



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 06:49 PM UTC

PDB ID : 4LF5 / pdb_00004lf5
Title : Crystal Structure of 30S ribosomal subunit from *Thermus thermophilus*
Authors : Demirci, H.; Belardinelli, R.; Carr, J.; Murphy IV, F.; Jogl, G.; Dahlberg, A.E.; Gregory, S.T.
Deposited on : 2013-06-26
Resolution : 3.75 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 ⓘ](#)) 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

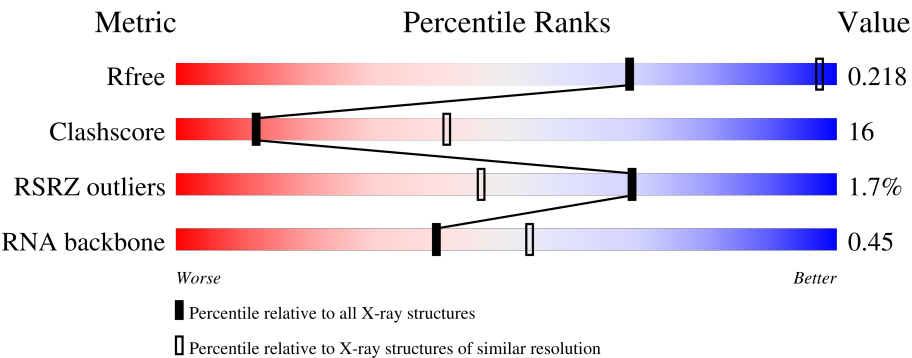
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.75 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	1029 (3.90-3.62)
Clashscore	190562	1061 (3.90-3.62)
RSRZ outliers	180081	1028 (3.90-3.62)
RNA backbone	3983	1001 (4.40-3.10)

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	0.2% 45% 44% 10% ..
2	B	256	0.2% 54% 37% 8% .
3	C	239	2% 45% 41% 13% .
4	D	209	5% 52% 45% .
5	E	162	51% 41% 7% .
6	F	101	62% 36% .

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Mol	Chain	Length	Quality of chain
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	

2 Entry composition

There are 26 unique types of molecules in this entry. The entry contains 51823 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	1513	Total	C	N	O	P	0	0	0
			32522	14483	6016	10511	1512			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1533	C	A	conflict	GB M26923.1
A	1534	A	C	conflict	GB M26923.1

- Molecule 2 is a protein called ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	236	Total	C	N	O	S	0	0	1
			1874	1195	336	338	5			

- Molecule 3 is a protein called 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 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 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 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 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 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 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 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 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 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 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 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 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 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 ribosomal protein S17.

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

- Molecule 18 is a protein called 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 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 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 ribosomal protein THX.

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

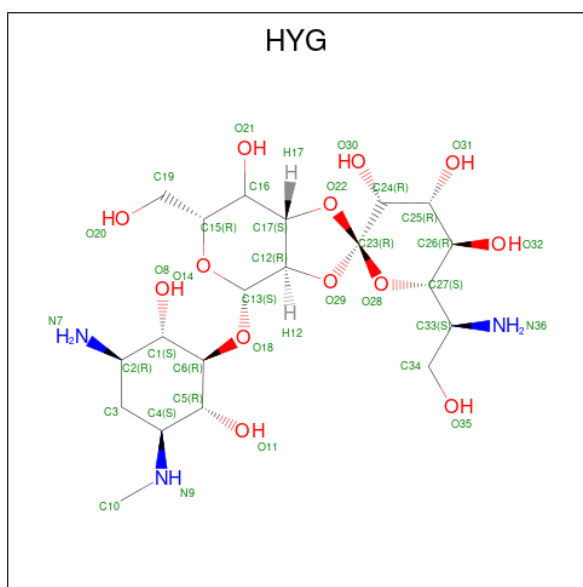
- Molecule 22 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	108	Total	Mg	0	0
			108	108		
22	B	1	Total	Mg	0	0
			1	1		
22	D	2	Total	Mg	0	0
			2	2		
22	E	1	Total	Mg	0	0
			1	1		
22	H	2	Total	Mg	0	0
			2	2		
22	K	1	Total	Mg	0	0
			1	1		
22	L	1	Total	Mg	0	0
			1	1		
22	M	1	Total	Mg	0	0
			1	1		
22	S	1	Total	Mg	0	0
			1	1		

- Molecule 23 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	A	8	Total	K	0	0
			8	8		

- Molecule 24 is HYGROMYCIN B (CCD ID: HYG) (formula: C₂₀H₃₇N₃O₁₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	A	1	Total	C	N	O	0	0
			36	20	3	13		

- Molecule 25 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

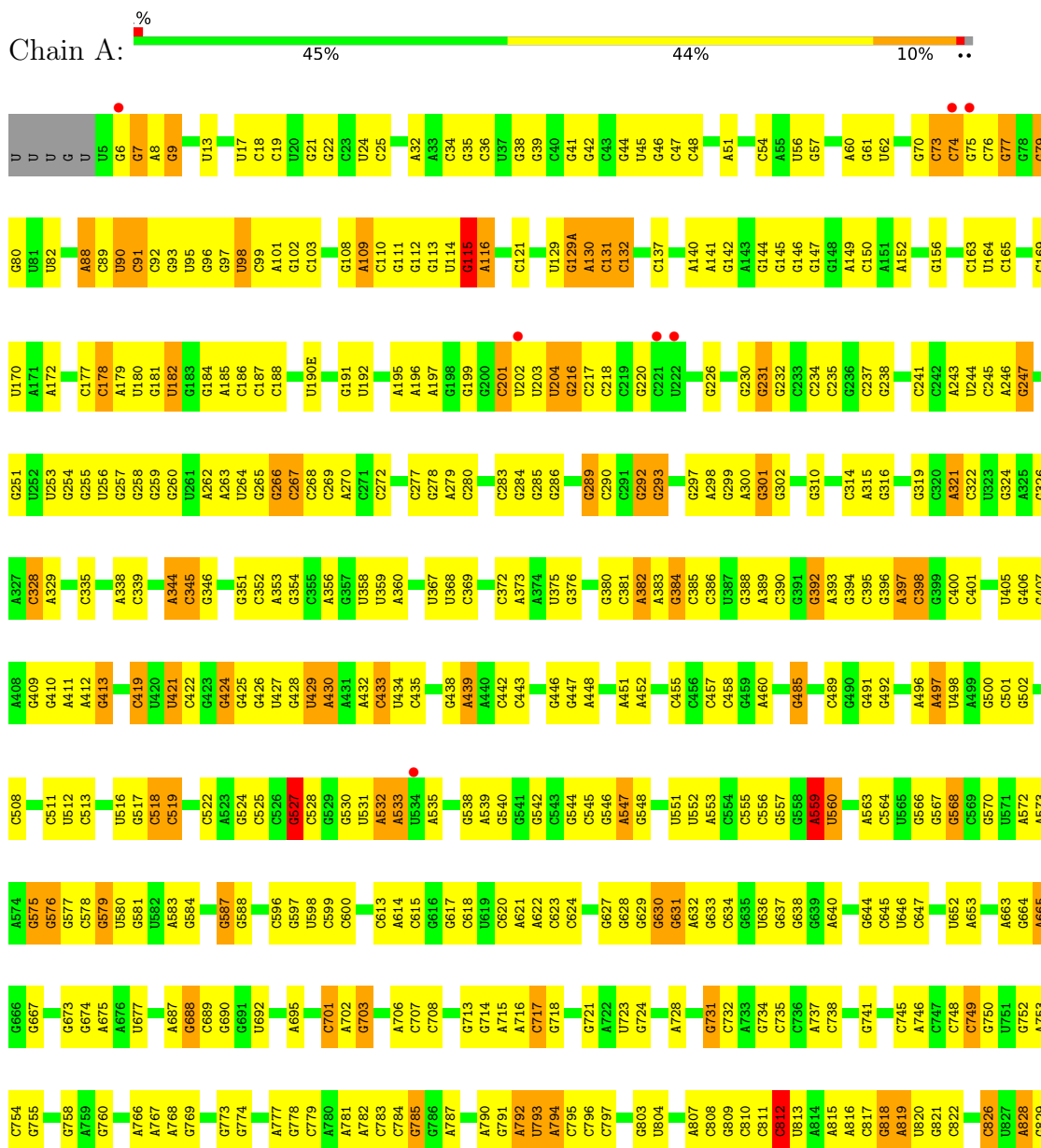
- Molecule 26 is water.

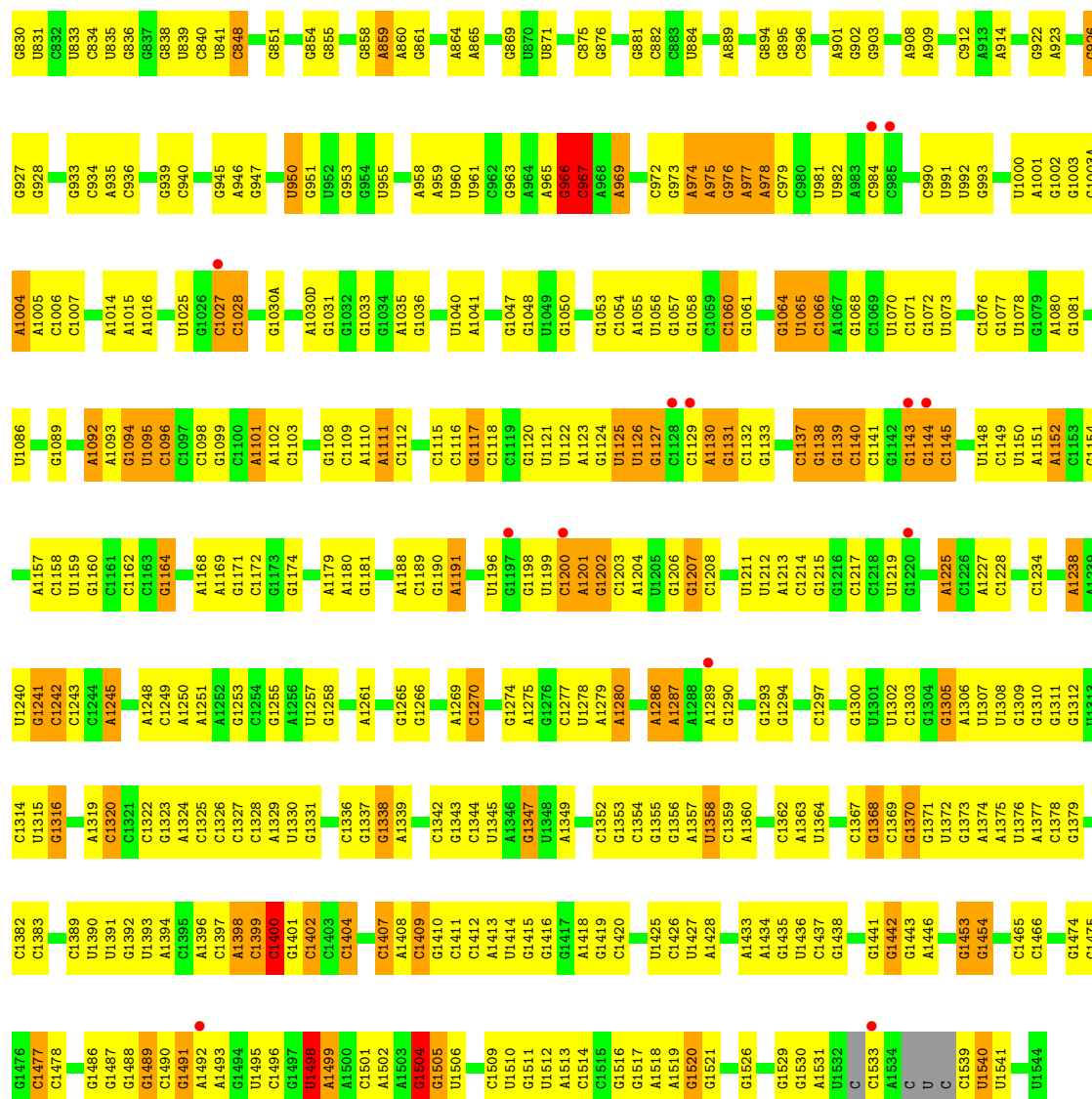
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
26	A	11	Total	O	0	0
			11	11		
26	E	6	Total	O	0	0
			6	6		
26	Q	1	Total	O	0	0
			1	1		

3 Residue-property plots

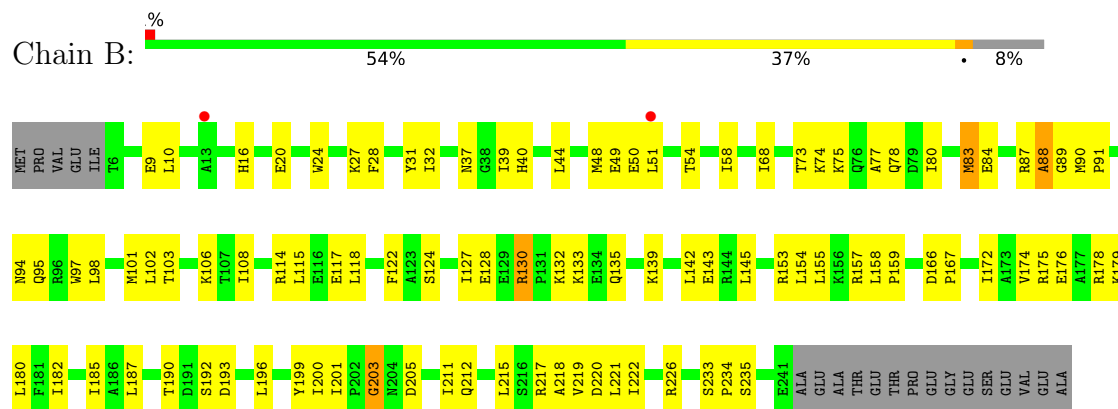
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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



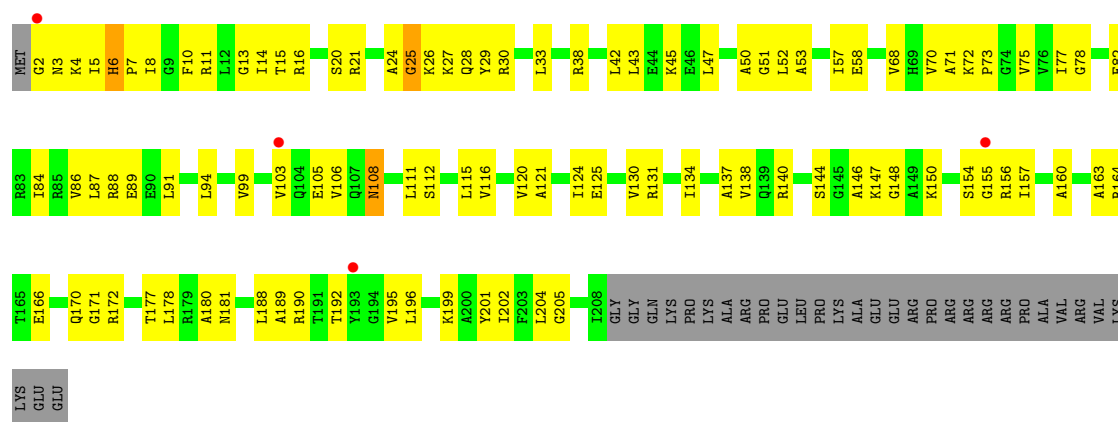


• Molecule 2: ribosomal protein S2

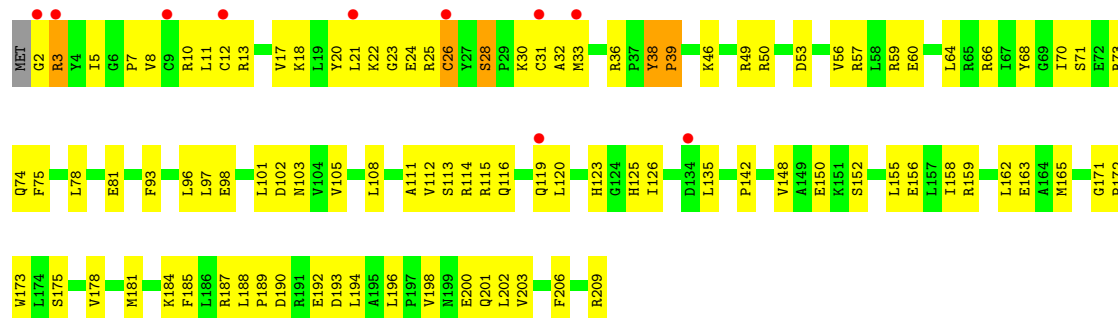


• Molecule 3: ribosomal protein S3

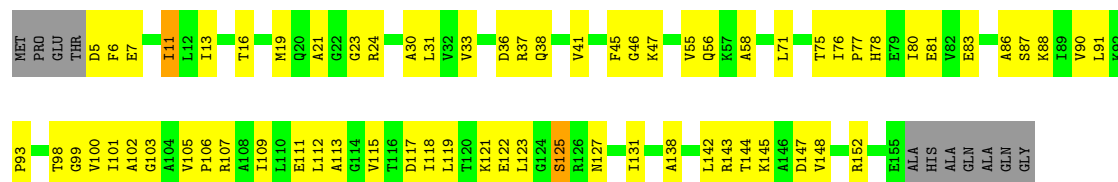




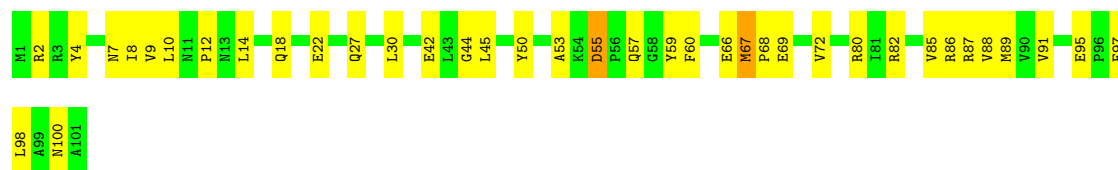
• Molecule 4: ribosomal protein S4



• Molecule 5: ribosomal protein S5

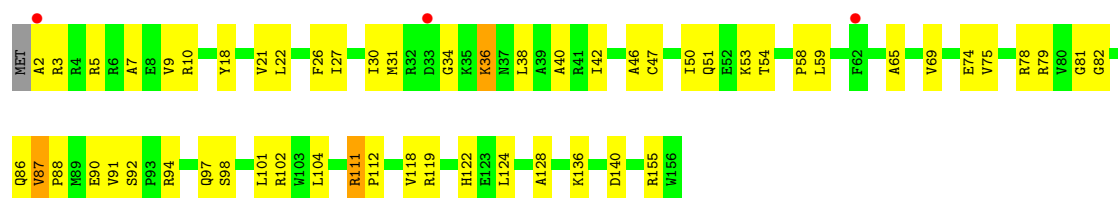


• Molecule 6: ribosomal protein S6



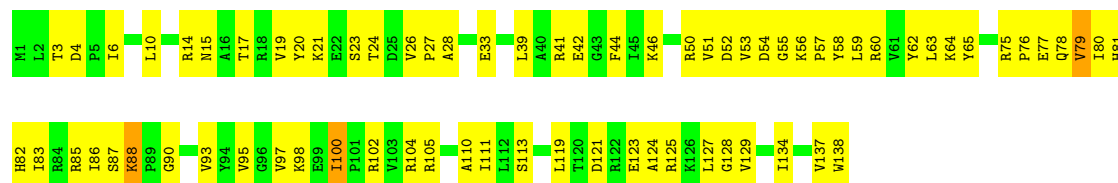
• Molecule 7: ribosomal protein S7





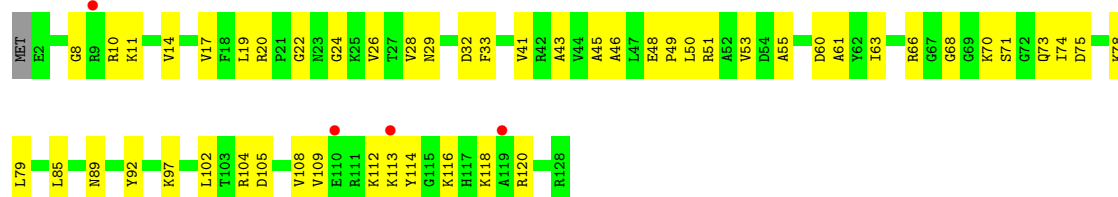
• Molecule 8: ribosomal protein S8

Chain H: 48% 50%



• Molecule 9: ribosomal protein S9

Chain I: 3% 59% 40%



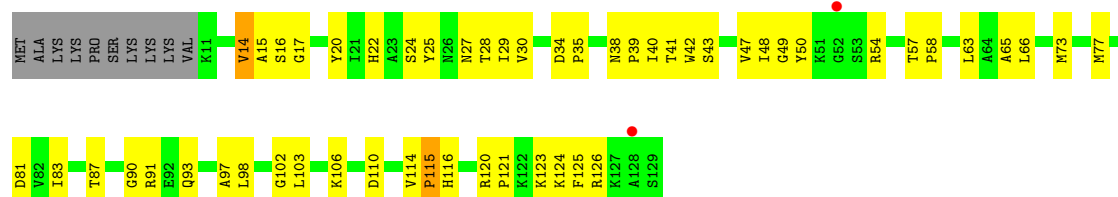
• Molecule 10: ribosomal protein S10

Chain J: 50% 39% 5% 6%

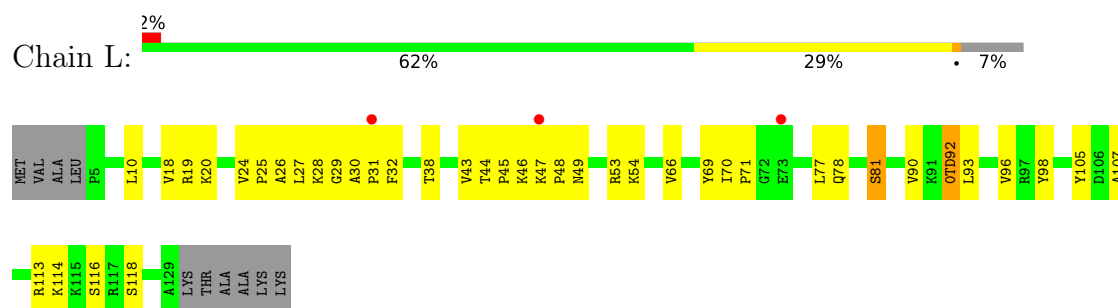


• Molecule 11: ribosomal protein S11

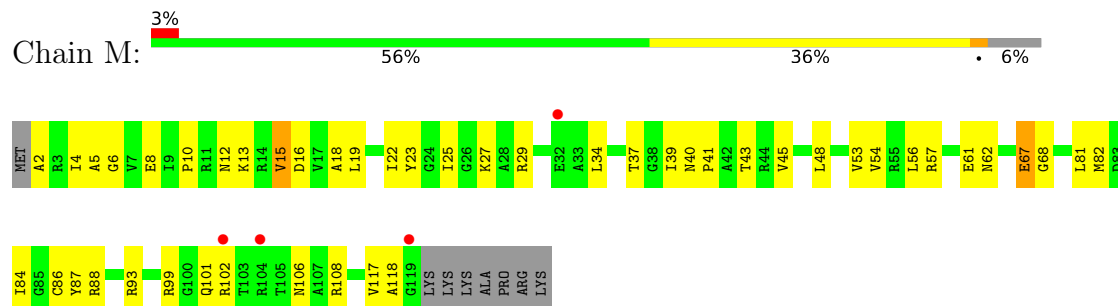
Chain K: 2% 51% 40% 8%



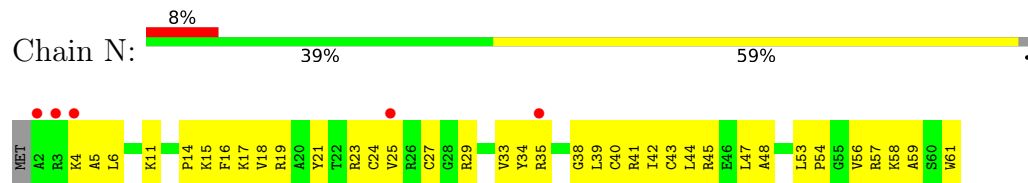
• Molecule 12: ribosomal protein S12



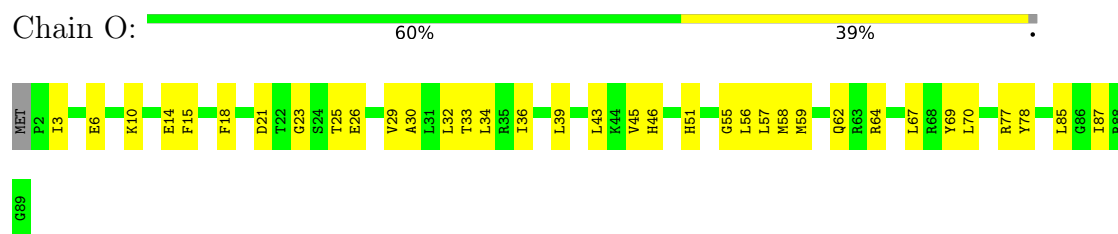
- Molecule 13: ribosomal protein S13



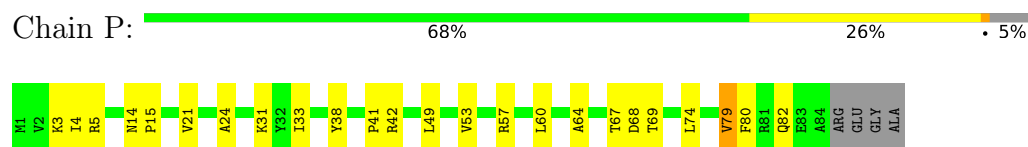
- Molecule 14: ribosomal protein S14



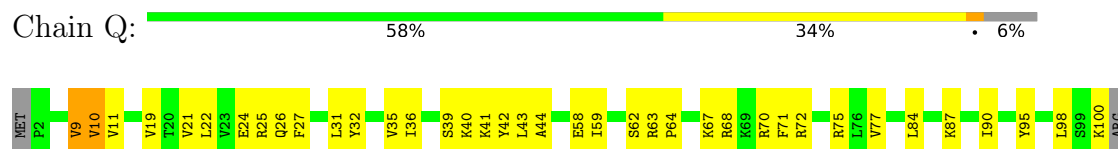
- Molecule 15: ribosomal protein S15



- Molecule 16: ribosomal protein S16



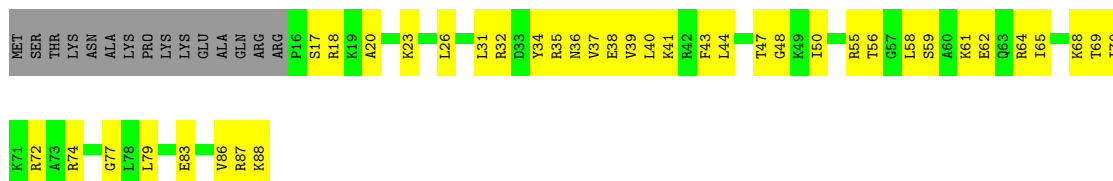
- Molecule 17: ribosomal protein S17



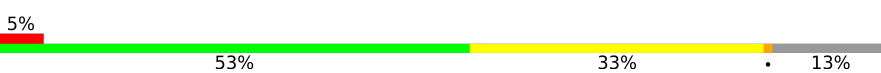
GLY
GLY
LYS
ALA

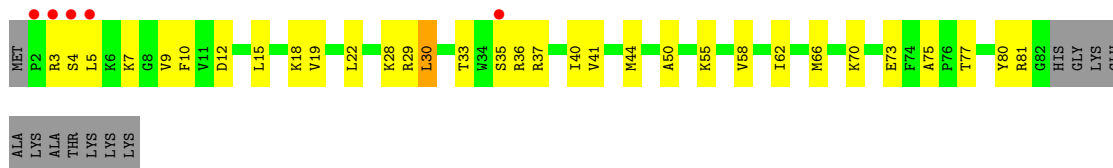
• Molecule 18: ribosomal protein S18

Chain R:  39% 44% 17%



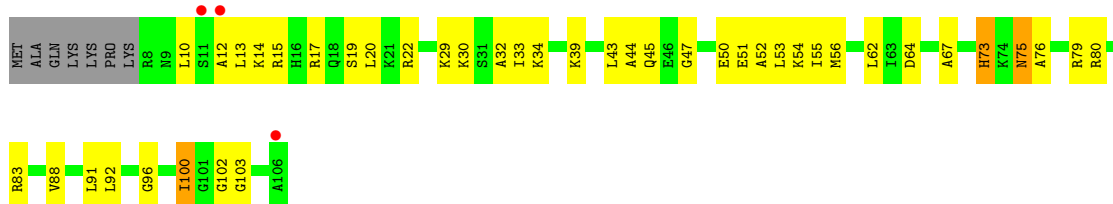
• Molecule 19: ribosomal protein S19

Chain S:  5% 53% 33% 13%



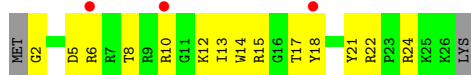
• Molecule 20: ribosomal protein S20

Chain T:  3% 54% 37% 7%



• Molecule 21: ribosomal protein THX

Chain U:  11% 41% 52% 7%



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	401.83Å 401.83Å 174.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.59 – 3.75 34.59 – 3.75	Depositor EDS
% Data completeness (in resolution range)	97.7 (34.59-3.75) 97.4 (34.59-3.75)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 3.76Å)	Xtriage
Refinement program	PHENIX dev_1119	Depositor
R, R_{free}	0.163 , 0.218 (Not available) , 0.218	Depositor DCC
R_{free} test set	7022 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	137.9	Xtriage
Anisotropy	0.350	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 115.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	51823	wwPDB-VP
Average B, all atoms (Å ²)	147.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.87% 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: M2G, 7MG, 0TD, K, PSU, 4OC, HYG, ZN, MG, 5MC, 2MG, UR3

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.45	0/36113	0.63	7/56360 (0.0%)
2	B	0.75	0/1909	1.08	5/2579 (0.2%)
3	C	0.54	0/1637	0.98	5/2207 (0.2%)
4	D	0.67	0/1733	1.14	16/2318 (0.7%)
5	E	0.96	1/1163 (0.1%)	1.32	11/1566 (0.7%)
6	F	0.60	0/856	1.04	5/1154 (0.4%)
7	G	0.62	0/1276	1.03	6/1709 (0.4%)
8	H	1.03	1/1136 (0.1%)	1.31	10/1527 (0.7%)
9	I	0.61	0/1029	1.01	1/1379 (0.1%)
10	J	0.58	0/806	1.19	9/1084 (0.8%)
11	K	0.74	0/900	1.19	7/1213 (0.6%)
12	L	0.77	0/978	1.24	9/1308 (0.7%)
13	M	0.68	1/947 (0.1%)	1.09	4/1270 (0.3%)
14	N	0.59	0/501	0.96	0/664
15	O	0.84	0/745	1.01	0/992
16	P	0.79	0/717	1.16	4/965 (0.4%)
17	Q	0.91	1/836 (0.1%)	1.24	3/1117 (0.3%)
18	R	0.68	0/604	1.13	5/801 (0.6%)
19	S	0.58	0/662	1.03	3/892 (0.3%)
20	T	0.74	0/765	1.14	6/1007 (0.6%)
21	U	0.51	0/213	0.90	0/279
All	All	0.56	4/55526 (0.0%)	0.82	116/82391 (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	2
3	C	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
8	H	0	1
10	J	0	2
18	R	0	1
All	All	0	7

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	11	ILE	CA-CB	-6.07	1.47	1.54
17	Q	9	VAL	CA-CB	-5.27	1.48	1.54
8	H	79	VAL	CA-CB	-5.24	1.47	1.54
13	M	106	ASN	CA-C	-5.09	1.48	1.53

All (116) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J	13	HIS	CB-CA-C	-10.11	104.91	116.54
4	D	26	CYS	N-CA-C	-9.18	102.08	113.28
12	L	26	ALA	N-CA-C	-8.99	102.45	113.15
10	J	13	HIS	N-CA-C	8.35	121.00	108.31
7	G	111	ARG	CA-C-N	8.13	127.71	118.85
7	G	111	ARG	C-N-CA	8.13	127.71	118.85
16	P	53	VAL	N-CA-C	7.85	117.91	110.53
4	D	38	TYR	CA-C-N	7.73	128.35	120.38
4	D	38	TYR	C-N-CA	7.73	128.35	120.38
8	H	75	ARG	CA-C-N	7.73	127.66	119.85
8	H	75	ARG	C-N-CA	7.73	127.66	119.85
8	H	80	ILE	CB-CA-C	-7.70	101.95	111.88
11	K	49	GLY	N-CA-C	7.55	122.05	112.83
4	D	56	VAL	CB-CA-C	-7.43	102.46	111.97
18	R	18	ARG	N-CA-C	7.33	122.40	113.17
16	P	79	VAL	N-CA-C	-7.02	102.21	112.04
3	C	6	HIS	CA-C-N	7.01	126.49	118.85
3	C	6	HIS	C-N-CA	7.01	126.49	118.85
3	C	108	ASN	CA-C-N	7.01	126.71	119.56
3	C	108	ASN	C-N-CA	7.01	126.71	119.56
11	K	91	ARG	N-CA-C	-6.99	102.88	111.40
5	E	100	VAL	CB-CA-C	-6.93	103.75	111.23
4	D	28	SER	CA-C-N	6.84	128.39	119.84
4	D	28	SER	C-N-CA	6.84	128.39	119.84
5	E	105	VAL	CA-C-N	-6.83	111.76	119.28
5	E	105	VAL	C-N-CA	-6.83	111.76	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	171	GLY	CA-C-N	6.83	126.45	119.56
4	D	171	GLY	C-N-CA	6.83	126.45	119.56
6	F	55	ASP	CA-C-N	6.70	126.33	119.56
6	F	55	ASP	C-N-CA	6.70	126.33	119.56
8	H	81	HIS	N-CA-C	-6.58	103.60	111.69
5	E	127	ASN	CA-C-N	6.56	126.06	119.24
5	E	127	ASN	C-N-CA	6.56	126.06	119.24
12	L	105	TYR	CB-CA-C	-6.53	109.05	116.63
10	J	71	LEU	N-CA-C	6.52	121.53	111.56
2	B	9	GLU	N-CA-C	6.51	119.96	109.02
5	E	103	GLY	N-CA-C	-6.41	104.56	111.93
7	G	36	LYS	N-CA-C	-6.41	105.28	113.23
17	Q	35	VAL	CB-CA-C	-6.40	103.22	110.96
20	T	12	ALA	N-CA-C	-6.39	105.34	113.02
1	A	115	G	C2'-C3'-O3'	6.39	119.08	109.50
6	F	67	MET	N-CA-C	6.38	113.75	108.07
13	M	106	ASN	CB-CA-C	-6.38	109.23	116.63
2	B	80	ILE	N-CA-C	-6.37	96.09	109.34
5	E	41	VAL	CB-CA-C	-6.27	101.88	110.90
13	M	67	GLU	CB-CA-C	-6.26	109.34	116.54
10	J	52	GLY	CA-C-N	6.25	126.16	119.28
10	J	52	GLY	C-N-CA	6.25	126.16	119.28
18	R	83	GLU	N-CA-C	6.21	117.61	108.86
5	E	11	ILE	CB-CA-C	-6.17	104.10	111.81
12	L	30	ALA	CA-C-N	6.15	127.53	119.84
12	L	30	ALA	C-N-CA	6.15	127.53	119.84
8	H	100	ILE	CA-C-N	6.13	126.64	120.14
8	H	100	ILE	C-N-CA	6.13	126.64	120.14
4	D	3	ARG	N-CA-C	6.09	119.93	111.90
20	T	76	ALA	N-CA-C	-6.08	104.66	111.28
8	H	88	LYS	CA-C-N	-5.98	113.37	119.83
8	H	88	LYS	C-N-CA	-5.98	113.37	119.83
2	B	203	GLY	N-CA-C	5.96	119.94	112.79
17	Q	9	VAL	CB-CA-C	-5.89	101.92	110.63
19	S	30	LEU	N-CA-C	5.85	119.42	111.17
1	A	1504	G	P-O3'-C3'	5.82	128.93	120.20
1	A	812	C	C2'-C3'-O3'	5.80	118.20	109.50
18	R	79	LEU	CA-C-N	5.78	125.54	119.76
18	R	79	LEU	C-N-CA	5.78	125.54	119.76
10	J	12	ASP	N-CA-C	5.76	118.18	107.99
13	M	15	VAL	N-CA-C	5.76	115.94	110.42
5	E	23	GLY	N-CA-C	5.73	117.78	110.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	102	GLY	N-CA-C	-5.72	107.20	115.27
5	E	115	VAL	CB-CA-C	-5.72	102.57	111.26
12	L	18	VAL	N-CA-C	5.67	116.03	107.80
19	S	10	PHE	N-CA-C	5.67	117.97	108.96
4	D	50	ARG	CA-C-N	5.64	125.40	119.76
4	D	50	ARG	C-N-CA	5.64	125.40	119.76
4	D	30	LYS	N-CA-C	5.63	119.99	113.18
13	M	67	GLU	N-CA-C	5.61	116.84	108.31
18	R	31	LEU	N-CA-C	-5.61	106.44	113.28
20	T	96	GLY	N-CA-C	5.57	121.36	111.73
4	D	12	CYS	N-CA-C	-5.50	104.67	111.33
7	G	92	SER	CA-C-N	5.50	124.95	119.24
7	G	92	SER	C-N-CA	5.50	124.95	119.24
20	T	100	ILE	N-CA-C	5.49	116.12	110.36
1	A	812	C	P-O3'-C3'	5.47	128.40	120.20
4	D	39	PRO	N-CA-C	5.45	117.35	110.70
12	L	66	VAL	CB-CA-C	-5.44	102.36	111.29
12	L	43	VAL	N-CA-C	5.41	117.88	108.90
1	A	559	A	C4'-C3'-O3'	5.36	117.45	109.40
9	I	22	GLY	N-CA-C	5.31	119.44	111.42
11	K	87	THR	CB-CA-C	-5.29	102.63	110.62
7	G	87	VAL	N-CA-C	5.28	113.75	107.73
10	J	38	ILE	CA-C-N	5.27	124.45	118.97
10	J	38	ILE	C-N-CA	5.27	124.45	118.97
10	J	87	THR	N-CA-C	5.26	117.38	108.02
20	T	73	HIS	CB-CA-C	-5.24	109.56	115.79
19	S	4	SER	N-CA-C	5.23	117.33	108.02
1	A	1504	G	C2'-C3'-O3'	5.21	117.32	109.50
8	H	3	THR	CA-C-N	-5.20	115.81	123.30
8	H	3	THR	C-N-CA	-5.20	115.81	123.30
12	L	81	SER	N-CA-C	5.20	117.42	110.35
2	B	10	LEU	N-CA-C	-5.19	106.54	112.92
1	A	1498	UR3	P-O3'-C3'	5.19	125.92	119.70
6	F	95	GLU	CA-C-N	5.16	125.08	119.76
6	F	95	GLU	C-N-CA	5.16	125.08	119.76
11	K	14	VAL	N-CA-C	5.15	115.43	110.74
12	L	38	THR	N-CA-C	-5.14	104.72	111.96
17	Q	10	VAL	CB-CA-C	-5.13	105.69	111.23
3	C	25	GLY	N-CA-C	-5.12	105.55	112.57
5	E	125	SER	N-CA-C	5.10	117.62	110.23
4	D	188	LEU	CA-C-N	5.08	124.98	119.85
4	D	188	LEU	C-N-CA	5.08	124.98	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	83	MET	N-CA-C	5.03	117.87	111.69
16	P	80	PHE	N-CA-C	5.02	119.41	113.28
20	T	75	ASN	N-CA-C	-5.02	106.75	112.92
11	K	115	PRO	CA-C-N	-5.01	115.35	122.77
11	K	115	PRO	C-N-CA	-5.01	115.35	122.77
16	P	31	LYS	N-CA-C	5.00	117.60	110.24

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	130	ARG	Peptide
2	B	88	ALA	Peptide
3	C	166	GLU	Peptide
8	H	90	GLY	Peptide
10	J	12	ASP	Peptide
10	J	87	THR	Peptide
18	R	20	ALA	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	32522	0	16437	647	0
2	B	1874	0	1887	78	0
3	C	1613	0	1677	79	0
4	D	1703	0	1763	84	0
5	E	1147	0	1207	53	0
6	F	843	0	857	34	0
7	G	1257	0	1296	48	0
8	H	1116	0	1177	52	0
9	I	1010	0	1037	42	0
10	J	793	0	835	43	0
11	K	885	0	904	37	0
12	L	973	0	1058	35	0
13	M	937	0	995	42	0
14	N	492	0	529	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	O	734	0	771	32	0
16	P	701	0	720	16	0
17	Q	823	0	891	36	0
18	R	598	0	670	30	0
19	S	648	0	673	24	0
20	T	763	0	861	34	0
21	U	209	0	221	20	0
22	A	108	0	0	0	0
22	B	1	0	0	0	0
22	D	2	0	0	0	0
22	E	1	0	0	0	0
22	H	2	0	0	0	0
22	K	1	0	0	0	0
22	L	1	0	0	0	0
22	M	1	0	0	0	0
22	S	1	0	0	0	0
23	A	8	0	0	0	0
24	A	36	0	37	4	0
25	D	1	0	0	0	0
25	N	1	0	0	0	0
26	A	11	0	0	0	0
26	E	6	0	0	0	0
26	Q	1	0	0	0	0
All	All	51823	0	36503	1355	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

All (1355) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:538:G:H5''	12:L:114:LYS:HB2	1.55	0.88
16:P:57:ARG:NH1	16:P:79:VAL:O	2.07	0.86
1:A:279:A:OP2	17:Q:95:TYR:OH	1.93	0.85
1:A:959:A:HO2'	1:A:984:C:HO2'	1.18	0.85
5:E:11:ILE:HB	5:E:31:LEU:HB3	1.57	0.85
2:B:75:LYS:HA	2:B:78:GLN:HB2	1.59	0.84
10:J:48:THR:HG1	10:J:62:HIS:HD1	0.85	0.84
1:A:144:G:H1	1:A:178:C:H42	1.26	0.84
13:M:86:CYS:SG	13:M:87:TYR:N	2.51	0.84
8:H:51:VAL:HG11	8:H:60:ARG:HG3	1.61	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:664:G:H22	1:A:741:G:H1	1.26	0.83
1:A:1133:G:H1	1:A:1141:C:H42	1.27	0.83
20:T:30:LYS:HE3	20:T:80:ARG:HH12	1.42	0.82
18:R:17:SER:HB3	18:R:55:ARG:HG2	1.62	0.81
10:J:48:THR:OG1	10:J:62:HIS:ND1	2.03	0.81
1:A:235:C:H5'	17:Q:70:ARG:HG2	1.62	0.81
5:E:80:ILE:HD11	5:E:138:ALA:HB1	1.62	0.81
19:S:7:LYS:O	19:S:7:LYS:NZ	2.13	0.80
1:A:1376:U:OP1	7:G:98:SER:OG	1.99	0.80
1:A:792:A:H4'	1:A:793:U:H5'	1.64	0.79
1:A:974:A:OP2	14:N:41:ARG:NH1	2.14	0.79
21:U:6:ARG:HH21	21:U:15:ARG:HH21	1.29	0.79
6:F:2:ARG:HE	6:F:69:GLU:HG2	1.46	0.79
2:B:103:THR:N	2:B:176:GLU:OE1	2.16	0.78
1:A:692:U:OP1	11:K:124:LYS:NZ	2.15	0.78
1:A:1028:C:N3	1:A:1033:G:N2	2.31	0.77
1:A:1060:C:OP1	14:N:45:ARG:NH2	2.16	0.77
13:M:4:ILE:HD12	13:M:56:LEU:HD12	1.64	0.77
1:A:1368:G:H5''	9:I:112:LYS:HB3	1.66	0.77
1:A:103:C:OP1	20:T:17:ARG:NH1	2.15	0.77
1:A:1028:C:H42	1:A:1033:G:H1	1.33	0.77
7:G:79:ARG:HG3	7:G:81:GLY:H	1.51	0.76
19:S:33:THR:HG22	19:S:35:SER:H	1.49	0.76
11:K:40:ILE:HG22	11:K:41:THR:HG22	1.69	0.75
2:B:78:GLN:O	2:B:94:ASN:ND2	2.17	0.75
2:B:158:LEU:HD12	2:B:158:LEU:H	1.52	0.75
9:I:97:LYS:HA	9:I:102:LEU:HD11	1.68	0.75
1:A:1356:G:H2'	1:A:1357:A:C8	2.22	0.75
13:M:16:ASP:OD1	13:M:16:ASP:N	2.19	0.75
13:M:81:LEU:HD23	13:M:84:ILE:HD11	1.68	0.75
1:A:427:U:OP1	4:D:13:ARG:NH2	2.18	0.75
1:A:413:G:N2	1:A:429:U:OP2	2.17	0.75
20:T:30:LYS:HE2	20:T:34:LYS:HE2	1.68	0.74
1:A:1219:U:OP1	14:N:19:ARG:NH2	2.15	0.74
20:T:53:LEU:HD12	20:T:102:GLY:HA3	1.70	0.74
10:J:17:ASP:HA	10:J:20:ALA:HB3	1.70	0.74
1:A:1086:U:H3	1:A:1099:G:H22	1.35	0.74
2:B:102:LEU:HB2	2:B:176:GLU:HG2	1.69	0.74
12:L:48:PRO:HD2	12:L:92:OTD:H3	1.69	0.74
13:M:5:ALA:HB3	13:M:22:ILE:HD11	1.69	0.74
1:A:1496:C:N4	24:A:1717:HYG:O11	2.22	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:112:LYS:NZ	9:I:116:LYS:O	2.21	0.73
1:A:955:U:H1'	1:A:1227:A:H61	1.52	0.73
16:P:21:VAL:HG12	16:P:33:ILE:HD12	1.70	0.73
2:B:77:ALA:HB2	2:B:211:ILE:HD13	1.70	0.73
9:I:50:LEU:HB3	9:I:55:ALA:HB2	1.68	0.73
18:R:32:ARG:HA	18:R:69:THR:HG21	1.70	0.73
16:P:68:ASP:OD1	16:P:68:ASP:N	2.18	0.73
1:A:290:C:H42	1:A:310:G:H1	1.36	0.72
16:P:4:ILE:HG12	16:P:21:VAL:HG22	1.71	0.72
1:A:258:G:H2'	1:A:259:G:H8	1.55	0.71
8:H:46:LYS:HG3	8:H:64:LYS:HB3	1.70	0.71
4:D:64:LEU:HD23	4:D:198:VAL:HG21	1.71	0.71
8:H:21:LYS:O	8:H:65:TYR:OH	2.09	0.71
1:A:946:A:H2'	1:A:947:G:C8	2.26	0.71
1:A:359:U:H2'	1:A:360:A:C8	2.24	0.71
13:M:34:LEU:HA	13:M:37:THR:HG22	1.72	0.71
1:A:285:G:H2'	1:A:286:G:H8	1.56	0.71
11:K:15:ALA:HA	11:K:77:MET:HA	1.71	0.71
20:T:56:MET:HG3	20:T:88:VAL:HG21	1.74	0.70
15:O:70:LEU:HD13	15:O:78:TYR:HA	1.71	0.70
1:A:1133:G:N2	1:A:1141:C:N3	2.35	0.70
5:E:98:THR:HB	5:E:117:ASP:HB3	1.72	0.70
1:A:299:G:H2'	1:A:300:A:C8	2.27	0.70
11:K:66:LEU:HG	11:K:97:ALA:HB1	1.74	0.70
10:J:50:ILE:HD11	10:J:57:LYS:HD2	1.74	0.69
1:A:1358:U:H5''	14:N:35:ARG:HD3	1.75	0.69
8:H:20:TYR:CE1	8:H:76:PRO:HD2	2.28	0.69
6:F:100:ASN:ND2	18:R:23:LYS:O	2.25	0.68
13:M:27:LYS:HE3	21:U:21:TYR:HE2	1.58	0.68
1:A:1266:G:N2	1:A:1269:A:OP2	2.26	0.68
5:E:83:GLU:HG2	5:E:88:LYS:HG3	1.75	0.68
13:M:57:ARG:HG2	13:M:61:GLU:HG3	1.76	0.68
1:A:129:U:O3'	1:A:129(A):G:H3'	1.93	0.68
12:L:10:LEU:HD23	17:Q:32:TYR:CZ	2.29	0.68
1:A:21:G:H2'	1:A:22:G:C8	2.29	0.68
1:A:1047:G:H5''	14:N:4:LYS:HG3	1.76	0.68
1:A:677:U:H3	1:A:713:G:H22	1.42	0.67
1:A:89:C:H2'	1:A:90:U:C6	2.29	0.67
1:A:407:G:OP1	4:D:115:ARG:NH2	2.26	0.67
9:I:48:GLU:OE2	9:I:51:ARG:NH2	2.23	0.67
1:A:9:G:OP2	5:E:121:LYS:NZ	2.16	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1415:G:C2	1:A:1486:G:C6	2.82	0.67
3:C:155:GLY:HA2	3:C:164:ARG:H	1.60	0.67
1:A:1189:C:H5'	3:C:5:ILE:HG12	1.77	0.67
2:B:212:GLN:HE21	2:B:235:SER:HB2	1.60	0.67
4:D:150:GLU:CD	4:D:150:GLU:H	2.02	0.67
1:A:811:C:O2'	1:A:901:A:N1	2.28	0.66
1:A:1058:G:OP1	3:C:199:LYS:NZ	2.28	0.66
12:L:113:ARG:NH1	12:L:116:SER:H	1.93	0.66
15:O:45:VAL:HB	15:O:46:HIS:CD2	2.30	0.66
8:H:41:ARG:NH1	8:H:123:GLU:OE2	2.28	0.66
10:J:4:ILE:HG21	10:J:77:PRO:HG3	1.75	0.66
1:A:76:C:H42	1:A:93:G:H1	1.42	0.66
18:R:38:GLU:HA	18:R:41:LYS:HE2	1.78	0.66
6:F:10:LEU:HB2	6:F:59:TYR:HB3	1.77	0.66
1:A:539:A:H2'	1:A:540:G:C8	2.31	0.66
1:A:316:G:OP2	1:A:351:G:O2'	2.14	0.66
2:B:20:GLU:HA	2:B:39:ILE:HG13	1.79	0.65
1:A:191:G:O2'	20:T:102:GLY:O	2.12	0.65
1:A:633:G:H2'	1:A:634:C:H6	1.62	0.65
7:G:79:ARG:HD2	7:G:82:GLY:H	1.61	0.65
1:A:101:A:H2'	1:A:102:G:H8	1.60	0.65
1:A:838:G:H1	1:A:848:C:H42	1.44	0.65
1:A:1286:A:H2'	1:A:1287:A:H4'	1.77	0.65
8:H:10:LEU:HD22	8:H:83:ILE:HD11	1.79	0.65
4:D:152:SER:HB3	4:D:155:LEU:HD12	1.78	0.65
10:J:13:HIS:HB3	10:J:14:LYS:HD3	1.77	0.65
13:M:54:VAL:HG22	13:M:57:ARG:HH12	1.61	0.65
1:A:263:A:OP2	20:T:79:ARG:NH1	2.30	0.65
1:A:1329:A:H5'	13:M:29:ARG:HD2	1.79	0.65
3:C:130:VAL:O	3:C:134:ILE:HG13	1.96	0.65
4:D:49:ARG:H	4:D:49:ARG:HD2	1.62	0.65
1:A:1401:G:O6	1:A:1504:G:N2	2.31	0.64
1:A:527:7MG:O2'	1:A:535:A:N1	2.30	0.64
1:A:1126:U:H2'	1:A:1127:G:H8	1.63	0.64
1:A:1148:U:H2'	1:A:1149:C:O4'	1.98	0.64
13:M:37:THR:HG23	13:M:39:ILE:H	1.62	0.64
17:Q:62:SER:OG	17:Q:72:ARG:HG3	1.97	0.64
1:A:633:G:H2'	1:A:634:C:C6	2.33	0.64
1:A:946:A:H2'	1:A:947:G:H8	1.60	0.64
3:C:78:GLY:HA3	3:C:82:GLU:HB3	1.78	0.64
18:R:86:VAL:HG12	18:R:87:ARG:HG3	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:835:U:H3	1:A:851:G:H1	1.44	0.64
14:N:16:PHE:HB2	14:N:19:ARG:HB2	1.79	0.64
1:A:875:C:O2'	8:H:14:ARG:NH1	2.31	0.64
3:C:156:ARG:H	3:C:163:ALA:HA	1.62	0.64
8:H:113:SER:HB2	8:H:134:ILE:HD11	1.80	0.64
9:I:46:ALA:HB2	9:I:74:ILE:HG23	1.80	0.64
1:A:266:G:H5'	1:A:268:C:H41	1.61	0.63
1:A:1309:G:OP2	13:M:99:ARG:NH2	2.31	0.63
11:K:43:SER:HA	11:K:47:VAL:HG21	1.78	0.63
13:M:4:ILE:HG22	13:M:5:ALA:H	1.64	0.63
16:P:3:LYS:HG3	16:P:24:ALA:HB2	1.79	0.63
10:J:82:ILE:HA	10:J:85:LEU:HB2	1.79	0.63
13:M:12:ASN:H	13:M:45:VAL:HB	1.63	0.63
15:O:85:LEU:HB3	15:O:87:ILE:HG23	1.81	0.63
1:A:1435:G:H2'	1:A:1436:U:C6	2.34	0.63
4:D:111:ALA:HB2	4:D:120:LEU:HD12	1.80	0.63
1:A:512:U:OP1	4:D:46:LYS:NZ	2.30	0.63
7:G:51:GLN:C	7:G:53:LYS:H	2.07	0.63
13:M:8:GLU:CD	13:M:22:ILE:HA	2.24	0.62
20:T:50:GLU:HA	20:T:100:ILE:HB	1.81	0.62
12:L:25:PRO:C	12:L:27:LEU:H	2.07	0.62
18:R:37:VAL:O	18:R:40:LEU:N	2.30	0.62
1:A:109:A:H2'	1:A:326:G:N2	2.14	0.62
1:A:951:G:OP2	13:M:102:ARG:NH2	2.32	0.62
8:H:23:SER:HB2	8:H:62:TYR:CD1	2.34	0.62
1:A:76:C:N4	1:A:93:G:H1	1.97	0.62
4:D:111:ALA:HB1	4:D:116:GLN:HG2	1.82	0.62
1:A:192:U:O4'	20:T:103:GLY:HA2	1.99	0.62
1:A:1411:C:H42	1:A:1490:C:N4	1.97	0.62
1:A:544:G:OP1	4:D:59:ARG:NH2	2.32	0.62
1:A:1149:C:O2'	1:A:1280:A:N1	2.33	0.62
3:C:202:ILE:HG22	3:C:204:LEU:HD23	1.81	0.62
11:K:30:VAL:HG21	11:K:65:ALA:HA	1.82	0.62
13:M:62:ASN:OD1	13:M:62:ASN:N	2.32	0.62
1:A:579:G:H5'	1:A:728:A:H1'	1.82	0.61
1:A:1347:G:N2	1:A:1373:G:H2'	2.15	0.61
1:A:1164:G:H1	1:A:1172:C:H42	1.47	0.61
3:C:116:VAL:HG21	3:C:202:ILE:HD11	1.80	0.61
7:G:90:GLU:HG2	7:G:91:VAL:H	1.65	0.61
1:A:976:G:OP2	1:A:1358:U:O2'	2.17	0.61
9:I:118:LYS:O	9:I:120:ARG:N	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1316:G:N1	1:A:1319:A:OP2	2.30	0.61
1:A:1412:C:N3	1:A:1489:G:N2	2.49	0.61
6:F:14:LEU:HD13	6:F:18:GLN:HB2	1.83	0.61
1:A:1278:U:H5''	1:A:1279:A:C8	2.36	0.61
4:D:31:CYS:C	4:D:33:MET:H	2.09	0.61
15:O:45:VAL:HG12	15:O:46:HIS:H	1.66	0.61
18:R:43:PHE:HD2	18:R:56:THR:HG22	1.64	0.61
13:M:19:LEU:O	13:M:22:ILE:HG22	2.00	0.60
15:O:39:LEU:HD12	15:O:56:LEU:HB2	1.82	0.60
1:A:1133:G:H1	1:A:1141:C:N4	1.99	0.60
1:A:1404:5MC:H1'	1:A:1499:A:C2	2.35	0.60
9:I:8:GLY:HA2	9:I:79:LEU:HD12	1.82	0.60
1:A:419:C:H42	1:A:424:G:H1	1.47	0.60
1:A:1425:U:H2'	1:A:1426:C:H6	1.66	0.60
4:D:78:LEU:HD11	4:D:96:LEU:HB3	1.84	0.60
1:A:501:C:H2'	1:A:502:G:C8	2.36	0.60
12:L:24:VAL:HG13	12:L:98:TYR:CE2	2.37	0.60
1:A:1162:C:H42	1:A:1174:G:H1	1.50	0.60
21:U:6:ARG:HE	21:U:15:ARG:NH2	1.99	0.60
12:L:24:VAL:HG13	12:L:98:TYR:HE2	1.66	0.60
21:U:6:ARG:HH21	21:U:15:ARG:NH2	1.98	0.60
1:A:1373:G:H5''	7:G:36:LYS:HE2	1.83	0.60
10:J:61:GLU:OE1	14:N:45:ARG:NH1	2.35	0.60
14:N:33:VAL:HA	14:N:40:CYS:HA	1.83	0.60
1:A:1190:G:O2'	3:C:3:ASN:HB3	2.02	0.59
1:A:1240:U:OP1	7:G:119:ARG:NH2	2.35	0.59
3:C:42:LEU:HA	3:C:45:LYS:HE3	1.83	0.59
4:D:53:ASP:OD1	4:D:53:ASP:N	2.34	0.59
9:I:19:LEU:HG	9:I:61:ALA:HB2	1.84	0.59
1:A:1397:C:O2'	1:A:1398:A:OP1	2.18	0.59
10:J:63:PHE:HE1	14:N:45:ARG:HA	1.66	0.59
20:T:33:ILE:HD12	20:T:62:LEU:HD13	1.83	0.59
4:D:187:ARG:NH2	4:D:193:ASP:OD1	2.36	0.59
1:A:1425:U:H2'	1:A:1426:C:C6	2.37	0.59
9:I:10:ARG:HD3	9:I:105:ASP:HB3	1.84	0.59
1:A:1056:U:H5'	3:C:163:ALA:HB2	1.84	0.59
1:A:1487:G:H2'	1:A:1488:G:C8	2.37	0.59
2:B:91:PRO:HG3	2:B:154:LEU:HB2	1.84	0.59
8:H:124:ALA:O	8:H:128:GLY:N	2.33	0.59
1:A:1510:U:H2'	1:A:1511:G:C8	2.38	0.59
14:N:27:CYS:HB3	14:N:43:CYS:SG	2.41	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:C:H5'	17:Q:68:ARG:HH12	1.68	0.59
1:A:438:G:N1	1:A:496:A:OP2	2.32	0.59
1:A:1191:A:OP1	3:C:4:LYS:NZ	2.36	0.59
2:B:84:GLU:OE2	2:B:235:SER:OG	2.21	0.59
1:A:384:G:H2'	1:A:385:C:C6	2.38	0.58
1:A:1238:A:H5'	1:A:1336:C:H41	1.68	0.58
10:J:14:LYS:HE3	10:J:15:THR:HG23	1.85	0.58
7:G:136:LYS:NZ	7:G:140:ASP:OD2	2.36	0.58
1:A:130:A:O2'	1:A:131:C:H5''	2.03	0.58
1:A:1399:C:H4'	1:A:1400:5MC:H5''	1.85	0.58
20:T:10:LEU:O	20:T:13:LEU:HB2	2.03	0.58
1:A:518:C:H4'	1:A:519:C:H5''	1.85	0.58
1:A:1188:A:O3'	14:N:58:LYS:NZ	2.33	0.58
1:A:232:G:H1'	1:A:262:A:N1	2.19	0.58
9:I:75:ASP:HA	9:I:78:LYS:HG3	1.84	0.58
1:A:1441:G:H4'	1:A:1442:G:C2	2.39	0.58
1:A:284:G:H2'	1:A:285:G:H8	1.69	0.58
1:A:580:U:H2'	1:A:581:G:O4'	2.04	0.58
1:A:1057:G:H5''	3:C:154:SER:HB2	1.85	0.58
2:B:97:TRP:HZ2	2:B:102:LEU:HD13	1.69	0.58
12:L:53:ARG:NH1	12:L:92:OTD:OD2	2.25	0.58
13:M:8:GLU:OE1	13:M:23:TYR:N	2.32	0.58
1:A:17:U:H2'	1:A:18:C:C6	2.39	0.58
1:A:457:C:H2'	1:A:458:C:H6	1.69	0.58
1:A:735:C:OP1	18:R:68:LYS:NZ	2.36	0.58
1:A:1498:UR3:O2'	1:A:1499:A:OP2	2.20	0.58
12:L:90:VAL:HG21	12:L:93:LEU:HD12	1.85	0.58
1:A:784:C:H2'	1:A:785:G:O4'	2.04	0.57
3:C:106:VAL:HG11	3:C:112:SER:HB3	1.86	0.57
1:A:79:G:C6	1:A:80:G:N7	2.72	0.57
1:A:836:G:C6	1:A:851:G:C6	2.92	0.57
1:A:963:G:O2'	1:A:1199:U:H5''	2.05	0.57
1:A:1241:G:H2'	1:A:1242:C:H6	1.69	0.57
2:B:211:ILE:O	2:B:215:LEU:HB2	2.03	0.57
8:H:86:ILE:HG22	8:H:87:SER:N	2.20	0.57
1:A:1137:C:H4'	1:A:1138:G:C2	2.39	0.57
1:A:1316:G:H4'	14:N:18:VAL:HG11	1.86	0.57
3:C:150:LYS:HB3	3:C:201:TYR:HB2	1.86	0.57
11:K:114:VAL:HG23	11:K:115:PRO:HD2	1.86	0.57
12:L:54:LYS:HB3	12:L:70:ILE:HD12	1.87	0.57
14:N:16:PHE:HD1	14:N:19:ARG:HD2	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:U:H2'	1:A:96:G:C8	2.39	0.57
1:A:614:A:H2'	1:A:615:C:C6	2.40	0.57
1:A:731:G:OP1	1:A:766:A:H1'	2.05	0.57
21:U:5:ASP:O	21:U:8:THR:OG1	2.23	0.57
9:I:53:VAL:HG21	9:I:85:LEU:HD11	1.86	0.57
1:A:392:G:H2'	1:A:393:A:H8	1.70	0.57
1:A:1200:C:O2	1:A:1204:A:N6	2.38	0.57
1:A:144:G:H1	1:A:178:C:N4	1.99	0.57
7:G:18:TYR:HB3	7:G:59:LEU:HD22	1.86	0.57
1:A:790:A:H2'	1:A:791:G:C8	2.40	0.56
1:A:1425:U:H3	1:A:1475:G:H1	1.51	0.56
3:C:43:LEU:HD21	3:C:91:LEU:HD11	1.86	0.56
8:H:54:ASP:OD2	8:H:55:GLY:N	2.37	0.56
8:H:82:HIS:C	8:H:82:HIS:CD2	2.83	0.56
15:O:45:VAL:HB	15:O:46:HIS:HD2	1.71	0.56
17:Q:21:VAL:HG21	17:Q:59:ILE:HG13	1.87	0.56
1:A:673:G:H5''	6:F:87:ARG:NH1	2.21	0.56
9:I:48:GLU:N	9:I:49:PRO:HD2	2.19	0.56
12:L:92:OTD:N	12:L:92:OTD:OD1	2.36	0.56
14:N:16:PHE:CD1	14:N:19:ARG:HD2	2.40	0.56
19:S:12:ASP:OD1	19:S:37:ARG:NH1	2.31	0.56
20:T:51:GLU:HA	20:T:54:LYS:HE2	1.87	0.56
1:A:184:G:H2'	1:A:185:A:H8	1.71	0.56
1:A:204:U:H5''	1:A:216:G:OP1	2.05	0.56
1:A:782:A:H2'	1:A:783:C:O4'	2.06	0.56
1:A:1412:C:H2'	1:A:1413:A:C8	2.40	0.56
4:D:162:LEU:HG	4:D:181:MET:HE3	1.88	0.56
6:F:10:LEU:HD23	6:F:85:VAL:HA	1.87	0.56
2:B:24:TRP:HB2	2:B:190:THR:HG22	1.88	0.56
5:E:31:LEU:HD23	5:E:45:PHE:HD1	1.70	0.56
5:E:145:LYS:O	5:E:148:VAL:HG23	2.06	0.56
6:F:80:ARG:NH2	6:F:88:VAL:O	2.39	0.56
3:C:156:ARG:NE	3:C:160:ALA:O	2.31	0.56
1:A:1305:G:N2	1:A:1331:G:H1'	2.20	0.56
1:A:1379:G:O6	7:G:2:ALA:N	2.39	0.56
10:J:38:ILE:HB	10:J:71:LEU:HB2	1.87	0.56
10:J:51:ARG:HD2	10:J:59:SER:HB2	1.87	0.56
12:L:27:LEU:O	12:L:29:GLY:N	2.37	0.56
13:M:40:ASN:HD22	13:M:43:THR:HG23	1.70	0.56
1:A:359:U:H2'	1:A:360:A:H8	1.67	0.56
1:A:1234:C:H1'	1:A:1364:U:O2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:102:ALA:O	5:E:107:ARG:NH1	2.38	0.56
19:S:28:LYS:HD3	19:S:29:ARG:H	1.71	0.56
1:A:413:G:O2'	1:A:428:G:N2	2.37	0.56
9:I:89:ASN:HB3	9:I:92:TYR:CE1	2.41	0.56
11:K:65:ALA:HB1	11:K:98:LEU:HD23	1.87	0.56
1:A:115:G:O2'	1:A:289:G:H5''	2.06	0.56
1:A:344:A:H5'	1:A:345:C:C5	2.41	0.56
1:A:1250:A:H4'	9:I:68:GLY:N	2.21	0.56
1:A:1414:U:C2	1:A:1415:G:C8	2.94	0.56
1:A:1441:G:O2'	1:A:1442:G:N2	2.38	0.56
1:A:614:A:H2'	1:A:615:C:H6	1.71	0.55
4:D:192:GLU:OE2	4:D:192:GLU:N	2.39	0.55
8:H:111:ILE:HG22	8:H:134:ILE:HD12	1.87	0.55
1:A:1408:A:H2'	1:A:1409:C:O4'	2.06	0.55
1:A:1486:G:C6	1:A:1487:G:C6	2.94	0.55
3:C:21:ARG:HB2	3:C:58:GLU:HB3	1.87	0.55
5:E:78:HIS:ND1	8:H:104:ARG:HG3	2.22	0.55
8:H:98:LYS:H	8:H:98:LYS:HZ3	1.54	0.55
1:A:328:C:H2'	1:A:328:C:O2	2.06	0.55
9:I:26:VAL:HB	9:I:33:PHE:HB2	1.89	0.55
11:K:27:ASN:OD1	11:K:28:THR:N	2.39	0.55
21:U:12:LYS:O	21:U:22:ARG:NH1	2.39	0.55
1:A:164:U:H2'	1:A:165:C:C6	2.41	0.55
8:H:83:ILE:HB	8:H:137:VAL:HG13	1.88	0.55
14:N:11:LYS:HE3	14:N:14:PRO:HA	1.88	0.55
1:A:581:G:O3'	15:O:64:ARG:NH2	2.40	0.55
18:R:38:GLU:CD	18:R:38:GLU:H	2.15	0.55
1:A:97:G:H2'	1:A:98:U:O4'	2.06	0.55
1:A:908:A:C2	1:A:909:A:C4	2.94	0.55
1:A:1198:G:H2'	1:A:1199:U:C6	2.42	0.55
4:D:7:PRO:HG2	4:D:10:ARG:HD2	1.89	0.55
1:A:278:G:C6	17:Q:95:TYR:HD2	2.25	0.55
1:A:1265:G:H1	1:A:1270:C:H42	1.55	0.55
1:A:1320:C:H5'	19:S:70:LYS:HD3	1.88	0.55
4:D:173:TRP:HB2	4:D:187:ARG:O	2.07	0.55
7:G:51:GLN:O	7:G:53:LYS:N	2.40	0.55
11:K:110:ASP:HB2	18:R:88:LYS:HD2	1.89	0.55
1:A:258:G:H2'	1:A:259:G:C8	2.40	0.55
7:G:88:PRO:O	7:G:155:ARG:NH1	2.40	0.55
11:K:123:LYS:HA	11:K:126:ARG:HG3	1.89	0.55
15:O:32:LEU:HD21	15:O:62:GLN:HB3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:113:SER:OG	4:D:114:ARG:N	2.39	0.55
10:J:34:VAL:HG11	10:J:74:ILE:HA	1.87	0.55
11:K:41:THR:OG1	11:K:42:TRP:N	2.40	0.55
1:A:321:A:H2'	1:A:322:C:H6	1.72	0.55
1:A:1150:U:O4	1:A:1151:A:N6	2.40	0.55
2:B:118:LEU:HB3	2:B:142:LEU:HG	1.89	0.55
3:C:91:LEU:HB3	3:C:99:VAL:HG21	1.88	0.55
8:H:97:VAL:HG23	8:H:129:VAL:O	2.06	0.55
16:P:14:ASN:OD1	16:P:42:ARG:NH2	2.39	0.55
1:A:1207:2MG:HM23	1:A:1208:C:H1'	1.89	0.54
2:B:178:ARG:HD2	2:B:196:LEU:O	2.07	0.54
4:D:93:PHE:CE1	4:D:97:LEU:HD11	2.41	0.54
9:I:108:VAL:HG12	9:I:109:VAL:H	1.72	0.54
19:S:33:THR:HG22	19:S:35:SER:N	2.20	0.54
1:A:279:A:OP1	1:A:280:C:O2'	2.21	0.54
1:A:858:G:O2'	1:A:859:A:H5''	2.07	0.54
1:A:1338:G:H2'	1:A:1339:A:C8	2.43	0.54
9:I:104:ARG:NH1	9:I:105:ASP:O	2.37	0.54
1:A:664:G:OP1	18:R:64:ARG:HD2	2.07	0.54
3:C:121:ALA:HA	3:C:124:ILE:HD12	1.89	0.54
5:E:88:LYS:HD2	5:E:123:LEU:HD12	1.89	0.54
8:H:65:TYR:HA	8:H:79:VAL:HG23	1.88	0.54
1:A:243:A:C2	1:A:246:A:C8	2.96	0.54
3:C:137:ALA:HA	3:C:140:ARG:HE	1.72	0.54
9:I:10:ARG:HH21	9:I:11:LYS:HE3	1.72	0.54
10:J:40:LEU:HD12	10:J:69:ASN:HB2	1.89	0.54
1:A:644:G:C5	1:A:645:C:C5	2.95	0.54
1:A:665:A:N3	1:A:732:C:H2'	2.22	0.54
1:A:560:U:H5'	1:A:566:G:N2	2.21	0.54
7:G:21:VAL:HG22	7:G:22:LEU:HD12	1.90	0.54
13:M:2:ALA:O	13:M:10:PRO:HD2	2.07	0.54
2:B:139:LYS:HE2	2:B:143:GLU:HG3	1.90	0.54
8:H:119:LEU:HD12	8:H:124:ALA:HA	1.90	0.54
14:N:25:VAL:HG23	14:N:38:GLY:HA3	1.89	0.54
1:A:345:C:OP2	1:A:345:C:H6	1.89	0.54
6:F:22:GLU:OE1	6:F:82:ARG:NH1	2.40	0.54
1:A:1207:2MG:H2'	1:A:1208:C:C6	2.43	0.54
1:A:1323:G:H2'	1:A:1324:A:C8	2.43	0.54
3:C:6:HIS:CE1	3:C:8:ILE:HB	2.43	0.54
5:E:144:THR:O	5:E:148:VAL:HG22	2.07	0.54
6:F:97:PHE:C	6:F:98:LEU:HD13	2.33	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:121:ALA:HB1	3:C:189:ALA:HB2	1.90	0.53
1:A:381:C:H2'	1:A:382:A:O4'	2.08	0.53
1:A:401:C:H1'	1:A:622:A:H1'	1.91	0.53
1:A:1139:G:H21	1:A:1143:G:H21	1.55	0.53
4:D:152:SER:O	4:D:155:LEU:HB2	2.08	0.53
14:N:48:ALA:HA	14:N:53:LEU:HB2	1.89	0.53
15:O:36:ILE:HG23	15:O:56:LEU:HD11	1.89	0.53
1:A:438:G:H4'	4:D:123:HIS:CD2	2.43	0.53
1:A:542:G:OP1	4:D:10:ARG:NH2	2.38	0.53
5:E:152:ARG:NE	8:H:44:PHE:HE1	2.07	0.53
6:F:67:MET:HB2	6:F:68:PRO:HD2	1.90	0.53
1:A:56:U:H2'	1:A:57:G:C8	2.43	0.53
1:A:1109:C:H2'	1:A:1110:A:O4'	2.07	0.53
1:A:1509:C:H42	1:A:1526:G:H1	1.57	0.53
3:C:84:ILE:HG23	3:C:88:ARG:HH21	1.74	0.53
10:J:19:SER:HA	10:J:22:LYS:HE2	1.91	0.53
1:A:1511:G:H2'	1:A:1512:U:O4'	2.08	0.53
3:C:52:LEU:HD12	3:C:70:VAL:HG12	1.90	0.53
4:D:32:ALA:O	4:D:36:ARG:N	2.29	0.53
1:A:421:U:H5'	1:A:422:C:H5	1.73	0.53
1:A:646:U:H2'	1:A:647:C:C6	2.43	0.53
1:A:1427:U:H2'	1:A:1428:A:C8	2.43	0.53
12:L:19:ARG:H	12:L:19:ARG:HD2	1.72	0.53
17:Q:87:LYS:HA	17:Q:90:ILE:HD12	1.89	0.53
1:A:74:C:H2'	1:A:75:G:O4'	2.08	0.53
1:A:141:A:H1'	1:A:182:U:O2	2.09	0.53
1:A:142:G:O2'	1:A:196:A:N1	2.37	0.53
8:H:23:SER:HB2	8:H:62:TYR:HD1	1.72	0.53
20:T:29:LYS:O	20:T:32:ALA:HB3	2.09	0.53
1:A:539:A:H2'	1:A:540:G:H8	1.71	0.53
1:A:1124:G:N7	1:A:1145:C:O2'	2.40	0.53
2:B:88:ALA:O	2:B:90:MET:N	2.42	0.53
12:L:93:LEU:O	12:L:96:VAL:HG23	2.08	0.53
14:N:17:LYS:HE2	14:N:18:VAL:HG13	1.91	0.53
1:A:199:G:H1	1:A:218:C:H42	1.57	0.53
1:A:1328:C:OP1	21:U:21:TYR:OH	2.27	0.53
12:L:27:LEU:HG	12:L:28:LYS:H	1.74	0.53
17:Q:10:VAL:HG13	17:Q:19:VAL:HB	1.91	0.53
1:A:673:G:H2'	1:A:674:G:C8	2.43	0.52
1:A:1342:C:H2'	1:A:1343:G:C8	2.44	0.52
2:B:87:ARG:HE	2:B:219:VAL:HG11	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:65:ALA:HB2	7:G:128:ALA:HB2	1.92	0.52
20:T:44:ALA:O	20:T:47:GLY:N	2.34	0.52
1:A:103:C:OP2	20:T:14:LYS:HD2	2.10	0.52
1:A:149:A:H2'	1:A:150:C:H6	1.74	0.52
1:A:587:G:N2	1:A:754:C:OP2	2.39	0.52
13:M:19:LEU:HD21	13:M:56:LEU:HD11	1.91	0.52
14:N:29:ARG:HH12	14:N:41:ARG:HH12	1.56	0.52
3:C:111:LEU:HD22	3:C:146:ALA:HB2	1.90	0.52
4:D:162:LEU:HD12	4:D:178:VAL:HG13	1.90	0.52
21:U:17:THR:HG22	21:U:18:TYR:H	1.75	0.52
1:A:443:C:H42	1:A:491:G:H1	1.57	0.52
1:A:1101:A:H4'	1:A:1102:A:O5'	2.08	0.52
1:A:1111:A:N1	3:C:177:THR:HG23	2.25	0.52
4:D:102:ASP:OD1	4:D:103:ASN:N	2.43	0.52
18:R:44:LEU:HD21	18:R:70:ILE:HD13	1.90	0.52
1:A:1065:U:O2'	1:A:1066:C:OP2	2.23	0.52
3:C:181:ASN:O	3:C:181:ASN:ND2	2.41	0.52
3:C:195:VAL:C	3:C:196:LEU:HD23	2.34	0.52
7:G:46:ALA:O	7:G:50:ILE:HG12	2.10	0.52
1:A:1000:U:H2'	1:A:1001:A:C8	2.45	0.52
5:E:7:GLU:CD	5:E:37:ARG:HE	2.17	0.52
1:A:79:G:N1	1:A:91:C:C4	2.78	0.52
1:A:1241:G:H2'	1:A:1242:C:C6	2.44	0.52
1:A:1255:G:OP1	3:C:26:LYS:NZ	2.33	0.52
6:F:7:ASN:HB2	6:F:89:MET:O	2.09	0.52
14:N:53:LEU:HD12	14:N:56:VAL:HG21	1.91	0.52
1:A:131:C:O2'	1:A:132:C:O5'	2.26	0.52
1:A:1140:C:H2'	1:A:1141:C:H6	1.75	0.52
6:F:12:PRO:HG3	6:F:57:GLN:HB2	1.92	0.52
20:T:39:LYS:HG2	20:T:55:ILE:HD13	1.91	0.52
1:A:278:G:OP2	17:Q:41:LYS:NZ	2.33	0.52
1:A:881:G:H2'	1:A:882:C:O4'	2.10	0.52
1:A:912:C:H5''	12:L:46:LYS:HE3	1.92	0.52
1:A:1356:G:H2'	1:A:1357:A:H8	1.74	0.52
15:O:25:THR:O	15:O:29:VAL:HG23	2.10	0.52
17:Q:31:LEU:HD23	17:Q:32:TYR:CE2	2.44	0.52
16:P:4:ILE:HG13	16:P:64:ALA:HB1	1.92	0.52
1:A:979:C:N4	14:N:18:VAL:O	2.30	0.51
2:B:167:PRO:HG2	2:B:192:SER:CB	2.41	0.51
4:D:60:GLU:HA	4:D:60:GLU:OE1	2.10	0.51
16:P:57:ARG:HG2	16:P:57:ARG:HH11	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:C:H2'	1:A:93:G:C8	2.45	0.51
1:A:940:C:OP1	7:G:102:ARG:HD3	2.10	0.51
3:C:77:ILE:HG12	3:C:103:VAL:HG21	1.91	0.51
3:C:130:VAL:HG21	3:C:157:ILE:HG23	1.92	0.51
1:A:392:G:H2'	1:A:393:A:C8	2.46	0.51
1:A:627:G:H2'	1:A:628:G:H8	1.75	0.51
2:B:32:ILE:HG21	2:B:40:HIS:HB3	1.92	0.51
11:K:121:PRO:HB2	11:K:125:PHE:HB2	1.92	0.51
1:A:234:C:H2'	1:A:235:C:C6	2.45	0.51
1:A:1157:A:H1'	1:A:1181:G:N2	2.25	0.51
2:B:217:ARG:O	2:B:220:ASP:HB2	2.09	0.51
5:E:107:ARG:O	5:E:111:GLU:HB2	2.10	0.51
14:N:47:LEU:HB3	14:N:53:LEU:HD23	1.92	0.51
1:A:74:C:C4	1:A:75:G:N7	2.78	0.51
1:A:552:U:H2'	1:A:553:A:C8	2.46	0.51
8:H:102:ARG:H	8:H:102:ARG:HD2	1.75	0.51
10:J:64:GLU:HB3	14:N:59:ALA:HB2	1.90	0.51
17:Q:59:ILE:HG23	17:Q:71:PHE:HB3	1.93	0.51
21:U:10:ARG:HG2	21:U:13:ILE:HD12	1.92	0.51
1:A:56:U:H2'	1:A:57:G:H8	1.75	0.51
1:A:833:U:H2'	1:A:834:C:H6	1.76	0.51
1:A:1035:A:H2'	1:A:1036:G:C8	2.45	0.51
1:A:1125:U:H3'	1:A:1126:U:C5	2.45	0.51
1:A:1305:G:OP1	21:U:2:GLY:N	2.44	0.51
1:A:1495:U:OP1	24:A:1717:HYG:N36	2.43	0.51
1:A:818:G:O2'	1:A:819:A:H5''	2.11	0.51
16:P:15:PRO:HG2	16:P:41:PRO:HG2	1.93	0.51
1:A:285:G:N3	1:A:286:G:C8	2.79	0.51
1:A:447:G:H2'	1:A:485:G:N2	2.26	0.51
1:A:1179:A:H2'	1:A:1180:A:O4'	2.10	0.51
1:A:1325:C:O3'	21:U:17:THR:HG21	2.10	0.51
1:A:1488:G:H2'	1:A:1489:G:C8	2.46	0.51
2:B:91:PRO:HG2	2:B:155:LEU:CD2	2.40	0.51
3:C:105:GLU:HG2	3:C:106:VAL:H	1.75	0.51
3:C:134:ILE:O	3:C:138:VAL:HG23	2.11	0.51
8:H:4:ASP:OD2	8:H:85:ARG:NH1	2.44	0.51
1:A:79:G:C2	1:A:80:G:C8	2.99	0.51
1:A:92:C:H2'	1:A:93:G:H8	1.75	0.51
1:A:216:G:O2'	1:A:217:C:O4'	2.28	0.51
5:E:71:LEU:HD11	5:E:113:ALA:O	2.10	0.51
6:F:82:ARG:HB2	6:F:85:VAL:HG23	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:46:LYS:HG2	12:L:47:LYS:H	1.75	0.51
13:M:101:GLN:N	13:M:101:GLN:OE1	2.44	0.51
17:Q:24:GLU:HA	17:Q:39:SER:HB3	1.93	0.51
1:A:953:G:H5'	1:A:965:A:H61	1.76	0.50
3:C:50:ALA:O	3:C:72:LYS:N	2.44	0.50
5:E:75:THR:OG1	5:E:76:ILE:N	2.43	0.50
1:A:75:G:C6	1:A:76:C:C4	2.99	0.50
1:A:184:G:H2'	1:A:185:A:C8	2.47	0.50
1:A:1201:A:H4'	1:A:1202:G:O5'	2.11	0.50
2:B:101:MET:C	2:B:102:LEU:HD12	2.36	0.50
1:A:981:U:H5'	14:N:21:TYR:CE1	2.45	0.50
1:A:1435:G:H2'	1:A:1436:U:H6	1.75	0.50
7:G:5:ARG:HG3	7:G:7:ALA:H	1.76	0.50
13:M:6:GLY:HA3	13:M:67:GLU:HG3	1.92	0.50
14:N:27:CYS:SG	14:N:29:ARG:HB2	2.51	0.50
4:D:142:PRO:HA	4:D:185:PHE:HD2	1.77	0.50
8:H:56:LYS:HD2	8:H:56:LYS:N	2.26	0.50
1:A:61:G:H2'	1:A:62:U:O4'	2.11	0.50
1:A:1000:U:H2'	1:A:1001:A:H8	1.76	0.50
2:B:98:LEU:HB2	2:B:101:MET:HG3	1.94	0.50
1:A:369:C:OP2	1:A:388:G:N2	2.44	0.50
1:A:380:G:N2	1:A:382:A:H3'	2.27	0.50
1:A:975:A:H5'	1:A:975:A:H8	1.76	0.50
2:B:167:PRO:HG2	2:B:192:SER:HB3	1.93	0.50
4:D:159:ARG:NH2	4:D:163:GLU:OE2	2.44	0.50
8:H:63:LEU:H	8:H:63:LEU:HD22	1.75	0.50
8:H:64:LYS:HG3	8:H:79:VAL:HG21	1.94	0.50
1:A:1048:G:H2'	1:A:1050:G:H8	1.77	0.50
2:B:54:THR:O	2:B:58:ILE:HG12	2.12	0.50
2:B:97:TRP:CZ2	2:B:101:MET:HB2	2.46	0.50
3:C:27:LYS:O	3:C:30:ARG:NH1	2.44	0.50
8:H:110:ALA:HB3	8:H:121:ASP:HB3	1.93	0.50
14:N:29:ARG:HH12	14:N:41:ARG:NH1	2.10	0.50
21:U:14:TRP:CE3	21:U:15:ARG:HG3	2.46	0.50
8:H:17:THR:O	8:H:78:GLN:NE2	2.42	0.50
1:A:1370:G:C2	1:A:1371:G:N7	2.80	0.50
3:C:11:ARG:NH1	3:C:177:THR:O	2.45	0.50
9:I:24:GLY:H	9:I:60:ASP:HB2	1.77	0.50
11:K:20:TYR:CE1	11:K:83:ILE:HD13	2.47	0.50
16:P:74:LEU:O	16:P:79:VAL:HG23	2.12	0.50
20:T:75:ASN:OD1	20:T:75:ASN:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:10:ARG:O	21:U:13:ILE:HB	2.12	0.50
1:A:35:G:O2'	12:L:118:SER:O	2.24	0.49
4:D:155:LEU:HD23	4:D:156:GLU:N	2.26	0.49
1:A:99:C:H2'	1:A:101:A:C8	2.46	0.49
1:A:234:C:H2'	1:A:235:C:H6	1.76	0.49
1:A:301:G:H2'	1:A:302:G:C8	2.48	0.49
4:D:194:LEU:H	4:D:194:LEU:HD22	1.77	0.49
12:L:31:PRO:HB2	12:L:32:PHE:CE2	2.48	0.49
1:A:41:G:H2'	1:A:42:G:C8	2.47	0.49
1:A:192:U:C1'	20:T:103:GLY:HA2	2.42	0.49
1:A:321:A:H2'	1:A:322:C:C6	2.47	0.49
1:A:1127:G:H5'	9:I:66:ARG:HH22	1.77	0.49
4:D:175:SER:O	4:D:184:LYS:N	2.41	0.49
1:A:584:G:OP2	17:Q:87:LYS:NZ	2.29	0.49
1:A:620:C:C2	4:D:135:LEU:HD22	2.47	0.49
1:A:1121:U:H2'	1:A:1122:U:C6	2.47	0.49
1:A:1411:C:H42	1:A:1490:C:H42	1.60	0.49
2:B:16:HIS:HB3	2:B:44:LEU:HD11	1.94	0.49
11:K:50:TYR:CD2	11:K:54:ARG:HB3	2.47	0.49
1:A:284:G:H2'	1:A:285:G:C8	2.48	0.49
1:A:538:G:H2'	1:A:539:A:H8	1.77	0.49
1:A:1131:G:H2'	1:A:1132:C:C6	2.48	0.49
3:C:155:GLY:O	3:C:196:LEU:HD22	2.13	0.49
4:D:119:GLN:HG3	4:D:123:HIS:ND1	2.27	0.49
13:M:5:ALA:HB2	13:M:61:GLU:HG2	1.93	0.49
13:M:37:THR:HG21	13:M:56:LEU:HD23	1.95	0.49
1:A:130:A:H1'	1:A:263:A:O2'	2.12	0.49
1:A:933:G:OP2	7:G:3:ARG:HB3	2.11	0.49
1:A:1064:G:H1'	1:A:1190:G:H21	1.78	0.49
1:A:1277:C:H2'	1:A:1279:A:H8	1.77	0.49
4:D:22:LYS:HB2	4:D:26:CYS:SG	2.52	0.49
6:F:4:TYR:CZ	6:F:72:VAL:HG21	2.48	0.49
9:I:102:LEU:HD12	9:I:102:LEU:H	1.76	0.49
15:O:26:GLU:OE2	15:O:77:ARG:HD3	2.12	0.49
20:T:43:LEU:HB3	20:T:52:ALA:HB2	1.95	0.49
1:A:149:A:H2'	1:A:150:C:C6	2.48	0.49
1:A:551:U:H2'	1:A:552:U:C6	2.47	0.49
1:A:578:C:O2'	1:A:728:A:N3	2.46	0.49
1:A:629:G:H2'	1:A:630:G:O4'	2.12	0.49
1:A:1127:G:H1	1:A:1145:C:H42	1.60	0.49
3:C:120:VAL:HG12	3:C:124:ILE:HD11	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:45:LEU:HD23	6:F:45:LEU:H	1.77	0.49
1:A:76:C:H2'	1:A:77:G:C8	2.47	0.49
1:A:767:A:H2'	1:A:768:A:O4'	2.12	0.49
1:A:958:A:N6	19:S:77:THR:O	2.45	0.49
1:A:1391:U:H2'	1:A:1392:G:C8	2.48	0.49
5:E:36:ASP:OD1	5:E:38:GLN:N	2.37	0.49
5:E:80:ILE:HA	8:H:104:ARG:NH2	2.28	0.49
1:A:152:A:N6	1:A:170:U:C2	2.81	0.49
1:A:1152:A:H5''	10:J:13:HIS:CE1	2.48	0.49
3:C:73:PRO:HG3	3:C:105:GLU:HB2	1.95	0.49
7:G:2:ALA:HB2	7:G:7:ALA:HB2	1.95	0.49
16:P:67:THR:HG22	16:P:69:THR:H	1.78	0.49
19:S:18:LYS:O	19:S:22:LEU:HG	2.12	0.49
19:S:29:ARG:HB3	19:S:30:LEU:HG	1.95	0.49
1:A:279:A:C5	17:Q:98:LEU:HD12	2.47	0.49
1:A:1358:U:H5'	14:N:35:ARG:H	1.77	0.49
5:E:33:VAL:HG12	5:E:112:LEU:HD12	1.94	0.49
6:F:91:VAL:HG21	18:R:72:ARG:CZ	2.43	0.49
1:A:292:G:H5''	1:A:293:G:OP2	2.12	0.48
1:A:432:A:H2'	1:A:433:C:O4'	2.13	0.48
1:A:1477:C:H2'	1:A:1478:C:C6	2.48	0.48
2:B:101:MET:HA	2:B:108:ILE:HG13	1.95	0.48
2:B:103:THR:HG23	2:B:176:GLU:HG3	1.94	0.48
2:B:114:ARG:O	2:B:117:GLU:HB2	2.13	0.48
3:C:30:ARG:HD3	3:C:30:ARG:H	1.78	0.48
4:D:196:LEU:O	4:D:198:VAL:N	2.44	0.48
7:G:47:CYS:HA	7:G:50:ILE:HG12	1.95	0.48
1:A:356:A:N3	1:A:368:U:O2'	2.41	0.48
1:A:1202:G:C2	14:N:42:ILE:HG21	2.48	0.48
1:A:1217:C:OP1	14:N:5:ALA:HB1	2.13	0.48
1:A:1502:A:C2	1:A:1504:G:C2	3.01	0.48
8:H:104:ARG:CZ	8:H:138:TRP:CZ2	2.97	0.48
13:M:22:ILE:CG2	13:M:25:ILE:HB	2.43	0.48
18:R:44:LEU:HD13	18:R:48:GLY:O	2.13	0.48
1:A:457:C:C2	1:A:458:C:C5	3.01	0.48
2:B:128:GLU:CD	2:B:128:GLU:H	2.20	0.48
3:C:13:GLY:HA3	14:N:57:ARG:CZ	2.43	0.48
4:D:17:VAL:HG22	4:D:18:LYS:H	1.78	0.48
7:G:111:ARG:HG2	7:G:112:PRO:HD2	1.95	0.48
9:I:43:ALA:HA	9:I:74:ILE:HD13	1.95	0.48
1:A:96:G:H2'	1:A:97:G:H8	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:G:OP1	17:Q:25:ARG:NH2	2.45	0.48
1:A:630:G:H3'	1:A:631:G:H8	1.78	0.48
1:A:753:A:OP1	15:O:69:TYR:OH	2.31	0.48
1:A:809:G:C6	1:A:810:C:C5	3.02	0.48
1:A:860:A:H2'	1:A:861:G:O4'	2.12	0.48
1:A:1250:A:H2'	1:A:1251:A:C8	2.48	0.48
4:D:73:ARG:HA	4:D:73:ARG:HD3	1.71	0.48
1:A:426:G:OP1	4:D:38:TYR:OH	2.27	0.48
1:A:1002:G:H2'	1:A:1003:G:C8	2.48	0.48
2:B:102:LEU:HD23	2:B:182:ILE:HD12	1.96	0.48
7:G:97:GLN:O	7:G:101:LEU:HD23	2.14	0.48
8:H:28:ALA:HB2	8:H:59:LEU:HG	1.94	0.48
1:A:547:A:OP2	4:D:2:GLY:N	2.46	0.48
1:A:1251:A:N3	1:A:1369:C:O2'	2.37	0.48
2:B:31:TYR:HE1	2:B:200:ILE:HG21	1.79	0.48
5:E:81:GLU:CD	5:E:88:LYS:HD3	2.38	0.48
7:G:79:ARG:HG3	7:G:81:GLY:N	2.25	0.48
14:N:6:LEU:HB3	14:N:23:ARG:NH2	2.28	0.48
1:A:1489:G:H2'	1:A:1490:C:C6	2.48	0.48
2:B:91:PRO:HG2	2:B:155:LEU:HD23	1.96	0.48
2:B:135:GLN:O	2:B:139:LYS:HB2	2.13	0.48
11:K:22:HIS:ND1	11:K:22:HIS:C	2.71	0.48
15:O:14:GLU:HG2	15:O:15:PHE:CD1	2.49	0.48
1:A:13:U:O2	1:A:914:A:H3'	2.13	0.48
1:A:1065:U:H5''	1:A:1190:G:N2	2.29	0.48
1:A:1391:U:H2'	1:A:1392:G:H8	1.79	0.48
1:A:1488:G:C5	1:A:1489:G:N7	2.81	0.48
7:G:50:ILE:CG2	7:G:58:PRO:HA	2.43	0.48
1:A:301:G:H2'	1:A:302:G:H8	1.77	0.48
1:A:1030(A):G:N2	1:A:1030(D):A:OP2	2.42	0.48
3:C:188:LEU:HD21	3:C:195:VAL:HB	1.95	0.48
1:A:358:U:H2'	1:A:359:U:H6	1.79	0.48
1:A:457:C:H2'	1:A:458:C:C6	2.48	0.48
1:A:1274:G:H2'	1:A:1275:A:C8	2.49	0.48
4:D:200:GLU:CD	4:D:200:GLU:H	2.22	0.48
10:J:40:LEU:HD22	10:J:41:PRO:HD2	1.96	0.48
10:J:49:VAL:HG13	14:N:41:ARG:HB2	1.95	0.48
19:S:15:LEU:O	19:S:19:VAL:HG12	2.14	0.48
1:A:80:G:H22	1:A:88:A:N6	2.11	0.47
2:B:187:LEU:HD22	2:B:205:ASP:HB3	1.96	0.47
6:F:2:ARG:NE	6:F:69:GLU:HG2	2.22	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:48:ILE:HD12	11:K:63:LEU:HB2	1.96	0.47
15:O:67:LEU:HD23	15:O:67:LEU:HA	1.73	0.47
1:A:830:G:C6	1:A:831:U:C4	3.02	0.47
1:A:838:G:H1	1:A:848:C:N4	2.09	0.47
2:B:124:SER:O	2:B:127:ILE:HG13	2.13	0.47
4:D:120:LEU:HD22	4:D:125:HIS:HB2	1.96	0.47
1:A:24:U:H2'	1:A:25:C:C6	2.49	0.47
1:A:575:G:N2	1:A:576:G:N7	2.54	0.47
1:A:1382:C:H2'	1:A:1383:C:H6	1.79	0.47
4:D:190:ASP:H	4:D:193:ASP:CG	2.22	0.47
7:G:50:ILE:HG21	7:G:58:PRO:HA	1.96	0.47
10:J:25:GLU:HA	10:J:28:ARG:HB2	1.96	0.47
11:K:17:GLY:HA3	11:K:77:MET:HE1	1.97	0.47
20:T:45:GLN:HA	20:T:91:LEU:HD12	1.95	0.47
1:A:92:C:C2	1:A:93:G:C8	3.03	0.47
1:A:375:U:H2'	1:A:376:G:H8	1.79	0.47
1:A:854:G:N1	1:A:855:G:N7	2.62	0.47
1:A:990:C:H42	1:A:1215:G:H1	1.61	0.47
1:A:1409:C:H3'	1:A:1410:G:H8	1.79	0.47
2:B:172:ILE:HD12	2:B:172:ILE:H	1.79	0.47
4:D:78:LEU:O	4:D:81:GLU:HB3	2.14	0.47
11:K:14:VAL:HG23	11:K:15:ALA:H	1.79	0.47
11:K:29:ILE:HG12	11:K:30:VAL:N	2.27	0.47
1:A:164:U:H2'	1:A:165:C:H6	1.80	0.47
1:A:410:G:H21	1:A:432:A:H62	1.62	0.47
1:A:854:G:C6	1:A:855:G:N7	2.83	0.47
1:A:1048:G:H2'	1:A:1050:G:C8	2.49	0.47
5:E:36:ASP:CG	5:E:38:GLN:H	2.21	0.47
6:F:44:GLY:HA2	6:F:59:TYR:CE1	2.49	0.47
7:G:38:LEU:O	7:G:42:ILE:HG13	2.15	0.47
8:H:53:VAL:HB	8:H:58:TYR:CD1	2.50	0.47
10:J:54:PHE:CD2	10:J:55:LYS:HG2	2.50	0.47
13:M:88:ARG:HH12	19:S:3:ARG:HD2	1.79	0.47
1:A:718:G:C8	11:K:116:HIS:HB3	2.50	0.47
1:A:966:M2G:HM22	1:A:967:5MC:C2	2.49	0.47
1:A:1314:C:H2'	1:A:1315:U:C6	2.50	0.47
1:A:1370:G:H5''	9:I:109:VAL:HG21	1.97	0.47
7:G:74:GLU:HG2	7:G:91:VAL:HG22	1.96	0.47
1:A:259:G:OP2	20:T:83:ARG:NE	2.48	0.47
1:A:267:C:OP1	17:Q:67:LYS:HE3	2.15	0.47
1:A:385:C:H2'	1:A:386:C:H6	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:636:U:H2'	1:A:637:G:C8	2.49	0.47
1:A:750:G:N3	15:O:23:GLY:HA3	2.30	0.47
1:A:950:U:H2'	1:A:951:G:C8	2.49	0.47
1:A:975:A:N6	1:A:1367:C:O4'	2.48	0.47
1:A:1061:G:N7	3:C:2:GLY:HA2	2.30	0.47
1:A:1326:C:OP2	21:U:6:ARG:NH2	2.40	0.47
1:A:1400:5MC:H3'	1:A:1401:G:H5'	1.97	0.47
1:A:1425:U:C2	1:A:1426:C:C5	3.03	0.47
2:B:54:THR:OG1	2:B:199:TYR:HB3	2.15	0.47
3:C:51:GLY:HA3	3:C:71:ALA:HB3	1.97	0.47
8:H:85:ARG:NH1	8:H:88:LYS:HA	2.30	0.47
10:J:51:ARG:HH21	10:J:61:GLU:HB2	1.80	0.47
11:K:90:GLY:HA2	11:K:93:GLN:HB2	1.97	0.47
19:S:22:LEU:HD13	19:S:28:LYS:HD2	1.96	0.47
19:S:62:ILE:HD12	19:S:66:MET:HE2	1.95	0.47
20:T:64:ASP:O	20:T:67:ALA:HB3	2.15	0.47
1:A:70:G:H2'	1:A:73:C:C6	2.50	0.47
1:A:114:U:H2'	1:A:115:G:C8	2.50	0.47
1:A:244:U:H4'	1:A:245:C:H5''	1.97	0.47
1:A:745:C:H2'	1:A:746:A:C8	2.50	0.47
1:A:1015:A:H2'	1:A:1016:A:C8	2.49	0.47
5:E:13:ILE:HG22	5:E:30:ALA:HA	1.95	0.47
1:A:555:C:H2'	1:A:556:C:C6	2.50	0.47
9:I:32:ASP:OD1	9:I:33:PHE:N	2.48	0.47
1:A:266:G:H5''	1:A:267:C:C5	2.50	0.47
1:A:803:G:C6	1:A:804:U:N3	2.83	0.47
1:A:1465:C:H2'	1:A:1466:C:O4'	2.15	0.47
1:A:1520:G:H2'	1:A:1521:G:H8	1.80	0.47
1:A:283:C:C2	1:A:284:G:C8	3.02	0.46
1:A:815:A:N6	1:A:1509:C:H1'	2.30	0.46
1:A:976:G:C8	1:A:1358:U:O2	2.68	0.46
1:A:1409:C:H3'	1:A:1410:G:C8	2.50	0.46
3:C:72:LYS:HB3	3:C:75:VAL:HG23	1.97	0.46
8:H:26:VAL:HG23	8:H:27:PRO:HD2	1.97	0.46
20:T:51:GLU:O	20:T:55:ILE:HG13	2.15	0.46
1:A:424:G:H2'	1:A:425:G:H8	1.79	0.46
1:A:551:U:H2'	1:A:552:U:H6	1.80	0.46
1:A:974:A:OP1	1:A:974:A:H8	1.98	0.46
1:A:977:A:H2'	1:A:978:A:H5'	1.98	0.46
3:C:170:GLN:HG2	3:C:171:GLY:H	1.80	0.46
4:D:23:GLY:HA3	4:D:112:VAL:HG12	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:47:PHE:HB3	14:N:34:TYR:CE2	2.50	0.46
19:S:36:ARG:NH2	19:S:75:ALA:O	2.48	0.46
1:A:617:G:N2	1:A:618:C:N3	2.63	0.46
1:A:689:C:H2'	1:A:690:G:O4'	2.15	0.46
1:A:854:G:C2	1:A:855:G:C8	3.04	0.46
1:A:1080:A:O3'	5:E:16:THR:OG1	2.33	0.46
1:A:1265:G:C6	1:A:1266:G:C6	3.04	0.46
4:D:119:GLN:NE2	4:D:123:HIS:HE1	2.13	0.46
5:E:99:GLY:N	5:E:117:ASP:OD1	2.39	0.46
10:J:52:GLY:HA2	10:J:53:PRO:HD3	1.82	0.46
12:L:49:ASN:HB2	12:L:92:OTD:SB	2.54	0.46
15:O:85:LEU:HA	15:O:85:LEU:HD23	1.40	0.46
18:R:43:PHE:C	18:R:44:LEU:HD23	2.41	0.46
1:A:567:G:H2'	1:A:568:G:O4'	2.16	0.46
3:C:190:ARG:HA	3:C:195:VAL:HG12	1.98	0.46
1:A:269:C:H2'	1:A:270:A:C8	2.50	0.46
1:A:748:C:H4'	1:A:749:C:O5'	2.15	0.46
1:A:1513:A:H2'	1:A:1514:C:C6	2.50	0.46
9:I:89:ASN:HB3	9:I:92:TYR:CZ	2.50	0.46
12:L:78:GLN:H	12:L:81:SER:HB2	1.81	0.46
15:O:18:PHE:CZ	15:O:21:ASP:HB2	2.50	0.46
15:O:45:VAL:HG12	15:O:46:HIS:N	2.30	0.46
1:A:7:G:H5'	1:A:298:A:H5'	1.97	0.46
1:A:110:C:H2'	1:A:111:G:O4'	2.16	0.46
1:A:1117:G:N2	1:A:1180:A:O2'	2.48	0.46
1:A:1130:A:OP1	1:A:1131:G:H8	1.98	0.46
1:A:1245:A:C2	1:A:1293:G:C2	3.04	0.46
3:C:108:ASN:HD21	3:C:144:SER:HB3	1.79	0.46
4:D:101:LEU:O	4:D:105:VAL:HG23	2.15	0.46
4:D:158:ILE:O	4:D:162:LEU:HB2	2.15	0.46
5:E:55:VAL:HG12	5:E:56:GLN:N	2.31	0.46
5:E:87:SER:HB3	5:E:131:ILE:HD13	1.97	0.46
1:A:45:U:H2'	1:A:46:G:C8	2.50	0.46
1:A:794:A:C6	1:A:795:C:C4	3.03	0.46
2:B:157:ARG:HG2	2:B:158:LEU:N	2.31	0.46
3:C:24:ALA:HB3	3:C:29:TYR:CD1	2.51	0.46
4:D:78:LEU:HD22	4:D:78:LEU:HA	1.84	0.46
7:G:40:ALA:HB1	9:I:41:VAL:HG21	1.98	0.46
1:A:7:G:H5'	1:A:298:A:O4'	2.16	0.46
1:A:8:A:H5'	5:E:101:ILE:HG22	1.97	0.46
1:A:186:C:H2'	1:A:187:C:C6	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:C:H2'	1:A:386:C:C6	2.50	0.46
1:A:1407:5MC:H2'	1:A:1408:A:O4'	2.16	0.46
24:A:1717:HYG:H341	24:A:1717:HYG:H13	1.98	0.46
7:G:75:VAL:HG21	7:G:86:GLN:HB3	1.97	0.46
7:G:90:GLU:HG2	7:G:91:VAL:N	2.31	0.46
12:L:77:LEU:HD21	12:L:107:ALA:HB2	1.97	0.46
13:M:117:VAL:HG12	13:M:118:ALA:H	1.80	0.46
1:A:112:G:O2'	1:A:113:G:H5'	2.15	0.46
1:A:259:G:H2'	1:A:260:G:C8	2.51	0.46
1:A:538:G:H2'	1:A:539:A:C8	2.50	0.46
1:A:620:C:C1'	4:D:135:LEU:HD13	2.45	0.46
1:A:1158:C:H4'	2:B:133:LYS:HG2	1.98	0.46
1:A:1168:A:H2'	1:A:1169:A:C8	2.51	0.46
2:B:73:THR:HG23	2:B:95:GLN:O	2.16	0.46
7:G:9:VAL:HG13	7:G:94:ARG:HH12	1.80	0.46
7:G:31:MET:SD	7:G:34:GLY:HA2	2.56	0.46
1:A:290:C:N4	1:A:310:G:H1	2.07	0.46
1:A:421:U:H5'	1:A:422:C:C5	2.51	0.46
1:A:627:G:H2'	1:A:628:G:C8	2.51	0.46
1:A:833:U:H2'	1:A:834:C:C6	2.50	0.46
4:D:64:LEU:HD12	4:D:75:PHE:CZ	2.50	0.46
9:I:114:TYR:CB	10:J:60:ARG:HG2	2.46	0.46
12:L:44:THR:HA	12:L:45:PRO:HD3	1.77	0.46
1:A:254:G:OP1	17:Q:67:LYS:O	2.35	0.45
1:A:1127:G:H1	1:A:1145:C:N4	2.13	0.45
1:A:1207:2MG:H2'	1:A:1208:C:H6	1.81	0.45
1:A:1316:G:H4'	14:N:18:VAL:CG1	2.45	0.45
5:E:112:LEU:HD23	5:E:112:LEU:HA	1.75	0.45
10:J:14:LYS:HD3	10:J:14:LYS:H	1.81	0.45
1:A:894:G:H2'	1:A:895:G:H8	1.81	0.45
2:B:130:ARG:HD3	2:B:130:ARG:HA	1.78	0.45
4:D:172:PRO:HD2	4:D:173:TRP:CZ3	2.51	0.45
6:F:53:ALA:C	6:F:55:ASP:H	2.23	0.45
13:M:67:GLU:HB3	13:M:68:GLY:H	1.45	0.45
1:A:255:G:C2	1:A:272:C:C2	3.05	0.45
1:A:300:A:H8	1:A:300:A:O5'	2.00	0.45
1:A:667:G:H4'	15:O:51:HIS:ND1	2.32	0.45
1:A:894:G:H2'	1:A:895:G:C8	2.51	0.45
1:A:1249:C:O2'	9:I:73:GLN:NE2	2.49	0.45
17:Q:63:ARG:HG2	17:Q:64:PRO:HD2	1.98	0.45
1:A:358:U:H2'	1:A:359:U:C6	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1151:A:H5'	10:J:40:LEU:O	2.17	0.45
1:A:1354:C:H2'	1:A:1355:G:H8	1.81	0.45
1:A:1363:A:H4'	1:A:1364:U:H2'	1.99	0.45
1:A:1399:C:O2	1:A:1401:G:C5	2.69	0.45
2:B:37:ASN:N	2:B:37:ASN:OD1	2.49	0.45
2:B:218:ALA:O	2:B:222:ILE:HG13	2.15	0.45
4:D:3:ARG:NH1	4:D:5:ILE:HD11	2.31	0.45
5:E:118:ILE:C	5:E:119:LEU:HD23	2.42	0.45
17:Q:58:GLU:O	17:Q:59:ILE:HD13	2.16	0.45
18:R:17:SER:HB3	18:R:55:ARG:CG	2.40	0.45
19:S:50:ALA:HA	19:S:58:VAL:O	2.16	0.45
1:A:1112:C:N3	3:C:178:LEU:HB2	2.31	0.45
1:A:1357:A:H2'	1:A:1358:U:C6	2.52	0.45
2:B:115:LEU:HD12	2:B:145:LEU:HB2	1.97	0.45
3:C:28:GLN:CD	3:C:28:GLN:H	2.24	0.45
3:C:38:ARG:HB3	3:C:94:LEU:HD21	1.98	0.45
10:J:54:PHE:HD2	10:J:55:LYS:HG2	1.81	0.45
17:Q:22:LEU:HD12	17:Q:22:LEU:HA	1.60	0.45
1:A:6:G:H4'	1:A:298:A:H4'	1.97	0.45
1:A:146:G:H2'	1:A:147:G:C8	2.52	0.45
1:A:191:G:N2	20:T:103:GLY:O	2.38	0.45
1:A:201:C:H42	1:A:216:G:H1	1.65	0.45
1:A:532:A:N3	1:A:532:A:H2'	2.32	0.45
1:A:737:A:H2'	1:A:738:C:C6	2.52	0.45
1:A:1092:A:C6	1:A:1093:A:C6	3.05	0.45
1:A:1343:G:H2'	1:A:1344:C:C6	2.51	0.45
1:A:1517:G:H2'	1:A:1518:A:O4'	2.17	0.45
2:B:27:LYS:HD2	2:B:193:ASP:OD2	2.16	0.45
6:F:50:TYR:CE1	18:R:77:GLY:HA2	2.52	0.45
18:R:47:THR:HG22	18:R:48:GLY:H	1.82	0.45
1:A:382:A:H2'	1:A:383:A:C8	2.52	0.45
1:A:491:G:C2	1:A:492:G:C8	3.05	0.45
1:A:1143:G:H2'	1:A:1144:G:C8	2.52	0.45
4:D:25:ARG:HA	4:D:28:SER:HB2	1.98	0.45
1:A:9:G:OP1	5:E:122:GLU:HG3	2.16	0.45
1:A:77:G:C6	1:A:93:G:N1	2.85	0.45
1:A:375:U:H2'	1:A:376:G:C8	2.52	0.45
1:A:524:G:H2'	1:A:525:C:C6	2.52	0.45
1:A:1056:U:O2'	1:A:1057:G:H5'	2.17	0.45
1:A:1130:A:H4'	9:I:20:ARG:NH2	2.31	0.45
8:H:100:ILE:CG2	8:H:125:ARG:HH11	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:10:LEU:HB3	17:Q:32:TYR:CD1	2.52	0.45
12:L:69:TYR:HE2	12:L:71:PRO:HA	1.82	0.45
1:A:42:G:H1	1:A:400:C:H42	1.63	0.45
1:A:113:G:H2'	1:A:114:U:H6	1.82	0.45
1:A:673:G:H5''	6:F:87:ARG:CZ	2.47	0.45
1:A:1372:U:OP1	9:I:71:SER:HB3	2.17	0.45
1:A:1392:G:H21	1:A:1502:A:H8	1.65	0.45
2:B:233:SER:HA	2:B:234:PRO:HD3	1.75	0.45
4:D:36:ARG:HB3	4:D:38:TYR:CE2	2.52	0.45
10:J:47:PHE:HB3	14:N:34:TYR:HE2	1.82	0.45
12:L:47:LYS:HB3	12:L:48:PRO:HD3	1.99	0.45
1:A:599:C:C2	1:A:640:A:C2	3.04	0.45
1:A:663:A:H2'	1:A:664:G:O4'	2.17	0.45
1:A:778:G:H2'	1:A:779:C:O4'	2.17	0.45
1:A:807:A:H2'	1:A:808:C:C6	2.52	0.45
1:A:1349:A:C2	1:A:1374:A:C4	3.05	0.45
1:A:1374:A:C4	1:A:1375:A:C8	3.05	0.45
1:A:1486:G:H2'	1:A:1487:G:O4'	2.17	0.45
1:A:1486:G:O6	1:A:1487:G:C6	2.70	0.45
1:A:1539:C:H2'	1:A:1540:PSU:C6	2.52	0.45
2:B:115:LEU:HD12	2:B:145:LEU:CB	2.47	0.45
11:K:73:MET:HG3	11:K:103:LEU:HD21	1.99	0.45
16:P:60:LEU:HD23	16:P:60:LEU:HA	1.74	0.45
1:A:241:C:H42	1:A:285:G:H1	1.64	0.44
1:A:1382:C:H2'	1:A:1383:C:C6	2.52	0.44
3:C:178:LEU:C	3:C:180:ALA:H	2.24	0.44
11:K:22:HIS:ND1	11:K:22:HIS:O	2.49	0.44
13:M:82:MET:HB3	13:M:93:ARG:NH1	2.32	0.44
19:S:41:VAL:HG23	19:S:44:MET:HG3	1.99	0.44
1:A:828:A:H2'	1:A:829:G:O4'	2.18	0.44
4:D:120:LEU:HA	4:D:120:LEU:HD23	1.56	0.44
8:H:87:SER:HB2	8:H:93:VAL:HB	1.99	0.44
20:T:62:LEU:HD23	20:T:62:LEU:HA	1.74	0.44
1:A:96:G:H2'	1:A:97:G:C8	2.53	0.44
1:A:103:C:O2'	1:A:172:A:N1	2.50	0.44
1:A:383:A:C5	1:A:384:G:H1'	2.52	0.44
1:A:652:U:O4	1:A:752:G:O2'	2.27	0.44
1:A:1115:C:O2'	1:A:1116:C:H5'	2.18	0.44
1:A:1352:C:H42	1:A:1370:G:H1	1.65	0.44
2:B:28:PHE:CD2	2:B:190:THR:HA	2.52	0.44
3:C:120:VAL:O	3:C:124:ILE:HG13	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:91:VAL:HG21	18:R:72:ARG:NH1	2.33	0.44
17:Q:43:LEU:HD23	17:Q:43:LEU:HA	1.68	0.44
21:U:5:ASP:HB3	21:U:8:THR:OG1	2.17	0.44
1:A:253:U:H2'	1:A:254:G:C8	2.52	0.44
1:A:597:G:H2'	1:A:598:U:H5'	1.98	0.44
1:A:854:G:H3'	1:A:871:U:O4	2.17	0.44
1:A:1309:G:N2	1:A:1329:A:H1'	2.32	0.44
5:E:5:ASP:CG	5:E:6:PHE:H	2.26	0.44
18:R:59:SER:H	18:R:62:GLU:HB2	1.82	0.44
1:A:409:G:H1	1:A:433:C:H42	1.65	0.44
1:A:701:C:O2	1:A:703:G:N1	2.50	0.44
1:A:923:A:OP1	5:E:21:ALA:HB2	2.17	0.44
10:J:60:ARG:N	10:J:60:ARG:HD2	2.32	0.44
11:K:34:ASP:HB2	11:K:35:PRO:HD2	1.99	0.44
15:O:3:ILE:H	15:O:3:ILE:HG13	1.53	0.44
20:T:92:LEU:HD23	20:T:92:LEU:HA	1.82	0.44
1:A:1053:G:HO2'	1:A:1199:U:H5	1.66	0.44
3:C:16:ARG:HD2	3:C:16:ARG:HA	1.63	0.44
3:C:147:LYS:HE2	3:C:205:GLY:H	1.81	0.44
12:L:54:LYS:HD2	12:L:54:LYS:N	2.33	0.44
14:N:59:ALA:HB1	14:N:61:TRP:HZ3	1.83	0.44
1:A:137:C:H42	1:A:226:G:H1	1.64	0.44
1:A:922:G:C2	1:A:1396:A:C6	3.05	0.44
1:A:1014:A:H2'	1:A:1015:A:C8	2.53	0.44
1:A:1061:G:H1'	10:J:56:HIS:CE1	2.52	0.44
1:A:1123:A:H4'	10:J:37:PRO:HD2	2.00	0.44
5:E:131:ILE:HD13	5:E:131:ILE:HA	1.56	0.44
5:E:143:ARG:NH1	8:H:77:GLU:OE2	2.51	0.44
11:K:54:ARG:O	11:K:57:THR:OG1	2.36	0.44
13:M:13:LYS:O	13:M:45:VAL:HG23	2.18	0.44
13:M:15:VAL:HG23	13:M:43:THR:O	2.17	0.44
1:A:1249:C:H2'	1:A:1250:A:H5'	2.00	0.44
1:A:1289:A:H2'	1:A:1290:G:H5'	2.00	0.44
3:C:6:HIS:HA	3:C:7:PRO:HD3	1.70	0.44
3:C:178:LEU:HD13	3:C:178:LEU:HA	1.82	0.44
4:D:98:GLU:HG2	4:D:189:PRO:HG3	2.00	0.44
16:P:38:TYR:O	16:P:49:LEU:HD12	2.18	0.44
18:R:39:VAL:HG13	18:R:40:LEU:HD23	2.00	0.44
20:T:67:ALA:O	20:T:73:HIS:ND1	2.50	0.44
1:A:758:G:O5'	1:A:758:G:H8	2.00	0.44
24:A:1717:HYG:H103	24:A:1717:HYG:H32A	1.68	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:116:VAL:O	3:C:120:VAL:HG23	2.18	0.44
9:I:28:VAL:HG12	9:I:29:ASN:OD1	2.17	0.44
9:I:112:LYS:HG2	9:I:113:LYS:N	2.32	0.44
17:Q:75:ARG:NH2	17:Q:77:VAL:HG13	2.33	0.44
1:A:98:U:H2'	1:A:99:C:C6	2.52	0.43
1:A:419:C:N4	1:A:424:G:H1	2.12	0.43
1:A:928:G:H5''	1:A:1533:C:H41	1.82	0.43
1:A:953:G:C5'	1:A:965:A:H61	2.30	0.43
2:B:98:LEU:HB2	2:B:101:MET:HE3	2.00	0.43
8:H:105:ARG:HD2	8:H:105:ARG:HA	1.81	0.43
12:L:77:LEU:HD23	12:L:77:LEU:HA	1.88	0.43
13:M:8:GLU:OE2	13:M:22:ILE:HA	2.18	0.43
19:S:36:ARG:HH21	19:S:75:ALA:HB3	1.83	0.43
1:A:285:G:C2	1:A:286:G:C8	3.07	0.43
1:A:376:G:N3	1:A:389:A:C2	2.86	0.43
1:A:393:A:C2	1:A:394:G:C8	3.07	0.43
1:A:394:G:H2'	1:A:395:C:C6	2.53	0.43
1:A:716:A:C6	1:A:717:C:C4	3.06	0.43
1:A:1228:C:OP1	13:M:108:ARG:NH2	2.46	0.43
1:A:1486:G:N1	1:A:1487:G:C2	2.86	0.43
3:C:25:GLY:O	3:C:29:TYR:HB2	2.18	0.43
3:C:29:TYR:CE2	3:C:33:LEU:HD23	2.53	0.43
6:F:18:GLN:O	6:F:22:GLU:HG2	2.18	0.43
8:H:28:ALA:CB	8:H:59:LEU:HG	2.49	0.43
8:H:95:VAL:HG11	8:H:100:ILE:HA	1.99	0.43
19:S:40:ILE:HD13	19:S:62:ILE:HD13	2.00	0.43
1:A:405:U:O4	4:D:2:GLY:HA2	2.18	0.43
1:A:429:U:H1'	1:A:430:A:H5''	2.00	0.43
1:A:517:G:N1	1:A:533:A:OP2	2.49	0.43
1:A:1139:G:H4'	1:A:1140:C:H5'	2.00	0.43
1:A:1372:U:H2'	1:A:1373:G:O4'	2.19	0.43
1:A:1392:G:H2'	1:A:1393:U:H6	1.82	0.43
11:K:16:SER:O	11:K:35:PRO:HD3	2.17	0.43
1:A:630:G:H3'	1:A:631:G:C8	2.54	0.43
1:A:821:G:H2'	1:A:822:C:H6	1.83	0.43
1:A:1001:A:H2'	1:A:1002:G:C8	2.54	0.43
1:A:1342:C:H2'	1:A:1343:G:H8	1.82	0.43
4:D:57:ARG:HG3	4:D:202:LEU:HD13	1.99	0.43
4:D:71:SER:OG	4:D:74:GLN:HB2	2.18	0.43
5:E:80:ILE:HD13	5:E:91:LEU:HB2	2.00	0.43
5:E:142:LEU:HA	5:E:142:LEU:HD23	1.69	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:27:GLN:HA	6:F:30:LEU:HD12	2.01	0.43
15:O:15:PHE:CD2	15:O:30:ALA:HB2	2.53	0.43
1:A:91:C:O2'	1:A:92:C:H5'	2.17	0.43
1:A:500:G:C5	1:A:546:G:N2	2.87	0.43
1:A:1140:C:H2'	1:A:1141:C:C6	2.53	0.43
1:A:1453:G:H5'	1:A:1454:G:OP2	2.18	0.43
20:T:53:LEU:HB2	20:T:100:ILE:HG21	2.00	0.43
1:A:376:G:C4	1:A:389:A:C2	3.07	0.43
1:A:575:G:H4'	1:A:575:G:OP1	2.19	0.43
1:A:636:U:H2'	1:A:637:G:H8	1.83	0.43
1:A:1306:A:C2	1:A:1307:U:H1'	2.52	0.43
2:B:201:ILE:O	2:B:203:GLY:N	2.51	0.43
3:C:20:SER:HA	3:C:57:ILE:O	2.19	0.43
4:D:148:VAL:HG11	4:D:158:ILE:HG21	2.00	0.43
14:N:24:CYS:SG	14:N:39:LEU:HA	2.59	0.43
21:U:18:TYR:CE2	21:U:24:ARG:HB3	2.53	0.43
1:A:297:G:N2	1:A:300:A:OP2	2.45	0.43
1:A:665:A:H2'	1:A:732:C:O2	2.17	0.43
1:A:812:C:OP1	1:A:903:G:H1'	2.18	0.43
1:A:895:G:H2'	1:A:896:C:C6	2.54	0.43
1:A:939:G:H2'	1:A:940:C:C6	2.54	0.43
1:A:1076:C:OP2	2:B:179:LYS:NZ	2.52	0.43
1:A:1089:G:H1	1:A:1096:C:H42	1.67	0.43
1:A:1415:G:C2	1:A:1416:G:C8	3.06	0.43
2:B:158:LEU:H	2:B:158:LEU:CD1	2.18	0.43
3:C:50:ALA:HB2	3:C:75:VAL:HB	2.00	0.43
4:D:24:GLU:HG2	4:D:25:ARG:N	2.34	0.43
5:E:46:GLY:H	5:E:58:ALA:HB2	1.84	0.43
5:E:90:VAL:C	5:E:91:LEU:HD23	2.43	0.43
10:J:19:SER:OG	10:J:94:VAL:HG21	2.19	0.43
12:L:113:ARG:HD3	12:L:114:LYS:H	1.83	0.43
13:M:34:LEU:HD12	13:M:41:PRO:HA	2.01	0.43
19:S:15:LEU:HA	19:S:18:LYS:HB2	1.99	0.43
1:A:44:G:H2'	1:A:45:U:O4'	2.18	0.43
1:A:864:A:H2'	1:A:865:A:C8	2.53	0.43
1:A:1027:C:H4'	1:A:1027:C:OP1	2.19	0.43
1:A:1399:C:C2	1:A:1401:G:C5	3.07	0.43
4:D:64:LEU:HD12	4:D:75:PHE:HZ	1.83	0.43
5:E:118:ILE:HG12	5:E:119:LEU:N	2.33	0.43
7:G:26:PHE:CE2	7:G:124:LEU:HD21	2.54	0.43
10:J:51:ARG:NH2	10:J:61:GLU:HB2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:80:TYR:CZ	19:S:81:ARG:HB2	2.53	0.43
20:T:100:ILE:HG13	20:T:102:GLY:N	2.34	0.43
1:A:389:A:C5	1:A:390:C:H1'	2.54	0.43
1:A:1068:G:N7	1:A:1094:G:H2'	2.33	0.43
1:A:1248:A:N3	9:I:70:LYS:NZ	2.67	0.43
1:A:1412:C:N4	1:A:1489:G:H1	2.16	0.43
2:B:49:GLU:HG3	2:B:50:GLU:N	2.34	0.43
2:B:89:GLY:H	2:B:226:ARG:HH22	1.67	0.43
4:D:98:GLU:O	4:D:103:ASN:ND2	2.52	0.43
8:H:19:VAL:HG23	8:H:19:VAL:O	2.18	0.43
14:N:25:VAL:HB	14:N:39:LEU:HD23	1.99	0.43
15:O:55:GLY:HA2	15:O:58:MET:HE2	2.01	0.43
17:Q:24:GLU:HG2	17:Q:39:SER:HB3	2.00	0.43
1:A:75:G:C2	1:A:96:G:C2	3.07	0.43
1:A:156:G:H1	1:A:165:C:H42	1.66	0.43
1:A:247:G:OP1	17:Q:100:LYS:HE3	2.18	0.43
1:A:600:C:H42	1:A:638:G:H1	1.67	0.43
1:A:1053:G:N2	1:A:1058:G:O6	2.52	0.43
1:A:1053:G:O2'	1:A:1199:U:H5	2.02	0.43
6:F:100:ASN:ND2	18:R:23:LYS:HG2	2.34	0.43
7:G:26:PHE:HE1	7:G:104:LEU:HB3	1.83	0.43
8:H:23:SER:OG	8:H:24:THR:N	2.52	0.43
8:H:56:LYS:HA	8:H:57:PRO:HD3	1.73	0.43
12:L:20:LYS:NZ	12:L:20:LYS:H	2.17	0.43
15:O:33:THR:HA	15:O:36:ILE:HD12	2.01	0.43
17:Q:27:PHE:CE2	17:Q:36:ILE:HG13	2.54	0.43
20:T:53:LEU:HG	20:T:100:ILE:HG21	2.00	0.43
1:A:8:A:C5	4:D:209:ARG:HB2	2.54	0.42
1:A:109:A:C6	1:A:326:G:C6	3.07	0.42
1:A:204:U:OP2	1:A:204:U:H3'	2.18	0.42
1:A:1377:A:H2'	7:G:7:ALA:CB	2.49	0.42
1:A:1378:C:H2'	1:A:1379:G:O4'	2.18	0.42
1:A:1433:A:N6	1:A:1434:A:C6	2.87	0.42
1:A:1487:G:C2	1:A:1488:G:C4	3.07	0.42
3:C:38:ARG:HD3	3:C:94:LEU:HD11	2.00	0.42
4:D:11:LEU:HD13	4:D:66:ARG:HG3	2.01	0.42
18:R:32:ARG:HH21	18:R:65:ILE:HD11	1.84	0.42
1:A:18:C:H2'	1:A:19:C:O4'	2.20	0.42
1:A:113:G:H2'	1:A:114:U:C6	2.54	0.42
1:A:1225:A:N3	1:A:1225:A:H2'	2.34	0.42
1:A:1419:G:C6	1:A:1420:C:C4	3.07	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1437:C:H2'	1:A:1438:G:C8	2.54	0.42
3:C:53:ALA:HB2	3:C:115:LEU:HD11	2.01	0.42
4:D:24:GLU:H	4:D:112:VAL:CG1	2.32	0.42
5:E:19:MET:SD	5:E:24:ARG:HG2	2.59	0.42
6:F:12:PRO:HD2	6:F:86:ARG:NH1	2.34	0.42
7:G:18:TYR:CG	7:G:59:LEU:HD13	2.54	0.42
7:G:78:ARG:HB3	7:G:87:VAL:HG21	2.00	0.42
11:K:66:LEU:HD23	11:K:66:LEU:HA	1.73	0.42
1:A:237:C:H2'	1:A:238:G:H8	1.84	0.42
1:A:630:G:H5'	1:A:631:G:OP2	2.19	0.42
1:A:936:C:H42	1:A:1379:G:H1	1.66	0.42
1:A:945:G:C2	1:A:1337:G:C2	3.07	0.42
1:A:1006:C:H2'	1:A:1007:C:C6	2.55	0.42
1:A:1040:U:H2'	1:A:1041:A:H8	1.84	0.42
1:A:1389:C:H2'	1:A:1390:U:O4'	2.20	0.42
1:A:1495:U:H2'	1:A:1496:C:O4'	2.19	0.42
9:I:8:GLY:HA3	9:I:79:LEU:HB3	2.01	0.42
10:J:55:LYS:HE3	10:J:55:LYS:HB2	1.63	0.42
15:O:56:LEU:HD12	15:O:59:MET:HE3	2.01	0.42
1:A:60:A:H4'	1:A:61:G:O5'	2.19	0.42
1:A:675:A:O2'	11:K:114:VAL:O	2.37	0.42
1:A:795:C:H5''	1:A:796:C:OP2	2.19	0.42
1:A:973:G:H3'	1:A:974:A:H5''	2.01	0.42
1:A:1064:G:H1'	1:A:1190:G:N2	2.34	0.42
1:A:1427:U:H2'	1:A:1428:A:H8	1.84	0.42
1:A:1486:G:O6	1:A:1487:G:N1	2.52	0.42
3:C:86:VAL:O	3:C:89:GLU:HB3	2.19	0.42
4:D:38:TYR:HA	4:D:39:PRO:HD3	1.91	0.42
5:E:87:SER:HB3	5:E:131:ILE:CD1	2.49	0.42
6:F:8:ILE:HG22	6:F:10:LEU:HG	2.00	0.42
9:I:114:TYR:HB2	10:J:60:ARG:HG2	2.01	0.42
15:O:29:VAL:O	15:O:33:THR:HB	2.19	0.42
18:R:34:TYR:HE1	18:R:35:ARG:HD3	1.84	0.42
1:A:397:A:H5'	1:A:398:C:OP1	2.19	0.42
1:A:1414:U:N3	1:A:1415:G:C8	2.88	0.42
1:A:1490:C:O2'	1:A:1491:G:H5'	2.20	0.42
3:C:131:ARG:HA	3:C:134:ILE:HD12	2.01	0.42
4:D:201:GLN:HE21	4:D:201:GLN:HB3	1.72	0.42
5:E:47:LYS:HB3	5:E:47:LYS:HE2	1.93	0.42
11:K:24:SER:OG	11:K:25:TYR:N	2.47	0.42
16:P:82:GLN:HE21	16:P:82:GLN:HB3	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:40:LYS:HG3	17:Q:41:LYS:N	2.32	0.42
1:A:230:G:H2'	1:A:231:G:O4'	2.19	0.42
1:A:256:U:H2'	1:A:257:G:C8	2.54	0.42
1:A:598:U:H2'	1:A:599:C:C6	2.54	0.42
2:B:98:LEU:HD13	2:B:98:LEU:HA	1.74	0.42
5:E:36:ASP:CG	5:E:38:GLN:HB2	2.44	0.42
6:F:22:GLU:OE2	6:F:82:ARG:HD3	2.19	0.42
8:H:82:HIS:C	8:H:82:HIS:HD2	2.28	0.42
10:J:51:ARG:HB2	10:J:59:SER:HB2	2.01	0.42
13:M:86:CYS:SG	19:S:73:GLU:HB3	2.60	0.42
1:A:278:G:C6	17:Q:95:TYR:CD2	3.05	0.42
1:A:338:A:C6	1:A:339:C:C4	3.08	0.42
1:A:383:A:C6	1:A:384:G:H1'	2.54	0.42
1:A:448:A:OP2	1:A:485:G:N1	2.44	0.42
1:A:556:C:H2'	1:A:557:G:O4'	2.20	0.42
1:A:1393:U:O2'	1:A:1501:C:O2'	2.31	0.42
1:A:1408:A:H3'	1:A:1409:C:H5''	2.01	0.42
3:C:14:ILE:HG22	3:C:15:THR:HG23	2.01	0.42
4:D:18:LYS:HE3	4:D:20:TYR:CE2	2.55	0.42
4:D:21:LEU:HD11	4:D:66:ARG:O	2.19	0.42
4:D:155:LEU:HD23	4:D:156:GLU:H	1.84	0.42
5:E:144:THR:HG23	5:E:147:ASP:OD2	2.20	0.42
6:F:86:ARG:O	6:F:87:ARG:HG2	2.20	0.42
8:H:19:VAL:HG22	8:H:21:LYS:HG3	2.02	0.42
13:M:27:LYS:HE3	21:U:21:TYR:CE2	2.45	0.42
20:T:15:ARG:HD3	20:T:15:ARG:HA	1.86	0.42
1:A:79:G:C2	1:A:91:C:C2	3.08	0.42
1:A:500:G:C6	1:A:546:G:C2	3.07	0.42
1:A:826:C:O2	8:H:15:ASN:ND2	2.53	0.42
1:A:859:A:H2'	1:A:860:A:O4'	2.19	0.42
2:B:83:MET:HB3	2:B:83:MET:HE2	1.73	0.42
2:B:102:LEU:HB3	2:B:180:LEU:HD12	2.01	0.42
2:B:174:VAL:HG12	2:B:175:ARG:N	2.34	0.42
2:B:221:LEU:HD22	2:B:221:LEU:HA	1.75	0.42
3:C:148:GLY:HA3	3:C:172:ARG:O	2.20	0.42
4:D:31:CYS:C	4:D:33:MET:N	2.77	0.42
1:A:93:G:C6	1:A:95:U:C4	3.07	0.42
1:A:1116:C:H2'	1:A:1117:G:H5''	2.01	0.42
1:A:1434:A:H2'	1:A:1435:G:O4'	2.19	0.42
2:B:74:LYS:HE3	2:B:166:ASP:HB2	2.02	0.42
3:C:47:LEU:HD11	3:C:87:LEU:HD13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:104:LEU:HD23	7:G:104:LEU:HA	1.66	0.42
15:O:43:LEU:HD23	15:O:43:LEU:HA	1.74	0.42
1:A:140:A:H2'	1:A:141:A:O4'	2.20	0.42
1:A:969:A:H4'	10:J:55:LYS:HZ3	1.84	0.42
1:A:1095:U:OP1	1:A:1108:G:N2	2.51	0.42
1:A:1308:U:OP2	13:M:99:ARG:HG3	2.20	0.42
2:B:48:MET:HA	2:B:51:LEU:HD12	2.02	0.42
2:B:132:LYS:HA	2:B:135:GLN:HB2	2.01	0.42
4:D:8:VAL:O	4:D:10:ARG:N	2.53	0.42
4:D:125:HIS:O	4:D:126:ILE:HD13	2.19	0.42
5:E:106:PRO:O	5:E:107:ARG:C	2.63	0.42
7:G:87:VAL:HA	7:G:88:PRO:HD3	1.81	0.42
9:I:118:LYS:C	9:I:120:ARG:H	2.24	0.42
20:T:43:LEU:HA	20:T:43:LEU:HD13	1.81	0.42
1:A:266:G:H8	1:A:266:G:H2'	1.61	0.41
1:A:324:G:OP1	20:T:22:ARG:NH1	2.52	0.41
1:A:570:G:H1'	1:A:820:U:C4	2.55	0.41
1:A:1103:C:H5'	2:B:98:LEU:HD12	2.02	0.41
1:A:1116:C:O2'	9:I:108:VAL:HG21	2.20	0.41
1:A:1250:A:C6	1:A:1251:A:C6	3.08	0.41
2:B:122:PHE:HE1	2:B:139:LYS:NZ	2.18	0.41
2:B:212:GLN:NE2	2:B:235:SER:HB2	2.32	0.41
6:F:97:PHE:CZ	18:R:61:LYS:HE3	2.54	0.41
11:K:38:ASN:HA	11:K:39:PRO:HD3	1.76	0.41
11:K:81:ASP:OD2	11:K:106:LYS:HB2	2.18	0.41
13:M:34:LEU:HD13	13:M:39:ILE:O	2.19	0.41
17:Q:67:LYS:HA	17:Q:70:ARG:HH12	1.85	0.41
1:A:145:G:H1	1:A:177:C:H42	1.67	0.41
1:A:926:G:C6	1:A:1505:G:C6	3.08	0.41
1:A:1098:C:H2'	1:A:1099:G:O4'	2.20	0.41
1:A:1286:A:H2	21:U:22:ARG:HH22	1.66	0.41
2:B:68:ILE:O	2:B:90:MET:HB3	2.20	0.41
3:C:10:PHE:CE1	3:C:178:LEU:HD11	2.55	0.41
5:E:76:ILE:HA	5:E:77:PRO:HD2	1.83	0.41
8:H:51:VAL:HG23	8:H:52:ASP:N	2.35	0.41
9:I:45:ALA:O	9:I:48:GLU:HB2	2.20	0.41
12:L:10:LEU:HD23	17:Q:32:TYR:CE1	2.55	0.41
14:N:6:LEU:HD13	14:N:6:LEU:HA	1.75	0.41
1:A:243:A:H4'	1:A:244:U:H5''	2.02	0.41
1:A:583:A:H2'	1:A:584:G:O4'	2.20	0.41
1:A:673:G:O3'	6:F:87:ARG:NH2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:836:G:H5''	1:A:836:G:H8	1.85	0.41
1:A:958:A:C2	19:S:55:LYS:HB2	2.56	0.41
1:A:1077:G:N2	1:A:1081:G:C4	2.87	0.41
1:A:1399:C:C2	1:A:1502:A:N6	2.88	0.41
5:E:33:VAL:HG11	5:E:109:ILE:HA	2.02	0.41
5:E:76:ILE:O	5:E:93:PRO:HB3	2.20	0.41
6:F:42:GLU:OE1	6:F:59:TYR:OH	2.31	0.41
7:G:51:GLN:HG3	7:G:58:PRO:HG3	2.02	0.41
9:I:17:VAL:HG13	9:I:63:ILE:HG12	2.01	0.41
11:K:57:THR:HG22	11:K:58:PRO:HD2	2.01	0.41
18:R:50:ILE:HG13	18:R:74:ARG:NH2	2.35	0.41
21:U:6:ARG:O	21:U:12:LYS:HE3	2.19	0.41
1:A:6:G:H2'	5:E:119:LEU:HD11	2.02	0.41
1:A:179:A:H2'	1:A:180:U:C6	2.55	0.41
1:A:237:C:H2'	1:A:238:G:C8	2.56	0.41
1:A:434:U:C4	1:A:435:C:N4	2.88	0.41
1:A:706:A:O2'	11:K:29:ILE:HD11	2.20	0.41
1:A:1070:U:H2'	1:A:1071:C:H6	1.85	0.41
1:A:1101:A:N6	2:B:176:GLU:OE2	2.54	0.41
1:A:1120:G:C2	1:A:1121:U:C2	3.08	0.41
1:A:1203:C:H2'	1:A:1204:A:O4'	2.20	0.41
1:A:1358:U:H5''	14:N:35:ARG:CD	2.48	0.41
3:C:70:VAL:O	3:C:105:GLU:HA	2.20	0.41
3:C:155:GLY:HA2	3:C:164:ARG:O	2.20	0.41
18:R:74:ARG:O	18:R:77:GLY:N	2.39	0.41
20:T:19:SER:OG	20:T:20:LEU:HD23	2.20	0.41
1:A:544:G:C6	1:A:545:C:C4	3.08	0.41
1:A:1190:G:OP1	3:C:4:LYS:HA	2.21	0.41
2:B:97:TRP:HH2	2:B:176:GLU:CD	2.28	0.41
3:C:47:LEU:CD2	3:C:68:VAL:HG11	2.50	0.41
7:G:51:GLN:C	7:G:53:LYS:N	2.73	0.41
8:H:33:GLU:OE1	8:H:50:ARG:NE	2.53	0.41
10:J:86:MET:HG3	10:J:87:THR:H	1.86	0.41
15:O:6:GLU:OE1	15:O:6:GLU:N	2.40	0.41
15:O:57:LEU:HA	15:O:57:LEU:HD12	1.84	0.41
21:U:6:ARG:NH2	21:U:15:ARG:HH21	2.07	0.41
1:A:7:G:C5'	1:A:298:A:H5'	2.50	0.41
1:A:455:C:H6	1:A:455:C:O5'	2.04	0.41
1:A:613:C:H2'	1:A:614:A:H8	1.85	0.41
1:A:790:A:C6	1:A:791:G:C6	3.08	0.41
1:A:945:G:H2'	1:A:945:G:N3	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:3:ARG:HH11	4:D:115:ARG:HE	1.67	0.41
4:D:108:LEU:O	4:D:165:MET:HE2	2.20	0.41
5:E:36:ASP:OD2	5:E:38:GLN:HB2	2.20	0.41
5:E:90:VAL:O	5:E:91:LEU:HD23	2.21	0.41
7:G:9:VAL:HG12	7:G:10:ARG:O	2.20	0.41
10:J:39:PRO:HA	10:J:70:ARG:NH1	2.36	0.41
17:Q:44:ALA:HA	17:Q:71:PHE:O	2.20	0.41
1:A:617:G:H1	1:A:623:C:H42	1.69	0.41
1:A:1057:G:H5''	3:C:154:SER:CB	2.51	0.41
1:A:1243:C:H42	1:A:1294:G:H1	1.68	0.41
1:A:1326:C:H2'	1:A:1327:C:C6	2.55	0.41
2:B:48:MET:HE2	2:B:48:MET:HB3	1.92	0.41
2:B:185:ILE:HA	2:B:199:TYR:O	2.21	0.41
4:D:64:LEU:HD22	4:D:64:LEU:HA	1.82	0.41
13:M:13:LYS:HB2	13:M:18:ALA:HB2	2.01	0.41
14:N:15:LYS:HG2	14:N:16:PHE:CE1	2.55	0.41
18:R:56:THR:HB	18:R:58:LEU:HG	2.02	0.41
1:A:41:G:H2'	1:A:42:G:H8	1.85	0.41
1:A:115:G:H1'	1:A:116:A:N7	2.35	0.41
1:A:446:G:C6	1:A:447:G:C4	3.08	0.41
1:A:714:G:H2'	1:A:715:A:O4'	2.21	0.41
1:A:1118:C:H1'	1:A:1179:A:C4	2.56	0.41
1:A:1329:A:H2'	1:A:1330:U:O4'	2.21	0.41
2:B:222:ILE:O	2:B:226:ARG:HG3	2.21	0.41
4:D:57:ARG:HB3	4:D:206:PHE:HB2	2.03	0.41
4:D:70:ILE:HG22	4:D:71:SER:O	2.21	0.41
7:G:118:VAL:O	7:G:122:HIS:HB2	2.21	0.41
8:H:39:LEU:O	8:H:42:GLU:N	2.54	0.41
14:N:53:LEU:HA	14:N:54:PRO:HD3	1.91	0.41
1:A:97:G:C2'	1:A:98:U:H5'	2.51	0.41
1:A:264:U:H2'	1:A:265:G:O4'	2.21	0.41
1:A:314:C:O2'	1:A:315:A:H5'	2.20	0.41
1:A:695:A:H61	1:A:797:C:H1'	1.85	0.41
1:A:768:A:C5	1:A:769:G:C8	3.09	0.41
1:A:1206:G:H4'	3:C:192:THR:O	2.21	0.41
1:A:1355:G:H2'	1:A:1356:G:H8	1.86	0.41
1:A:1378:C:C5	1:A:1379:G:C8	3.09	0.41
1:A:1410:G:N1	1:A:1411:C:C4	2.89	0.41
1:A:1486:G:C6	1:A:1487:G:N1	2.89	0.41
4:D:25:ARG:O	4:D:25:ARG:HG2	2.19	0.41
4:D:126:ILE:HD13	4:D:126:ILE:HA	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:27:ILE:HD11	7:G:40:ALA:HA	2.01	0.41
10:J:32:ALA:O	10:J:34:VAL:HG23	2.20	0.41
10:J:76:ASN:HB3	10:J:78:ASN:ND2	2.36	0.41
16:P:74:LEU:HB3	16:P:79:VAL:CG2	2.51	0.41
17:Q:40:LYS:HG2	17:Q:42:TYR:CE1	2.56	0.41
17:Q:84:LEU:HD12	17:Q:84:LEU:H	1.86	0.41
18:R:36:ASN:O	18:R:40:LEU:HG	2.21	0.41
19:S:5:LEU:HG	19:S:9:VAL:HG22	2.03	0.41
1:A:439:A:C4	1:A:497:A:C2	3.09	0.41
1:A:559:A:H4'	1:A:560:U:O5'	2.21	0.41
1:A:688:G:H2'	1:A:689:C:H6	1.85	0.41
1:A:859:A:OP2	1:A:869:G:N1	2.35	0.41
1:A:1345:U:OP1	9:I:120:ARG:NH1	2.50	0.41
1:A:1370:G:O5'	1:A:1370:G:H8	2.04	0.41
2:B:158:LEU:HB3	2:B:159:PRO:HD2	2.03	0.41
6:F:2:ARG:O	6:F:66:GLU:HA	2.21	0.41
7:G:65:ALA:O	7:G:69:VAL:HG23	2.20	0.41
12:L:113:ARG:C	12:L:114:LYS:HD2	2.46	0.41
13:M:48:LEU:HD12	13:M:53:VAL:HG23	2.03	0.41
1:A:76:C:H2'	1:A:77:G:H8	1.84	0.40
1:A:129(A):G:H1'	1:A:190(E):U:H2'	2.03	0.40
1:A:376:G:H5''	16:P:5:ARG:HB2	2.02	0.40
1:A:451:A:O5'	1:A:451:A:H8	2.05	0.40
1:A:522:C:H41	12:L:53:ARG:HH22	1.69	0.40
1:A:707:C:H2'	1:A:708:C:C6	2.56	0.40
1:A:981:U:H5'	14:N:21:TYR:CZ	2.56	0.40
1:A:1518:A:H2'	1:A:1519:A:C8	2.56	0.40
3:C:121:ALA:O	3:C:125:GLU:HG3	2.21	0.40
8:H:6:ILE:O	8:H:10:LEU:HG	2.20	0.40
10:J:49:VAL:HG21	14:N:44:LEU:HD23	2.03	0.40
11:K:73:MET:HE3	11:K:73:MET:HB2	1.98	0.40
12:L:46:LYS:HB3	12:L:92:OTD:H8	2.03	0.40
15:O:26:GLU:CD	15:O:77:ARG:HD3	2.46	0.40
1:A:35:G:C6	1:A:36:C:C4	3.09	0.40
1:A:1003(A):G:H2'	1:A:1004:A:H4'	2.03	0.40
1:A:1328:C:H2'	1:A:1329:A:O4'	2.21	0.40
1:A:1413:A:N1	1:A:1489:G:C2	2.89	0.40
2:B:115:LEU:CD2	2:B:153:ARG:HH21	2.34	0.40
4:D:203:VAL:O	4:D:206:PHE:HB3	2.21	0.40
8:H:127:LEU:HD23	8:H:127:LEU:HA	1.84	0.40
11:K:98:LEU:HD22	11:K:98:LEU:HA	1.61	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:26:LEU:HA	18:R:26:LEU:HD12	1.73	0.40
1:A:285:G:C4	1:A:286:G:C8	3.09	0.40
1:A:401:C:O2'	1:A:621:A:N3	2.48	0.40
1:A:446:G:N2	1:A:489:C:C2	2.89	0.40
1:A:923:A:H8	1:A:923:A:O5'	2.04	0.40
1:A:1148:U:O3'	9:I:14:VAL:HG11	2.22	0.40
1:A:1435:G:H8	1:A:1435:G:O5'	2.03	0.40
1:A:1516:G:N2	1:A:1520:G:C4	2.89	0.40
5:E:86:ALA:O	5:E:125:SER:N	2.51	0.40
7:G:26:PHE:HA	7:G:101:LEU:HD12	2.02	0.40
7:G:51:GLN:HA	7:G:54:THR:O	2.21	0.40
11:K:120:ARG:HH11	11:K:120:ARG:HD3	1.73	0.40
19:S:40:ILE:HD13	19:S:62:ILE:CD1	2.52	0.40
1:A:34:C:H1'	12:L:32:PHE:CZ	2.57	0.40
1:A:258:G:N3	1:A:259:G:C8	2.90	0.40
1:A:1072:G:C5	1:A:1073:U:C4	3.10	0.40
2:B:31:TYR:N	2:B:31:TYR:CD2	2.89	0.40
5:E:98:THR:HG21	5:E:119:LEU:HD21	2.03	0.40
7:G:27:ILE:HA	7:G:30:ILE:HD12	2.04	0.40
15:O:10:LYS:HD2	15:O:10:LYS:HA	1.85	0.40
15:O:30:ALA:HA	15:O:85:LEU:HD11	2.03	0.40
15:O:34:LEU:C	15:O:34:LEU:HD13	2.46	0.40
17:Q:26:GLN:O	17:Q:27:PHE:HB3	2.21	0.40
1:A:36:C:O2'	1:A:501:C:OP1	2.36	0.40
1:A:79:G:C6	1:A:91:C:N4	2.89	0.40
1:A:241:C:N4	1:A:285:G:H1	2.19	0.40
1:A:268:C:H2'	1:A:269:C:H6	1.86	0.40
1:A:1117:G:N2	1:A:1180:A:H1'	2.37	0.40
1:A:1499:A:H1'	1:A:1520:G:H5'	2.02	0.40
2:B:106:LYS:HA	2:B:106:LYS:HD3	1.81	0.40
4:D:68:TYR:OH	4:D:98:GLU:OE1	2.26	0.40
6:F:9:VAL:HG22	6:F:60:PHE:CE2	2.57	0.40
17:Q:9:VAL:O	17:Q:11:VAL:HG13	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1511/1522 (99%)	288 (19%)	0

All (288) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	7	G
1	A	9	G
1	A	32	A
1	A	38	G
1	A	39	G
1	A	47	C
1	A	48	C
1	A	51	A
1	A	54	C
1	A	73	C
1	A	74	C
1	A	77	G
1	A	79	G
1	A	82	U
1	A	88	A
1	A	90	U
1	A	91	C
1	A	98	U
1	A	108	G
1	A	109	A
1	A	115	G
1	A	116	A
1	A	121	C
1	A	129(A)	G
1	A	130	A
1	A	131	C
1	A	132	C
1	A	163	C
1	A	169	C
1	A	178	C
1	A	181	G

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Mol	Chain	Res	Type
1	A	182	U
1	A	188	C
1	A	195	A
1	A	197	A
1	A	201	C
1	A	202	U
1	A	203	U
1	A	204	U
1	A	216	G
1	A	220	G
1	A	231	G
1	A	247	G
1	A	251	G
1	A	266	G
1	A	267	C
1	A	289	G
1	A	292	G
1	A	293	G
1	A	301	G
1	A	319	G
1	A	321	A
1	A	328	C
1	A	329	A
1	A	335	C
1	A	344	A
1	A	345	C
1	A	346	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	382	A
1	A	384	G
1	A	392	G
1	A	396	G
1	A	397	A
1	A	398	C
1	A	406	G
1	A	411	A
1	A	412	A

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Mol	Chain	Res	Type
1	A	413	G
1	A	419	C
1	A	421	U
1	A	424	G
1	A	429	U
1	A	430	A
1	A	433	C
1	A	439	A
1	A	442	C
1	A	452	A
1	A	460	A
1	A	485	G
1	A	497	A
1	A	498	U
1	A	508	C
1	A	511	C
1	A	513	C
1	A	518	C
1	A	519	C
1	A	527	7MG
1	A	528	C
1	A	530	G
1	A	531	U
1	A	532	A
1	A	533	A
1	A	547	A
1	A	548	G
1	A	559	A
1	A	560	U
1	A	563	A
1	A	564	C
1	A	568	G
1	A	572	A
1	A	573	A
1	A	575	G
1	A	576	G
1	A	577	G
1	A	579	G
1	A	587	G
1	A	588	G
1	A	596	C
1	A	624	C

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Mol	Chain	Res	Type
1	A	630	G
1	A	631	G
1	A	632	A
1	A	653	A
1	A	665	A
1	A	687	A
1	A	688	G
1	A	701	C
1	A	702	A
1	A	703	G
1	A	717	C
1	A	721	G
1	A	723	U
1	A	724	G
1	A	731	G
1	A	734	G
1	A	749	C
1	A	755	G
1	A	760	G
1	A	773	G
1	A	774	G
1	A	777	A
1	A	781	A
1	A	785	G
1	A	787	A
1	A	792	A
1	A	793	U
1	A	794	A
1	A	812	C
1	A	813	U
1	A	816	A
1	A	817	C
1	A	818	G
1	A	819	A
1	A	826	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	876	G

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Mol	Chain	Res	Type
1	A	884	U
1	A	889	A
1	A	902	G
1	A	926	G
1	A	927	G
1	A	934	C
1	A	935	A
1	A	950	U
1	A	960	U
1	A	961	U
1	A	966	M2G
1	A	967	5MC
1	A	969	A
1	A	972	C
1	A	974	A
1	A	975	A
1	A	976	G
1	A	977	A
1	A	978	A
1	A	982	U
1	A	991	U
1	A	992	U
1	A	993	G
1	A	1004	A
1	A	1005	A
1	A	1025	U
1	A	1027	C
1	A	1028	C
1	A	1031	G
1	A	1054	C
1	A	1055	A
1	A	1060	C
1	A	1064	G
1	A	1065	U
1	A	1066	C
1	A	1078	U
1	A	1092	A
1	A	1094	G
1	A	1095	U
1	A	1096	C
1	A	1101	A
1	A	1111	A

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Mol	Chain	Res	Type
1	A	1117	G
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	1137	C
1	A	1138	G
1	A	1139	G
1	A	1140	C
1	A	1143	G
1	A	1144	G
1	A	1145	C
1	A	1152	A
1	A	1154	G
1	A	1159	U
1	A	1160	G
1	A	1164	G
1	A	1171	G
1	A	1191	A
1	A	1196	U
1	A	1200	C
1	A	1201	A
1	A	1202	G
1	A	1211	U
1	A	1212	U
1	A	1213	A
1	A	1214	C
1	A	1225	A
1	A	1238	A
1	A	1241	G
1	A	1242	C
1	A	1245	A
1	A	1253	G
1	A	1257	U
1	A	1258	G
1	A	1261	A
1	A	1270	C
1	A	1280	A
1	A	1286	A
1	A	1287	A

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Mol	Chain	Res	Type
1	A	1297	C
1	A	1300	G
1	A	1302	U
1	A	1303	C
1	A	1305	G
1	A	1310	G
1	A	1311	G
1	A	1312	G
1	A	1316	G
1	A	1320	C
1	A	1322	C
1	A	1338	G
1	A	1347	G
1	A	1353	G
1	A	1358	U
1	A	1359	C
1	A	1360	A
1	A	1362	C
1	A	1368	G
1	A	1370	G
1	A	1394	A
1	A	1398	A
1	A	1399	C
1	A	1400	5MC
1	A	1402	4OC
1	A	1409	C
1	A	1418	A
1	A	1442	G
1	A	1443	G
1	A	1446	A
1	A	1453	G
1	A	1454	G
1	A	1474	G
1	A	1477	C
1	A	1489	G
1	A	1491	G
1	A	1492	A
1	A	1493	A
1	A	1498	UR3
1	A	1499	A
1	A	1504	G
1	A	1505	G

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Mol	Chain	Res	Type
1	A	1506	U
1	A	1520	G
1	A	1529	G
1	A	1530	G
1	A	1531	A

There are no RNA pucker outliers to report.

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

13 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	516	22,1	18,21,22	1.11	1 (5%)	21,30,33	1.62	3 (14%)
1	7MG	A	527	1	23,26,27	4.08	4 (17%)	27,39,42	2.26	9 (33%)
1	5MC	A	1404	1	19,22,23	0.93	2 (10%)	26,32,35	1.04	4 (15%)
1	UR3	A	1498	1	19,22,23	0.91	1 (5%)	26,32,35	1.14	0
1	5MC	A	1407	1	19,22,23	1.66	3 (15%)	26,32,35	1.28	4 (15%)
1	PSU	A	1541	1	18,21,22	1.11	1 (5%)	21,30,33	1.92	4 (19%)
1	PSU	A	1540	1	18,21,22	1.17	2 (11%)	21,30,33	1.94	6 (28%)
1	M2G	A	966	1	24,27,28	1.32	2 (8%)	33,40,43	0.90	2 (6%)
12	0TD	L	92	12	8,9,10	1.70	1 (12%)	6,11,13	2.64	4 (66%)
1	4OC	A	1402	1	20,23,24	1.13	1 (5%)	25,32,35	0.68	0
1	2MG	A	1207	1	23,26,27	1.51	5 (21%)	33,38,41	1.10	3 (9%)
1	5MC	A	1400	1	19,22,23	1.34	2 (10%)	26,32,35	0.99	1 (3%)
1	5MC	A	967	1	19,22,23	0.95	0	26,32,35	1.02	1 (3%)

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	516	22,1	-	0/7/25/26	0/2/2/2
1	7MG	A	527	1	-	2/7/37/38	0/3/3/3
1	5MC	A	1404	1	-	0/7/25/26	0/2/2/2
1	UR3	A	1498	1	-	2/7/25/26	0/2/2/2
1	5MC	A	1407	1	-	0/7/25/26	0/2/2/2
1	PSU	A	1541	1	-	0/7/25/26	0/2/2/2
1	PSU	A	1540	1	-	0/7/25/26	0/2/2/2
1	M2G	A	966	1	-	4/11/29/30	0/3/3/3
12	0TD	L	92	12	-	2/7/12/14	-
1	4OC	A	1402	1	-	2/9/29/30	0/2/2/2
1	2MG	A	1207	1	-	1/9/27/28	0/3/3/3
1	5MC	A	1400	1	-	6/7/25/26	0/2/2/2
1	5MC	A	967	1	-	2/7/25/26	0/2/2/2

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	527	7MG	C8-N9	-17.79	1.34	1.45
1	A	527	7MG	C5-N7	4.99	1.42	1.35
1	A	1407	5MC	C5-C4	4.88	1.47	1.44
1	A	527	7MG	C2-N2	4.57	1.44	1.34
1	A	966	M2G	C2-N2	4.05	1.42	1.35
1	A	1407	5MC	C2-N1	4.04	1.48	1.40
12	L	92	0TD	CB-CA	-3.94	1.53	1.54
1	A	1540	PSU	C6-C5	3.77	1.39	1.35
1	A	1541	PSU	C6-C5	3.76	1.39	1.35
1	A	1207	2MG	C2-N2	3.73	1.41	1.33
1	A	1400	5MC	C5-C4	3.59	1.46	1.44
1	A	1207	2MG	C2-N1	3.57	1.42	1.36
1	A	516	PSU	C6-C5	3.43	1.39	1.35
1	A	527	7MG	C4-N3	3.21	1.41	1.34
1	A	966	M2G	C4-N3	3.01	1.41	1.34
1	A	1498	UR3	C2-N1	2.71	1.42	1.38
1	A	1207	2MG	C6-N1	2.58	1.43	1.38
1	A	1404	5MC	C2-N3	2.58	1.41	1.36
1	A	1407	5MC	C2-N3	2.54	1.41	1.36
1	A	1402	4OC	C2-N3	2.34	1.41	1.36
1	A	1207	2MG	C4-N3	2.27	1.39	1.34
1	A	1540	PSU	C4-C5	-2.12	1.38	1.44
1	A	1400	5MC	C2-N3	2.12	1.40	1.36
1	A	1207	2MG	C8-N9	2.11	1.42	1.37
1	A	1404	5MC	C5-C4	-2.02	1.42	1.44

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	527	7MG	C5-C6-N1	5.37	120.40	110.94
1	A	1540	PSU	C4-N3-C2	-4.82	119.73	126.37
1	A	1541	PSU	N1-C2-N3	4.78	120.21	115.17
1	A	1541	PSU	C4-N3-C2	-4.73	119.86	126.37
1	A	527	7MG	C2-N3-C4	4.73	120.44	112.30
1	A	1540	PSU	N1-C2-N3	4.57	119.98	115.17
1	A	527	7MG	N9-C4-N3	4.49	132.03	125.46
1	A	516	PSU	C4-N3-C2	-4.23	120.55	126.37
1	A	527	7MG	C5-C4-N3	-4.05	120.53	128.13
1	A	516	PSU	N1-C2-N3	3.82	119.20	115.17
12	L	92	0TD	CSB-SB-CB	-3.51	96.05	102.36
1	A	527	7MG	C6-C5-N7	3.34	137.11	131.93
1	A	1541	PSU	O2-C2-N1	-3.32	119.36	122.79
12	L	92	0TD	OD1-CG-CB	-3.26	115.61	122.44
1	A	527	7MG	C6-C5-C4	-3.11	116.93	122.40
1	A	1407	5MC	N4-C4-N3	-3.09	112.91	118.51
12	L	92	0TD	CB-CA-N	-2.82	103.37	109.10
1	A	527	7MG	C2-N1-C6	-2.80	120.03	125.11
1	A	1540	PSU	O2-C2-N1	-2.76	119.94	122.79
1	A	1404	5MC	C5-C4-N3	2.76	124.58	121.75
1	A	1400	5MC	N4-C4-N3	-2.65	113.70	118.51
1	A	527	7MG	N9-C8-N7	2.63	107.10	103.37
1	A	966	M2G	C5-C4-N3	-2.60	124.25	128.39
1	A	1541	PSU	C6-N1-C2	-2.56	120.32	122.69
1	A	516	PSU	C6-N1-C2	-2.48	120.39	122.69
1	A	1540	PSU	C6-N1-C2	-2.46	120.41	122.69
1	A	527	7MG	O6-C6-C5	-2.43	121.66	127.62
1	A	1207	2MG	C5-C4-N3	-2.41	124.56	128.39
1	A	1407	5MC	C5-C4-N3	2.38	124.19	121.75
12	L	92	0TD	O-C-CA	-2.31	118.82	124.77
1	A	1404	5MC	N4-C4-N3	-2.31	114.32	118.51
1	A	1207	2MG	O6-C6-N1	-2.22	115.93	120.11
1	A	967	5MC	N4-C4-N3	-2.22	114.48	118.51
1	A	1407	5MC	C1'-N1-C6	-2.22	117.50	121.15
1	A	966	M2G	O6-C6-N1	-2.15	116.08	120.11
1	A	1540	PSU	C6-C5-C4	2.15	119.62	118.17
1	A	1207	2MG	N9-C4-N3	2.15	130.24	125.95
1	A	1404	5MC	C4-N3-C2	-2.12	117.87	120.81
1	A	1540	PSU	O4-C4-C5	-2.11	118.77	124.01
1	A	1407	5MC	C5-C6-N1	-2.04	121.09	123.31
1	A	1404	5MC	C5-C6-N1	-2.02	121.12	123.31

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	527	7MG	O4'-C4'-C5'-O5'
1	A	966	M2G	N1-C2-N2-CM1
1	A	1400	5MC	O4'-C4'-C5'-O5'
1	A	1402	4OC	O4'-C4'-C5'-O5'
1	A	527	7MG	C3'-C4'-C5'-O5'
1	A	967	5MC	O4'-C4'-C5'-O5'
1	A	1400	5MC	C3'-C4'-C5'-O5'
1	A	1402	4OC	C3'-C4'-C5'-O5'
1	A	1400	5MC	C2'-C1'-N1-C6
1	A	1400	5MC	C2'-C1'-N1-C2
1	A	967	5MC	C3'-C4'-C5'-O5'
1	A	1498	UR3	O4'-C4'-C5'-O5'
1	A	1498	UR3	C3'-C4'-C5'-O5'
1	A	966	M2G	N3-C2-N2-CM1
12	L	92	0TD	CG-CB-SB-CSB
1	A	1400	5MC	O4'-C1'-N1-C2
1	A	1400	5MC	O4'-C1'-N1-C6
1	A	1207	2MG	O4'-C4'-C5'-O5'
12	L	92	0TD	SB-CB-CG-OD1
1	A	966	M2G	N3-C2-N2-CM2
1	A	966	M2G	N1-C2-N2-CM2

There are no ring outliers.

10 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	527	7MG	1	0
1	A	1404	5MC	1	0
1	A	1498	UR3	1	0
1	A	1407	5MC	1	0
1	A	1540	PSU	1	0
1	A	966	M2G	1	0
12	L	92	0TD	5	0
1	A	1207	2MG	3	0
1	A	1400	5MC	2	0
1	A	967	5MC	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 129 ligands modelled in this entry, 128 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
24	HYG	A	1717	-	36,39,39	1.94	8 (22%)	44,60,60	2.69	14 (31%)

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
24	HYG	A	1717	-	-	6/12/87/87	0/4/4/4

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	1717	HYG	C27-C33	6.55	1.60	1.52
24	A	1717	HYG	C34-C33	3.73	1.58	1.52
24	A	1717	HYG	C5-C4	3.51	1.59	1.52
24	A	1717	HYG	C4-N9	3.23	1.50	1.47
24	A	1717	HYG	C16-C15	3.22	1.59	1.53
24	A	1717	HYG	C13-C12	2.79	1.59	1.52
24	A	1717	HYG	C26-C25	2.22	1.58	1.52
24	A	1717	HYG	O28-C27	-2.04	1.40	1.44

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	1717	HYG	O29-C12-C13	7.25	129.40	110.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	1717	HYG	O18-C13-C12	7.20	123.08	109.09
24	A	1717	HYG	O28-C27-C26	6.21	117.19	108.50
24	A	1717	HYG	C13-O14-C15	4.73	122.96	113.72
24	A	1717	HYG	O14-C15-C16	4.61	118.00	109.70
24	A	1717	HYG	C23-O28-C27	4.53	120.63	112.00
24	A	1717	HYG	C3-C4-C5	3.83	117.79	109.89
24	A	1717	HYG	C26-C25-C24	3.75	116.54	111.18
24	A	1717	HYG	C5-C6-C1	-3.36	106.19	110.86
24	A	1717	HYG	C16-C17-C12	-3.28	105.67	113.50
24	A	1717	HYG	C25-C26-C27	3.18	116.91	109.68
24	A	1717	HYG	O18-C6-C1	2.75	114.23	107.23
24	A	1717	HYG	O35-C34-C33	-2.32	106.52	111.55
24	A	1717	HYG	C3-C2-C1	2.20	113.38	110.08

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	A	1717	HYG	C26-C27-C33-C34
24	A	1717	HYG	O28-C27-C33-C34
24	A	1717	HYG	O14-C13-O18-C6
24	A	1717	HYG	O14-C15-C19-O20
24	A	1717	HYG	C16-C15-C19-O20
24	A	1717	HYG	C12-C13-O18-C6

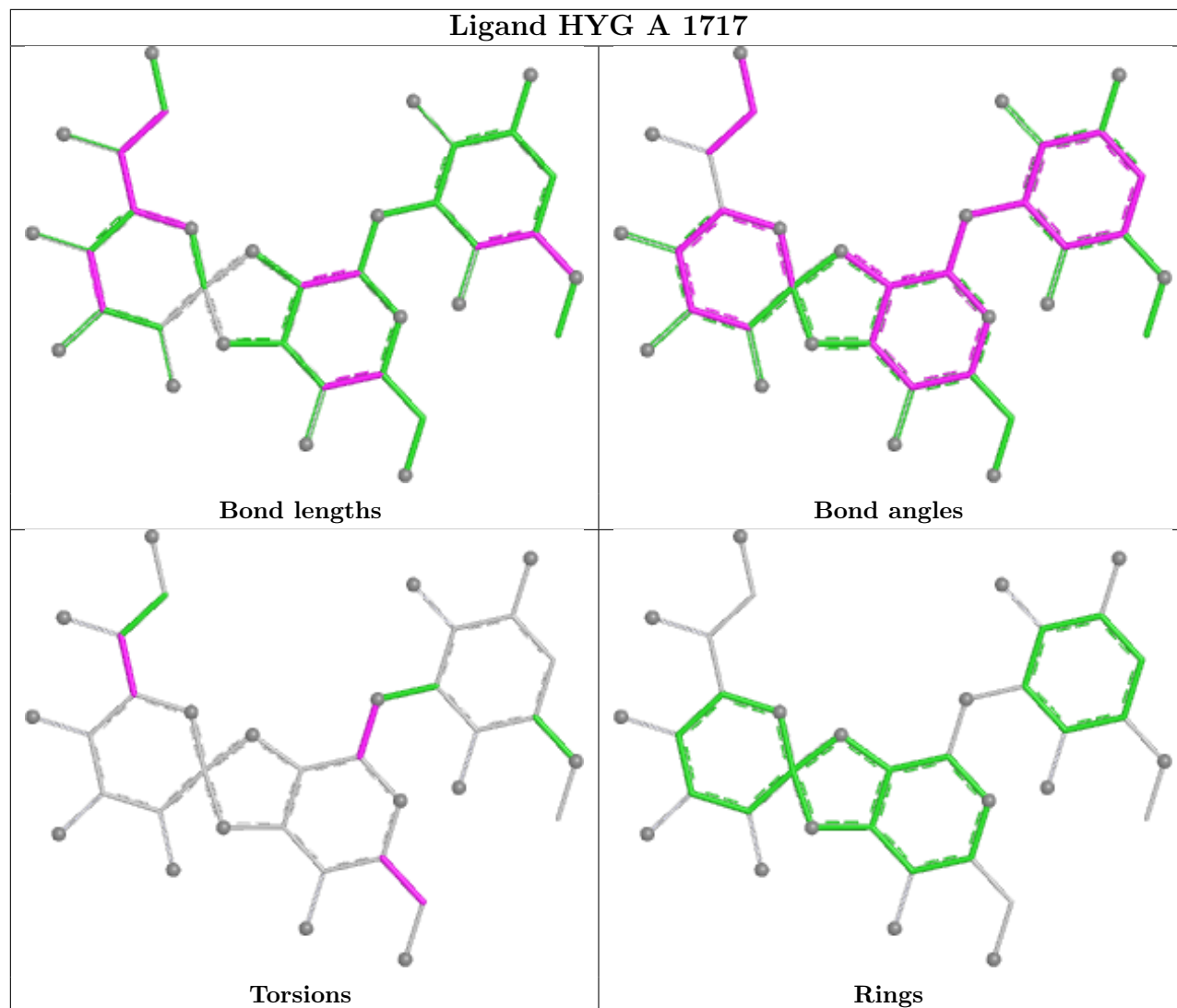
There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	A	1717	HYG	4	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	1501/1522 (98%)	-0.38	20 (1%) 75 52	69, 132, 256, 360	0
2	B	236/256 (92%)	-0.46	2 (0%) 82 62	77, 136, 231, 275	0
3	C	207/239 (86%)	-0.17	4 (1%) 66 44	94, 196, 235, 248	0
4	D	208/209 (99%)	-0.16	10 (4%) 35 26	87, 136, 186, 207	0
5	E	151/162 (93%)	-0.55	0 100 100	62, 100, 148, 192	0
6	F	101/101 (100%)	-0.52	0 100 100	114, 152, 178, 202	0
7	G	155/156 (99%)	-0.25	3 (1%) 66 44	125, 174, 240, 276	0
8	H	138/138 (100%)	-0.67	0 100 100	65, 91, 134, 149	0
9	I	127/128 (99%)	0.01	4 (3%) 51 34	145, 190, 236, 264	0
10	J	99/105 (94%)	-0.02	0 100 100	81, 213, 309, 332	0
11	K	119/129 (92%)	-0.38	2 (1%) 69 46	88, 126, 169, 206	0
12	L	124/135 (91%)	-0.23	3 (2%) 59 40	64, 126, 162, 245	0
13	M	118/126 (93%)	-0.17	4 (3%) 48 32	133, 163, 190, 230	0
14	N	60/61 (98%)	0.41	5 (8%) 17 16	152, 187, 233, 271	0
15	O	88/89 (98%)	-0.48	0 100 100	85, 119, 169, 220	0
16	P	84/88 (95%)	-0.31	0 100 100	89, 128, 167, 247	0
17	Q	99/105 (94%)	-0.45	0 100 100	73, 110, 148, 169	0
18	R	73/88 (82%)	-0.48	0 100 100	82, 126, 207, 231	0
19	S	81/93 (87%)	0.08	5 (6%) 26 21	96, 206, 253, 294	0
20	T	99/106 (93%)	-0.23	3 (3%) 52 35	98, 133, 180, 200	0
21	U	25/27 (92%)	0.58	3 (12%) 9 11	80, 173, 190, 263	0
All	All	3893/4063 (95%)	-0.32	68 (1%) 69 46	62, 141, 236, 360	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
14	N	3	ARG	5.5
1	A	202	U	5.2
20	T	106	ALA	4.9
12	L	73	GLU	4.0
1	A	985	C	3.9
4	D	9	CYS	3.8
4	D	31	CYS	3.7
4	D	2	GLY	3.7
7	G	33	ASP	3.7
9	I	110	GLU	3.6
4	D	21	LEU	3.6
13	M	102	ARG	3.5
1	A	1128	C	3.5
1	A	984	C	3.4
14	N	2	ALA	3.4
7	G	2	ALA	3.3
3	C	155	GLY	3.3
9	I	9	ARG	3.3
1	A	1129	C	3.2
11	K	52	GLY	3.1
1	A	1197	G	3.0
19	S	3	ARG	3.0
21	U	10	ARG	3.0
1	A	1220	G	2.9
19	S	35	SER	2.9
21	U	6	ARG	2.9
4	D	134	ASP	2.8
4	D	119	GLN	2.7
2	B	51	LEU	2.7
19	S	2	PRO	2.7
2	B	13	ALA	2.6
13	M	119	GLY	2.6
3	C	193	TYR	2.6
3	C	103	VAL	2.6
9	I	119	ALA	2.6
21	U	18	TYR	2.5
1	A	1492	A	2.5
19	S	5	LEU	2.5
19	S	4	SER	2.5
1	A	221	C	2.5
1	A	1200	C	2.5
4	D	26	CYS	2.4
9	I	113	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	1144	G	2.4
13	M	104	ARG	2.3
13	M	32	GLU	2.3
1	A	1143	G	2.3
4	D	33	MET	2.3
1	A	74	C	2.3
1	A	75	G	2.3
1	A	222	U	2.3
12	L	47	LYS	2.2
1	A	1289	A	2.2
7	G	62	PHE	2.2
11	K	128	ALA	2.2
1	A	6	G	2.2
14	N	25	VAL	2.2
1	A	1027	C	2.2
12	L	31	PRO	2.2
20	T	12	ALA	2.1
4	D	12	CYS	2.1
1	A	1533	C	2.1
14	N	4	LYS	2.1
1	A	534	U	2.0
4	D	3	ARG	2.0
20	T	11	SER	2.0
3	C	2	GLY	2.0
14	N	35	ARG	2.0

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	0.85	0.12	325,348,352,353	0
1	PSU	A	1541	20/21	0.91	0.10	333,344,359,360	0
1	PSU	A	516	20/21	0.94	0.10	137,146,155,158	0
1	2MG	A	1207	24/25	0.95	0.09	200,220,224,230	0
1	7MG	A	527	24/25	0.96	0.07	97,110,123,130	0
1	5MC	A	1407	21/22	0.96	0.10	142,156,190,190	0
1	UR3	A	1498	21/22	0.96	0.11	115,129,138,150	0
1	M2G	A	966	25/26	0.96	0.09	130,149,169,172	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	5MC	A	967	21/22	0.96	0.07	128,135,143,146	0
1	5MC	A	1400	21/22	0.97	0.06	100,115,125,129	0
1	5MC	A	1404	21/22	0.97	0.06	97,110,130,136	0
12	0TD	L	92	10/11	0.97	0.09	130,150,216,313	0
1	4OC	A	1402	22/23	0.98	0.09	102,122,130,137	0

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
22	MG	A	1711	1/1	0.33	0.27	122,122,122,122	0
22	MG	A	1609	1/1	0.69	0.22	119,119,119,119	0
23	K	A	1704	1/1	0.70	0.22	148,148,148,148	0
22	MG	D	302	1/1	0.73	0.23	112,112,112,112	0
22	MG	A	1709	1/1	0.74	0.20	130,130,130,130	0
22	MG	A	1643	1/1	0.74	0.27	131,131,131,131	0
22	MG	H	202	1/1	0.75	0.14	100,100,100,100	0
22	MG	A	1641	1/1	0.77	0.21	80,80,80,80	0
22	MG	A	1663	1/1	0.79	0.11	107,107,107,107	0
22	MG	A	1715	1/1	0.80	0.06	434,434,434,434	0
22	MG	A	1710	1/1	0.80	0.13	71,71,71,71	0
22	MG	A	1633	1/1	0.81	0.12	92,92,92,92	0
22	MG	A	1666	1/1	0.81	0.20	130,130,130,130	0
22	MG	A	1690	1/1	0.81	0.27	84,84,84,84	0
22	MG	A	1608	1/1	0.81	0.36	70,70,70,70	0
22	MG	A	1629	1/1	0.81	0.21	46,46,46,46	0
23	K	A	1706	1/1	0.81	0.15	146,146,146,146	0
22	MG	A	1610	1/1	0.82	0.30	62,62,62,62	0
22	MG	A	1664	1/1	0.82	0.22	75,75,75,75	0
22	MG	A	1635	1/1	0.82	0.36	74,74,74,74	0
22	MG	A	1713	1/1	0.83	0.15	136,136,136,136	0
22	MG	A	1646	1/1	0.84	0.08	127,127,127,127	0
23	K	A	1699	1/1	0.85	0.24	142,142,142,142	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	MG	D	303	1/1	0.85	0.18	88,88,88,88	0
22	MG	A	1712	1/1	0.85	0.21	88,88,88,88	0
22	MG	A	1619	1/1	0.86	0.21	79,79,79,79	0
23	K	A	1702	1/1	0.86	0.18	161,161,161,161	0
22	MG	H	201	1/1	0.86	0.18	72,72,72,72	0
23	K	A	1705	1/1	0.86	0.17	157,157,157,157	0
22	MG	A	1606	1/1	0.86	0.48	99,99,99,99	0
22	MG	A	1655	1/1	0.87	0.20	102,102,102,102	0
22	MG	A	1658	1/1	0.87	0.34	70,70,70,70	0
22	MG	A	1644	1/1	0.87	0.21	109,109,109,109	0
22	MG	A	1648	1/1	0.88	0.20	81,81,81,81	0
22	MG	A	1603	1/1	0.88	0.15	64,64,64,64	0
22	MG	S	101	1/1	0.88	0.19	114,114,114,114	0
22	MG	A	1637	1/1	0.88	0.27	63,63,63,63	0
24	HYG	A	1717	36/36	0.88	0.15	144,215,236,246	0
22	MG	A	1657	1/1	0.89	0.08	127,127,127,127	0
22	MG	A	1670	1/1	0.89	0.11	91,91,91,91	0
22	MG	A	1651	1/1	0.89	0.21	73,73,73,73	0
22	MG	A	1654	1/1	0.89	0.42	84,84,84,84	0
22	MG	A	1614	1/1	0.89	0.33	46,46,46,46	0
22	MG	A	1630	1/1	0.90	0.18	56,56,56,56	0
22	MG	A	1650	1/1	0.90	0.28	59,59,59,59	0
22	MG	A	1616	1/1	0.90	0.16	101,101,101,101	0
22	MG	B	301	1/1	0.90	0.16	101,101,101,101	0
22	MG	A	1652	1/1	0.90	0.36	71,71,71,71	0
22	MG	A	1665	1/1	0.91	0.34	86,86,86,86	0
22	MG	A	1645	1/1	0.91	0.08	135,135,135,135	0
22	MG	A	1634	1/1	0.91	0.30	83,83,83,83	0
22	MG	A	1671	1/1	0.91	0.23	94,94,94,94	0
22	MG	A	1675	1/1	0.91	0.16	91,91,91,91	0
22	MG	A	1611	1/1	0.91	0.23	106,106,106,106	0
22	MG	A	1612	1/1	0.92	0.21	66,66,66,66	0
22	MG	A	1632	1/1	0.92	0.29	86,86,86,86	0
22	MG	A	1667	1/1	0.92	0.14	73,73,73,73	0
22	MG	A	1618	1/1	0.92	0.25	40,40,40,40	0
23	K	A	1701	1/1	0.92	0.13	100,100,100,100	0
22	MG	A	1692	1/1	0.93	0.22	167,167,167,167	0
22	MG	A	1696	1/1	0.93	0.29	73,73,73,73	0
22	MG	A	1628	1/1	0.93	0.16	55,55,55,55	0
22	MG	M	201	1/1	0.93	0.08	113,113,113,113	0
22	MG	A	1685	1/1	0.93	0.19	91,91,91,91	0
22	MG	A	1668	1/1	0.93	0.31	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	MG	A	1615	1/1	0.94	0.23	40,40,40,40	0
22	MG	A	1631	1/1	0.94	0.18	57,57,57,57	0
22	MG	A	1687	1/1	0.94	0.20	89,89,89,89	0
22	MG	A	1642	1/1	0.94	0.15	103,103,103,103	0
22	MG	A	1607	1/1	0.94	0.26	90,90,90,90	0
22	MG	A	1649	1/1	0.94	0.29	80,80,80,80	0
22	MG	A	1707	1/1	0.94	0.08	76,76,76,76	0
22	MG	A	1673	1/1	0.94	0.17	48,48,48,48	0
22	MG	A	1674	1/1	0.94	0.25	49,49,49,49	0
22	MG	A	1677	1/1	0.95	0.12	40,40,40,40	0
22	MG	K	201	1/1	0.95	0.14	59,59,59,59	0
22	MG	A	1684	1/1	0.95	0.05	141,141,141,141	0
22	MG	A	1669	1/1	0.95	0.30	59,59,59,59	0
22	MG	A	1636	1/1	0.95	0.26	54,54,54,54	0
23	K	A	1700	1/1	0.95	0.16	130,130,130,130	0
22	MG	A	1604	1/1	0.95	0.14	98,98,98,98	0
22	MG	A	1617	1/1	0.95	0.17	29,29,29,29	0
23	K	A	1703	1/1	0.95	0.20	166,166,166,166	0
22	MG	A	1602	1/1	0.95	0.33	54,54,54,54	0
22	MG	A	1647	1/1	0.95	0.10	50,50,50,50	0
22	MG	E	201	1/1	0.95	0.05	301,301,301,301	0
22	MG	A	1676	1/1	0.95	0.13	89,89,89,89	0
22	MG	A	1682	1/1	0.96	0.30	61,61,61,61	0
22	MG	A	1672	1/1	0.96	0.24	37,37,37,37	0
22	MG	A	1662	1/1	0.96	0.55	64,64,64,64	0
22	MG	A	1639	1/1	0.96	0.23	72,72,72,72	0
22	MG	A	1656	1/1	0.96	0.50	66,66,66,66	0
22	MG	A	1716	1/1	0.96	0.05	320,320,320,320	0
22	MG	A	1653	1/1	0.96	0.09	74,74,74,74	0
22	MG	A	1694	1/1	0.96	0.11	82,82,82,82	0
22	MG	A	1627	1/1	0.96	0.19	47,47,47,47	0
22	MG	A	1679	1/1	0.96	0.26	78,78,78,78	0
22	MG	A	1708	1/1	0.96	0.07	65,65,65,65	0
22	MG	A	1681	1/1	0.96	0.10	76,76,76,76	0
22	MG	A	1625	1/1	0.97	0.10	65,65,65,65	0
22	MG	A	1686	1/1	0.97	0.32	102,102,102,102	0
22	MG	A	1601	1/1	0.97	0.40	52,52,52,52	0
22	MG	A	1688	1/1	0.97	0.09	62,62,62,62	0
22	MG	A	1678	1/1	0.97	0.11	72,72,72,72	0
22	MG	A	1714	1/1	0.97	0.08	118,118,118,118	0
22	MG	A	1638	1/1	0.97	0.13	55,55,55,55	0
22	MG	A	1613	1/1	0.97	0.21	65,65,65,65	0

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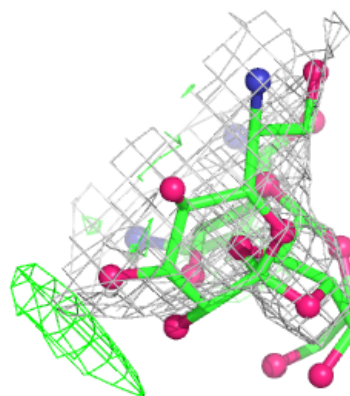
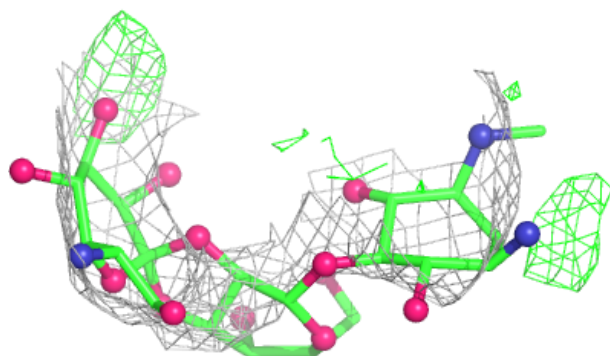
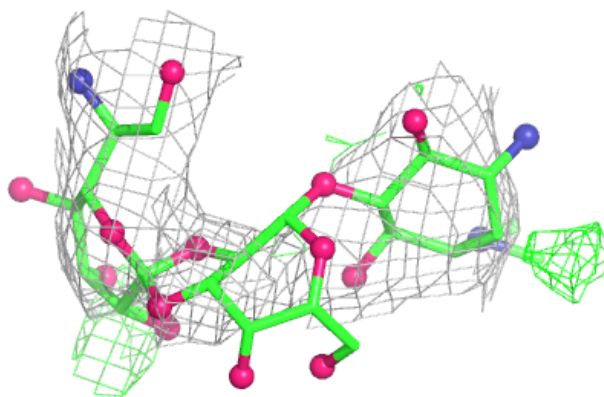
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	MG	A	1695	1/1	0.97	0.04	103,103,103,103	0
22	MG	A	1620	1/1	0.97	0.15	89,89,89,89	0
22	MG	A	1697	1/1	0.97	0.11	117,117,117,117	0
22	MG	A	1683	1/1	0.97	0.11	76,76,76,76	0
22	MG	A	1623	1/1	0.97	0.22	55,55,55,55	0
22	MG	A	1622	1/1	0.98	0.24	55,55,55,55	0
22	MG	A	1640	1/1	0.98	0.07	88,88,88,88	0
22	MG	A	1698	1/1	0.98	0.07	70,70,70,70	0
22	MG	A	1689	1/1	0.98	0.05	86,86,86,86	0
22	MG	A	1605	1/1	0.98	0.14	67,67,67,67	0
22	MG	A	1691	1/1	0.98	0.07	81,81,81,81	0
22	MG	A	1621	1/1	0.98	0.10	61,61,61,61	0
22	MG	A	1693	1/1	0.98	0.04	60,60,60,60	0
22	MG	A	1626	1/1	0.98	0.03	88,88,88,88	0
22	MG	A	1660	1/1	0.98	0.04	64,64,64,64	0
22	MG	L	201	1/1	0.98	0.03	107,107,107,107	0
25	ZN	D	301	1/1	0.98	0.21	119,119,119,119	0
22	MG	A	1659	1/1	0.99	0.10	84,84,84,84	0
22	MG	A	1624	1/1	0.99	0.04	71,71,71,71	0
22	MG	A	1661	1/1	0.99	0.04	41,41,41,41	0
22	MG	A	1680	1/1	0.99	0.11	88,88,88,88	0
25	ZN	N	101	1/1	0.99	0.06	199,199,199,199	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.

Electron density around HYG A 1717:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.