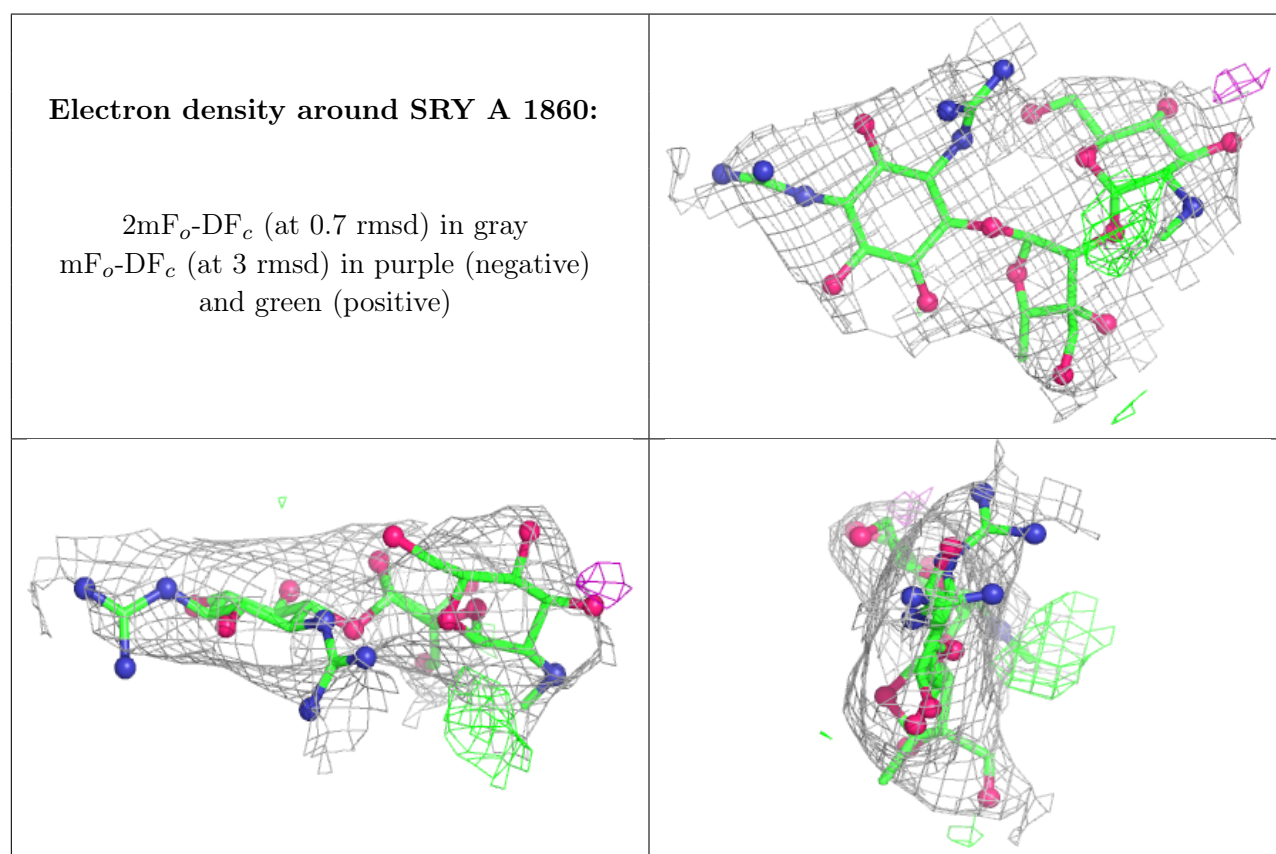
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	MG	A	1838	1/1	0.97	0.13	181,181,181,181	0
24	MG	A	1670	1/1	0.97	0.08	109,109,109,109	0
24	MG	A	1703	1/1	0.97	0.16	106,106,106,106	0
24	MG	A	1648	1/1	0.97	0.05	96,96,96,96	0
24	MG	A	1816	1/1	0.97	0.14	318,318,318,318	0
24	MG	A	1607	1/1	0.97	0.05	102,102,102,102	0
24	MG	A	1665	1/1	0.97	0.06	99,99,99,99	0
24	MG	A	1759	1/1	0.97	0.17	75,75,75,75	0
24	MG	A	1693	1/1	0.97	0.11	192,192,192,192	0
25	SRY	A	1860	40/40	0.97	0.07	60,79,97,101	0
24	MG	A	1694	1/1	0.97	0.11	116,116,116,116	0
24	MG	A	1831	1/1	0.98	0.09	160,160,160,160	0
24	MG	A	1743	1/1	0.98	0.05	76,76,76,76	0
24	MG	A	1636	1/1	0.98	0.04	94,94,94,94	0
24	MG	A	1814	1/1	0.98	0.04	113,113,113,113	0
24	MG	A	1835	1/1	0.98	0.20	299,299,299,299	0
24	MG	A	1647	1/1	0.98	0.18	127,127,127,127	0
24	MG	A	1712	1/1	0.98	0.07	107,107,107,107	0
24	MG	A	1625	1/1	0.98	0.31	194,194,194,194	0
24	MG	A	1601	1/1	0.98	0.15	86,86,86,86	0
24	MG	A	1676	1/1	0.98	0.28	138,138,138,138	0
24	MG	A	1820	1/1	0.98	0.07	152,152,152,152	0
24	MG	A	1627	1/1	0.98	0.07	102,102,102,102	0
24	MG	A	1640	1/1	0.98	0.07	98,98,98,98	0
24	MG	A	1720	1/1	0.98	0.10	64,64,64,64	0
24	MG	A	1736	1/1	0.98	0.06	119,119,119,119	0
24	MG	P	101	1/1	0.98	0.20	67,67,67,67	0
24	MG	A	1628	1/1	0.98	0.12	104,104,104,104	0
24	MG	A	1629	1/1	0.98	0.06	151,151,151,151	0
24	MG	A	1630	1/1	0.98	0.04	82,82,82,82	0
24	MG	A	1623	1/1	0.98	0.06	84,84,84,84	0
24	MG	A	1708	1/1	0.98	0.15	211,211,211,211	0
24	MG	A	1624	1/1	0.98	0.07	97,97,97,97	0
24	MG	A	1631	1/1	0.99	0.03	101,101,101,101	0
24	MG	A	1660	1/1	0.99	0.04	104,104,104,104	0
24	MG	A	1635	1/1	0.99	0.05	75,75,75,75	0
24	MG	A	1632	1/1	0.99	0.10	76,76,76,76	0
24	MG	A	1649	1/1	0.99	0.08	51,51,51,51	0
24	MG	A	1696	1/1	0.99	0.03	99,99,99,99	0
24	MG	A	1715	1/1	0.99	0.05	89,89,89,89	0
24	MG	A	1843	1/1	0.99	0.05	115,115,115,115	0
24	MG	A	1716	1/1	0.99	0.03	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	MG	A	1605	1/1	0.99	0.03	72,72,72,72	0
24	MG	A	1657	1/1	0.99	0.15	189,189,189,189	0
24	MG	A	1651	1/1	0.99	0.12	143,143,143,143	0
24	MG	A	1775	1/1	0.99	0.06	114,114,114,114	0
26	ZN	N	101	1/1	1.00	0.03	129,129,129,129	0

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



6.5 Other polymers [i](#)

There are no such residues in this entry.