



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 11:39 PM UTC

PDB ID : 4DV4 / pdb_00004dv4
Title : Crystal structure of the *Thermus thermophilus* 30S ribosomal subunit with a 16S rRNA mutation, A914G
Authors : Demirci, H.; Murphy IV, F.; Murphy, E.; Gregory, S.T.; Dahlberg, A.E.; Jogl, G.
Deposited on : 2012-02-22
Resolution : 3.65 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
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

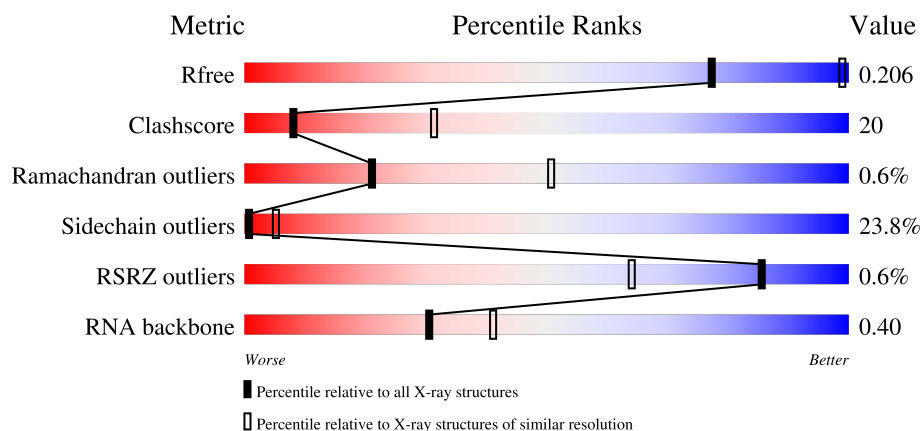
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

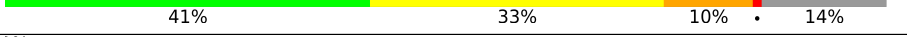
The reported resolution of this entry is 3.65 Å.

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.



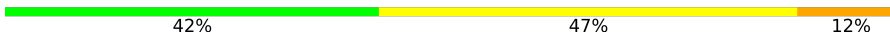
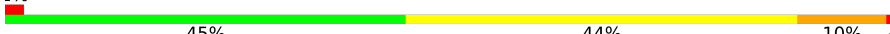
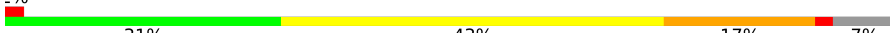
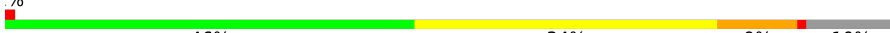
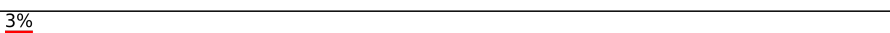
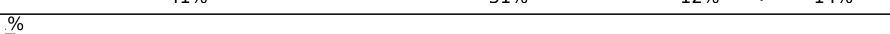
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1062 (3.78-3.54)
Clashscore	190562	1009 (3.76-3.56)
Ramachandran outliers	187476	1054 (3.78-3.54)
Sidechain outliers	187428	1052 (3.78-3.54)
RSRZ outliers	180081	1061 (3.78-3.54)
RNA backbone	3983	1027 (4.26-3.06)

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	 40% 43% 16% 2% 1%
2	B	256	 36% 39% 14% 9% 2%
3	C	239	 41% 33% 10% 14% 2%
4	D	209	 2% 42% 39% 17% 2%

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	MG	A	1714	-	-	-	X

2 Entry composition

There are 24 unique types of molecules in this entry. The entry contains 52434 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1512	Total	C	N	O	P	0	6	0
			32645	14540	6039	10548	1518			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	914	G	A	engineered mutation	GB M26923.1
A	1534	C	A	conflict	GB M26923.1
A	1535	A	C	conflict	GB M26923.1

- Molecule 2 is a protein called ribosomal protein S2.

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

- Molecule 3 is a protein called ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	206	Total	C	N	O	S	0	0	0
			1612	1016	314	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	150	Total	C	N	O	S	0	0	0
			1146	724	217	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	98	Total	C	N	O	S	0	0	0
			792	498	156	137	1			

- Molecule 11 is a protein called ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	116	Total	C	N	O	S	0	0	0
			864	537	164	160	3			

- Molecule 12 is a protein called ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	124	Total	C	N	O	S	0	0	0
			972	612	195	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	87	Total	C	N	O	S	0	0	0
			729	457	146	124	2			

- Molecule 16 is a protein called ribosomal protein S16.

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

- Molecule 17 is a protein called ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	99	Total	C	N	O	S	0	0	0
			823	528	152	141	2			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	96	GLN	GLU	conflict	UNP Q5SHP7

- Molecule 18 is a protein called ribosomal protein S18.

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

- Molecule 19 is a protein called ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	S	80	Total	C	N	O	S	0	0	0
			647	414	119	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	24	Total	C	N	O	0	0	0
			208	128	50	30			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	268	Total	Mg	0	0
			268	268		
22	B	2	Total	Mg	0	0
			2	2		
22	C	2	Total	Mg	0	0
			2	2		
22	D	3	Total	Mg	0	0
			3	3		
22	E	1	Total	Mg	0	0
			1	1		
22	F	1	Total	Mg	0	0
			1	1		
22	J	2	Total	Mg	0	0
			2	2		
22	M	1	Total	Mg	0	0
			1	1		
22	N	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	P	3	Total 3	Mg 3	0	0
22	Q	2	Total 2	Mg 2	0	0
22	S	1	Total 1	Mg 1	0	0

- Molecule 23 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

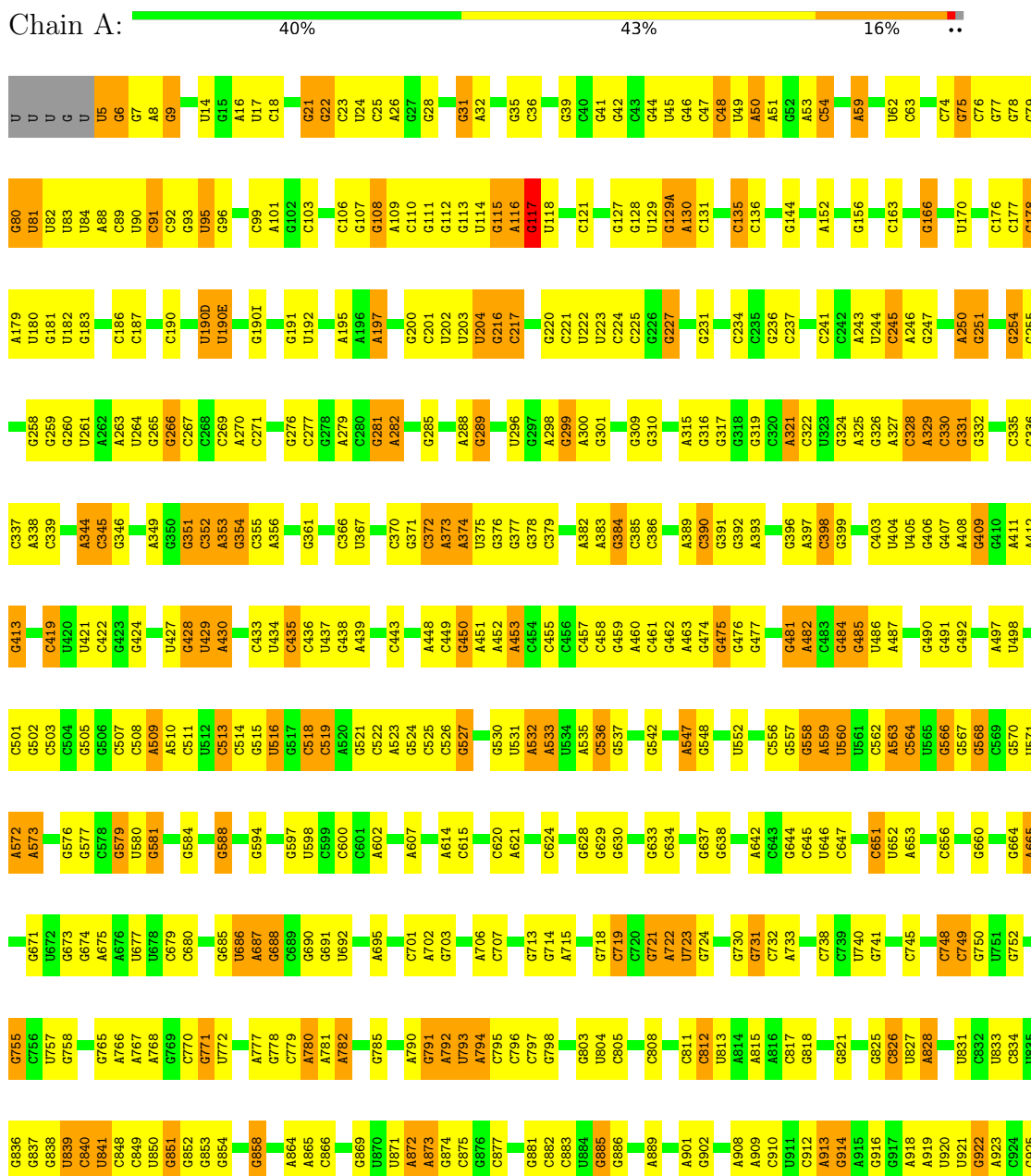
- Molecule 24 is water.

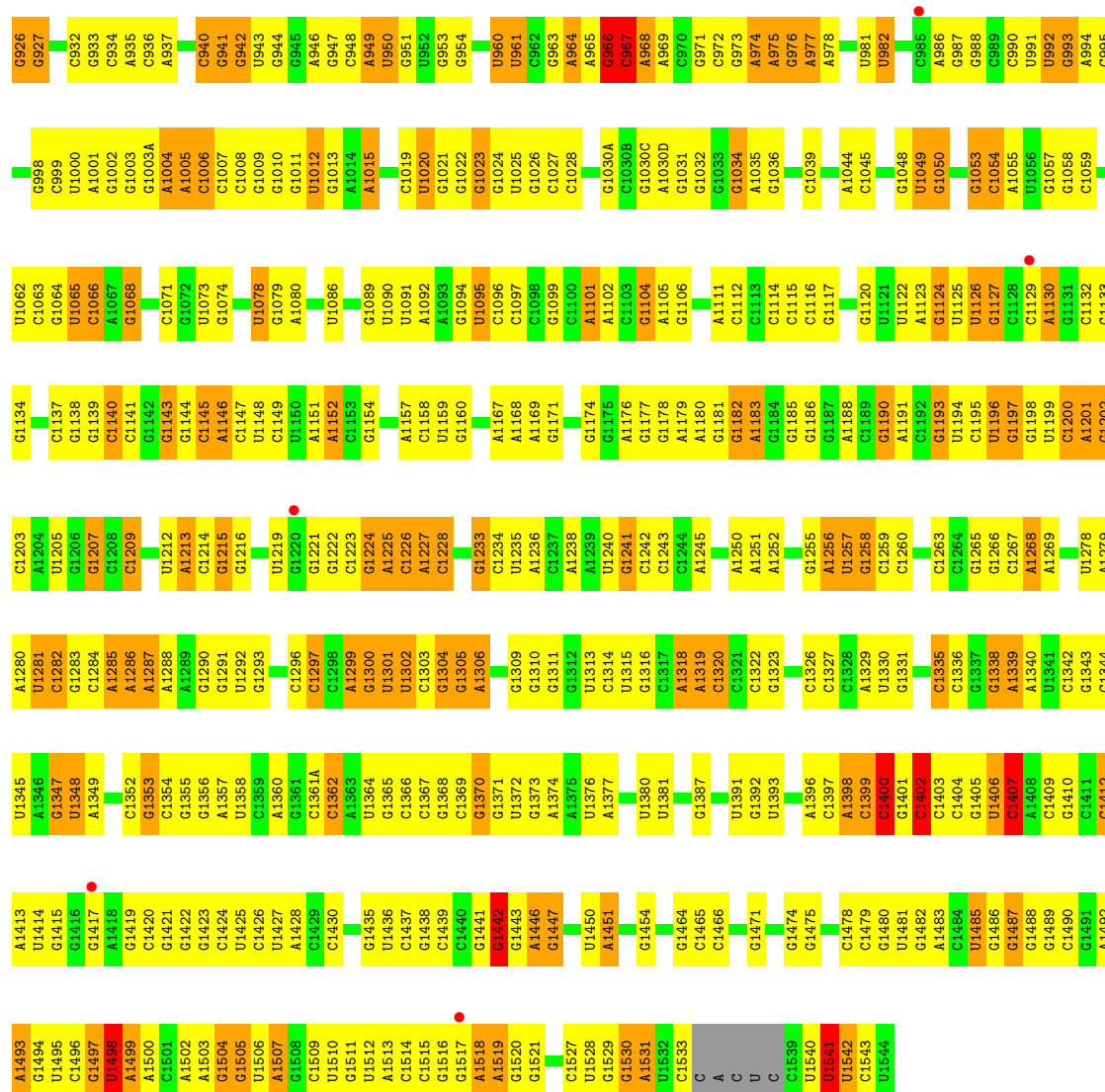
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	A	383	Total 383	O 383	0	0
24	E	3	Total 3	O 3	0	0
24	G	2	Total 2	O 2	0	0
24	I	1	Total 1	O 1	0	0
24	J	3	Total 3	O 3	0	0
24	L	1	Total 1	O 1	0	0
24	M	7	Total 7	O 7	0	0
24	N	2	Total 2	O 2	0	0
24	P	8	Total 8	O 8	0	0
24	Q	1	Total 1	O 1	0	0
24	T	1	Total 1	O 1	0	0

3 Residue-property plots

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

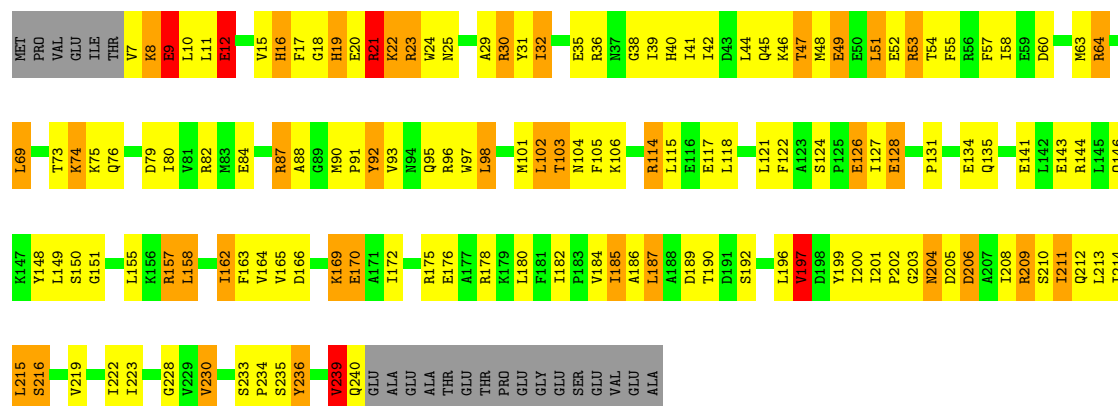
• Molecule 1: 16S rRNA



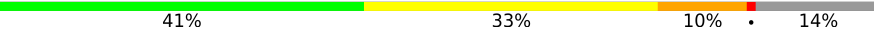


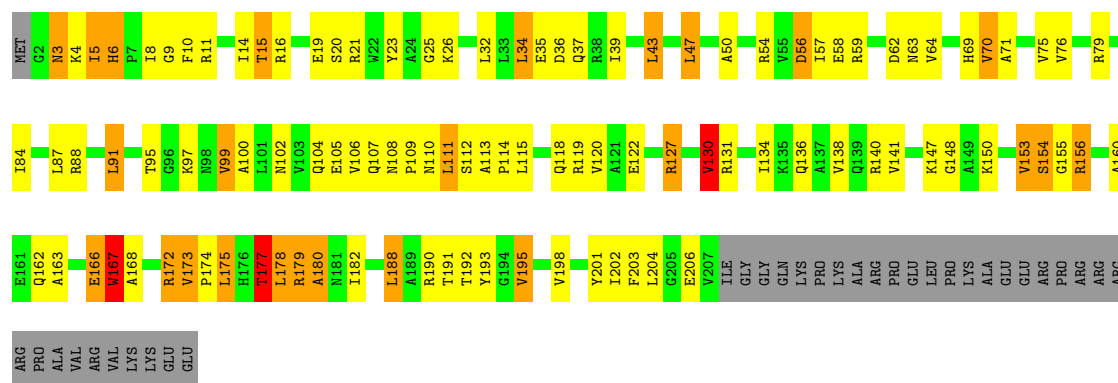
• Molecule 2: ribosomal protein S2

Chain B: 36% 39% 14% 9%



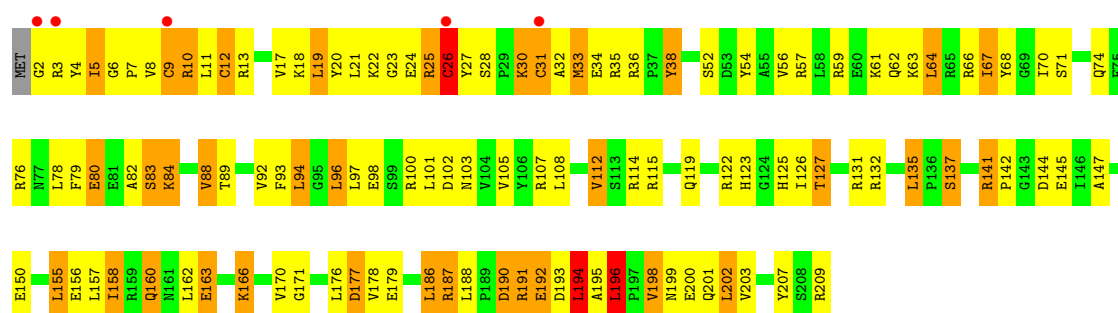
• Molecule 3: ribosomal protein S3

Chain C:  41% 33% 10% 14%

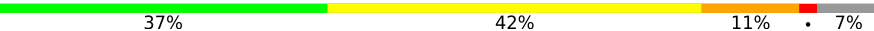


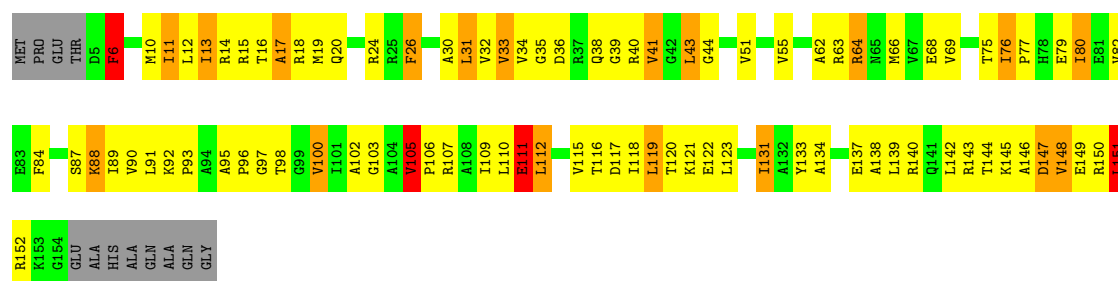
• Molecule 4: ribosomal protein S4

Chain D:  42% 39% 17%



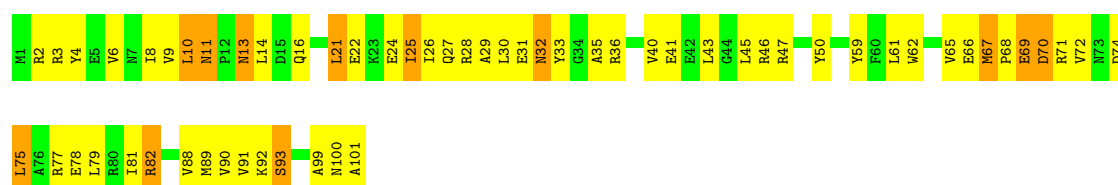
• Molecule 5: ribosomal protein S5

Chain E:  37% 42% 11% 7%

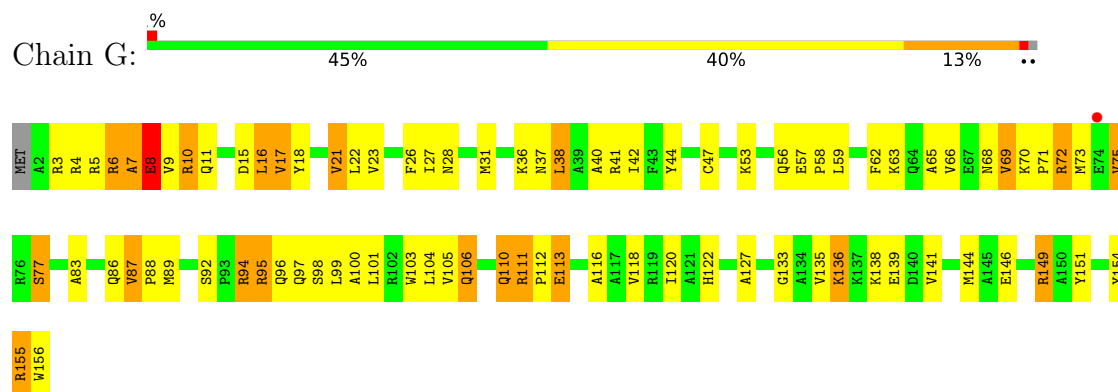


• Molecule 6: ribosomal protein S6

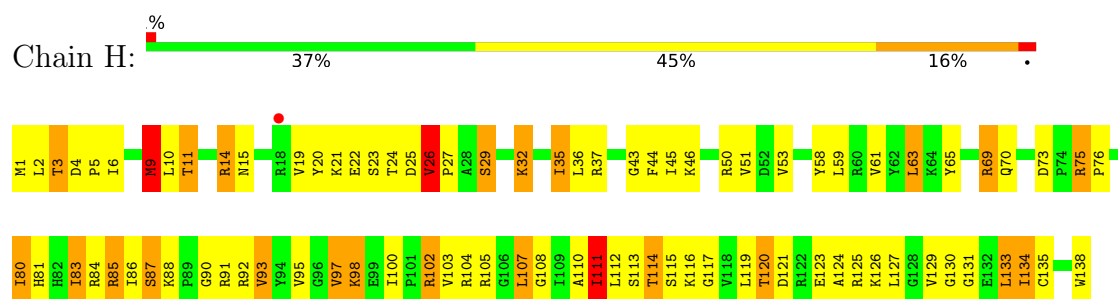
Chain F:  42% 47% 12%



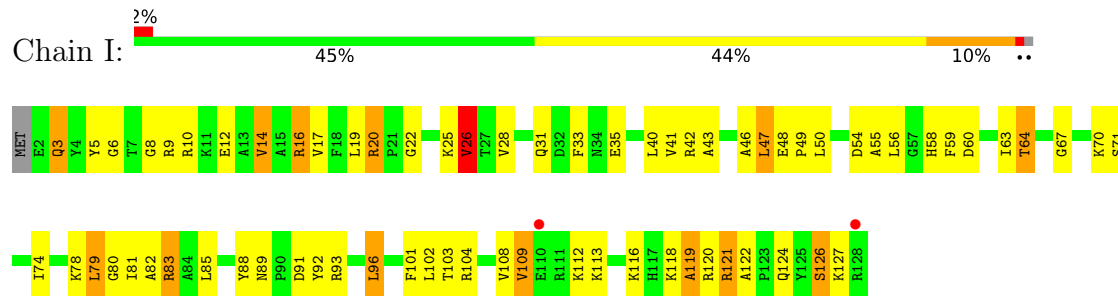
- Molecule 7: ribosomal protein S7



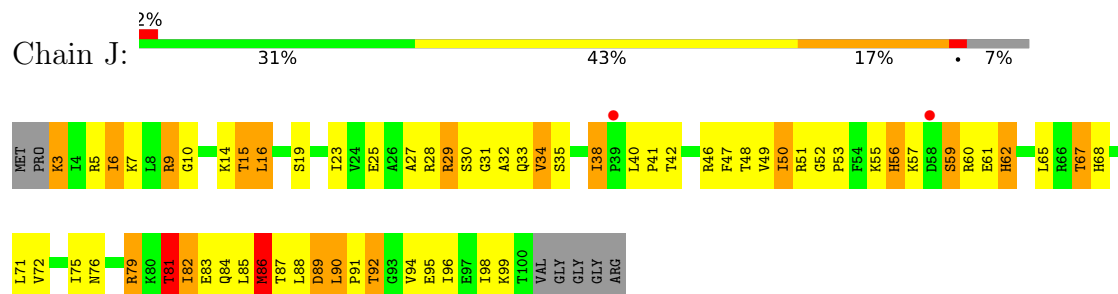
- Molecule 8: ribosomal protein S8



- Molecule 9: ribosomal protein S9

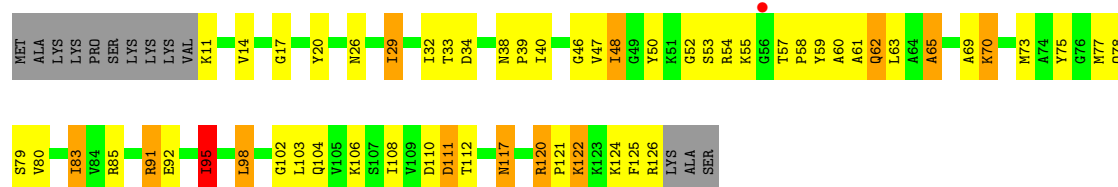


- Molecule 10: ribosomal protein S10

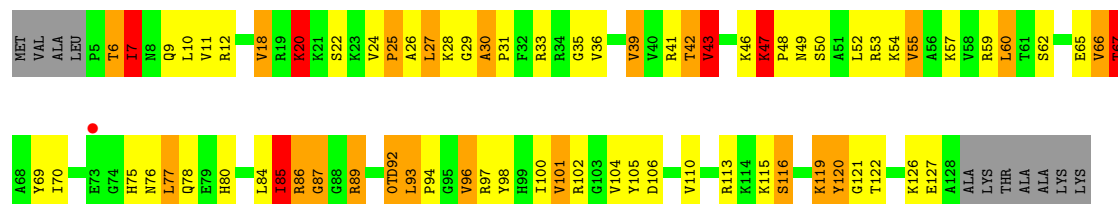


- Molecule 11: ribosomal protein S11

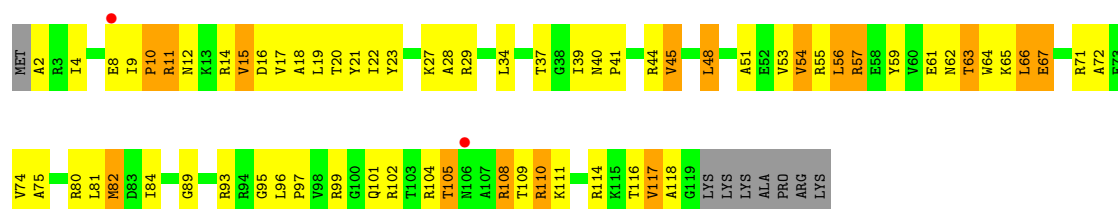




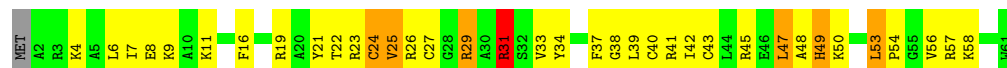
• Molecule 12: ribosomal protein S12



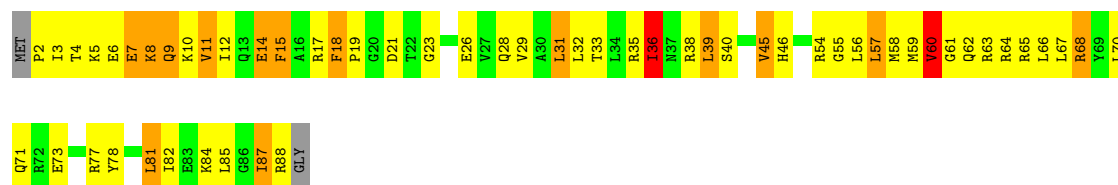
• Molecule 13: ribosomal protein S13



• Molecule 14: ribosomal protein S14

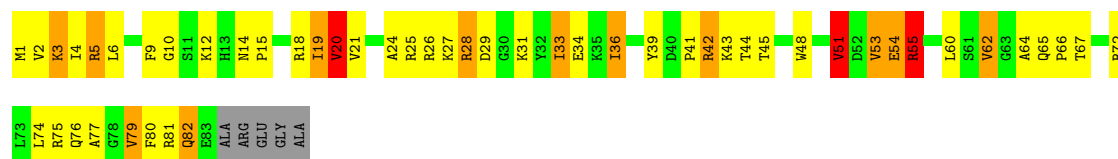


• Molecule 15: ribosomal protein S15

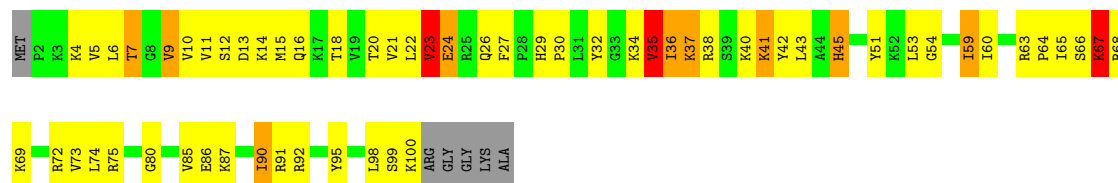
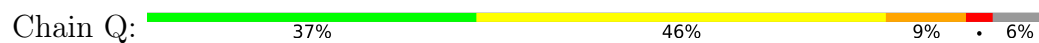


• Molecule 16: ribosomal protein S16

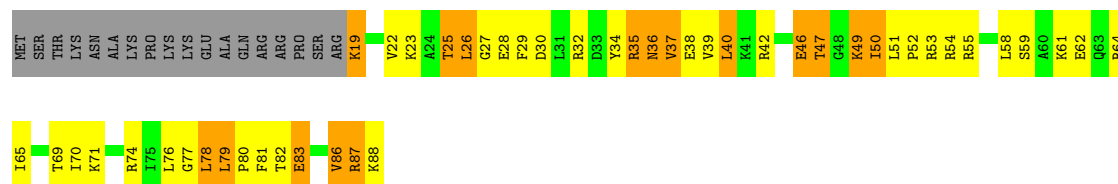
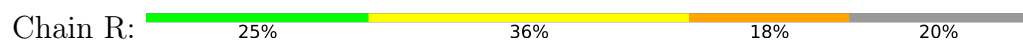




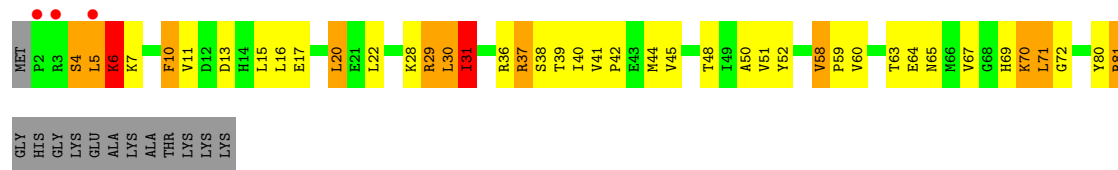
- Molecule 17: ribosomal protein S17



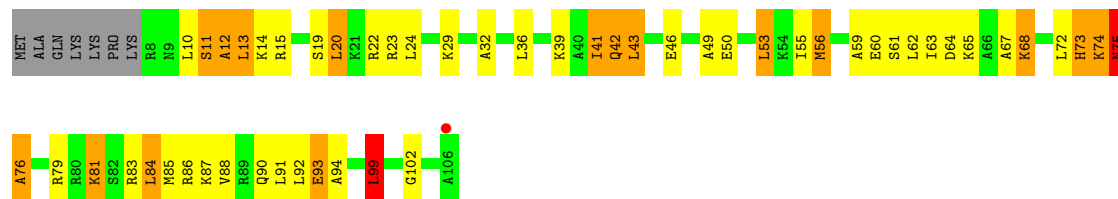
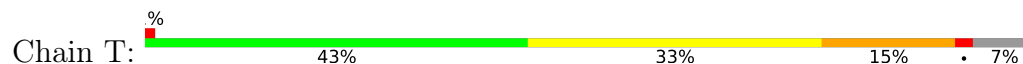
- Molecule 18: ribosomal protein S18



- Molecule 19: ribosomal protein S19



- Molecule 20: ribosomal protein S20



- Molecule 21: ribosomal protein THX





4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	402.64Å 402.64Å 174.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.66 – 3.65 34.66 – 3.65	Depositor EDS
% Data completeness (in resolution range)	98.2 (34.66-3.65) 97.8 (34.66-3.65)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 3.66Å)	Xtriage
Refinement program	PHENIX dev_978	Depositor
R, R_{free}	0.153 , 0.208 0.151 , 0.206	Depositor DCC
R_{free} test set	7745 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	138.2	Xtriage
Anisotropy	0.202	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 134.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	52434	wwPDB-VP
Average B, all atoms (Å ²)	168.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.89% 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: 7MG, 0TD, M2G, UR3, 4OC, ZN, 2MG, MA6, PSU, MG, 5MC

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	0.64	1/36140 (0.0%)	0.64	6/56398 (0.0%)
2	B	1.03	4/1935 (0.2%)	1.34	19/2609 (0.7%)
3	C	0.84	1/1636 (0.1%)	1.21	12/2205 (0.5%)
4	D	0.94	2/1733 (0.1%)	1.44	29/2318 (1.3%)
5	E	1.25	7/1162 (0.6%)	1.53	22/1564 (1.4%)
6	F	0.85	0/856	1.20	3/1154 (0.3%)
7	G	0.87	2/1276 (0.2%)	1.33	16/1709 (0.9%)
8	H	1.31	5/1136 (0.4%)	1.64	17/1527 (1.1%)
9	I	0.74	0/1029	1.15	4/1379 (0.3%)
10	J	0.87	0/805	1.29	7/1082 (0.6%)
11	K	1.07	3/879 (0.3%)	1.42	9/1187 (0.8%)
12	L	1.07	2/977 (0.2%)	1.61	24/1306 (1.8%)
13	M	0.83	0/947	1.16	4/1270 (0.3%)
14	N	0.83	0/501	1.23	3/664 (0.5%)
15	O	1.03	2/740 (0.3%)	1.32	8/987 (0.8%)
16	P	1.18	4/716 (0.6%)	1.55	12/963 (1.2%)
17	Q	1.27	5/836 (0.6%)	1.53	11/1117 (1.0%)
18	R	1.03	1/579 (0.2%)	1.40	9/768 (1.2%)
19	S	0.88	1/661 (0.2%)	1.28	5/890 (0.6%)
20	T	1.06	2/765 (0.3%)	1.44	9/1007 (0.9%)
21	U	0.70	0/212	1.34	3/277 (1.1%)
All	All	0.79	42/55521 (0.1%)	0.94	232/82381 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
4	D	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
7	G	0	1
8	H	0	1
10	J	0	2
12	L	0	2
13	M	0	1
15	O	0	1
18	R	0	1
20	T	0	2
All	All	0	13

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	P	19	ILE	CA-CB	-9.24	1.45	1.54
12	L	7	ILE	CA-CB	-7.82	1.45	1.54
17	Q	35	VAL	CA-CB	-7.67	1.45	1.54
7	G	118	VAL	CA-CB	-7.04	1.46	1.54
1	A	1498	UR3	O3'-P	6.93	1.63	1.56
8	H	111	ILE	CA-CB	-6.92	1.45	1.54
5	E	148	VAL	CA-CB	-6.91	1.46	1.54
4	D	30	LYS	CA-C	6.76	1.61	1.52
18	R	50	ILE	CA-CB	-6.68	1.47	1.54
16	P	36	ILE	CA-CB	-6.47	1.45	1.54
11	K	48	ILE	CA-CB	-6.46	1.45	1.54
16	P	20	VAL	CA-CB	-6.34	1.49	1.55
8	H	134	ILE	CA-CB	-6.27	1.46	1.54
17	Q	9	VAL	CA-CB	-6.27	1.46	1.54
8	H	80	ILE	CA-CB	-6.26	1.46	1.53
20	T	12	ALA	CA-CB	-6.22	1.43	1.53
17	Q	23	VAL	CA-CB	-6.18	1.46	1.53
11	K	120	ARG	CA-C	-6.16	1.46	1.53
5	E	115	VAL	CA-CB	-6.14	1.47	1.54
16	P	51	VAL	CA-CB	-6.10	1.46	1.54
2	B	182	ILE	CA-CB	-5.97	1.46	1.54
8	H	51	VAL	CA-CB	-5.96	1.49	1.55
17	Q	7	THR	CA-CB	-5.93	1.43	1.53
5	E	109	ILE	CA-CB	-5.87	1.47	1.54
17	Q	99	SER	CA-C	5.76	1.60	1.52
15	O	60	VAL	CA-CB	-5.68	1.48	1.54
20	T	12	ALA	CA-C	5.66	1.60	1.52
7	G	155	ARG	CA-C	5.53	1.60	1.52
5	E	34	VAL	CA-CB	-5.50	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	31	CYS	N-CA	5.35	1.53	1.46
11	K	95	ILE	CA-CB	-5.33	1.47	1.54
3	C	180	ALA	CA-CB	-5.30	1.45	1.53
12	L	67	THR	CA-CB	-5.29	1.45	1.53
2	B	197	VAL	CA-CB	-5.26	1.47	1.54
2	B	103	THR	CA-CB	-5.26	1.45	1.53
19	S	6	LYS	N-CA	5.23	1.53	1.47
5	E	41	VAL	CA-CB	-5.22	1.47	1.54
2	B	165	VAL	CA-CB	-5.20	1.47	1.54
8	H	61	VAL	CA-CB	-5.20	1.48	1.54
5	E	41	VAL	CA-C	-5.11	1.46	1.52
5	E	89	ILE	CA-C	-5.11	1.46	1.52
15	O	45	VAL	CA-CB	-5.08	1.47	1.54

All (232) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	L	26	ALA	N-CA-C	-13.27	95.19	111.11
4	D	26	CYS	N-CA-C	-12.31	98.31	113.20
7	G	111	ARG	CA-C-N	11.19	130.61	118.97
7	G	111	ARG	C-N-CA	11.19	130.61	118.97
4	D	56	VAL	CB-CA-C	-10.97	97.84	111.88
8	H	75	ARG	CA-C-N	10.48	130.57	119.78
8	H	75	ARG	C-N-CA	10.48	130.57	119.78
16	P	62	VAL	N-CA-C	10.38	122.05	112.29
19	S	6	LYS	N-CA-C	10.22	125.74	108.67
8	H	100	ILE	CA-C-N	10.10	130.84	120.14
8	H	100	ILE	C-N-CA	10.10	130.84	120.14
3	C	167	TRP	N-CA-C	9.58	121.45	108.23
6	F	67	MET	N-CA-C	9.49	116.52	108.07
11	K	91	ARG	N-CA-C	-9.47	100.29	112.23
17	Q	67	LYS	N-CA-C	-9.11	96.81	110.28
2	B	165	VAL	N-CA-C	9.06	119.61	110.82
17	Q	14	LYS	N-CA-C	9.03	122.26	111.33
4	D	6	GLY	CA-C-N	8.98	129.53	119.93
4	D	6	GLY	C-N-CA	8.98	129.53	119.93
3	C	166	GLU	N-CA-C	8.65	119.35	108.45
2	B	23	ARG	N-CA-C	-8.64	92.40	110.80
11	K	117	ASN	N-CA-C	8.61	129.14	110.80
4	D	33	MET	N-CA-C	-8.60	102.05	112.54
4	D	12	CYS	N-CA-C	-8.35	101.09	111.11
12	L	77	LEU	N-CA-C	8.26	121.89	109.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	S	4	SER	N-CA-C	8.20	122.62	108.02
4	D	30	LYS	N-CA-C	8.17	124.25	113.30
20	T	94	ALA	N-CA-C	-8.06	94.27	108.13
12	L	30	ALA	CA-C-N	8.05	128.24	119.87
12	L	30	ALA	C-N-CA	8.05	128.24	119.87
12	L	18	VAL	N-CA-C	8.03	120.43	108.46
17	Q	99	SER	N-CA-C	8.01	127.87	110.80
18	R	79	LEU	CA-C-N	7.99	128.28	119.90
18	R	79	LEU	C-N-CA	7.99	128.28	119.90
5	E	115	VAL	CB-CA-C	-7.97	99.45	111.33
7	G	133	GLY	N-CA-C	7.90	122.47	112.83
5	E	64	ARG	N-CA-C	-7.82	98.36	110.17
12	L	119	LYS	N-CA-C	-7.81	98.72	110.28
3	C	6	HIS	CA-C-N	7.81	127.36	118.85
3	C	6	HIS	C-N-CA	7.81	127.36	118.85
4	D	38	TYR	CA-C-N	7.69	128.30	120.38
4	D	38	TYR	C-N-CA	7.69	128.30	120.38
4	D	196	LEU	N-CA-C	7.54	118.85	109.57
2	B	16	HIS	N-CA-C	7.53	122.71	111.04
17	Q	10	VAL	CB-CA-C	-7.51	103.12	111.23
8	H	26	VAL	CA-C-N	-7.48	112.22	120.14
8	H	26	VAL	C-N-CA	-7.48	112.22	120.14
20	T	79	ARG	N-CA-C	-7.36	103.20	111.07
20	T	75	ASN	N-CA-C	-7.32	104.34	113.28
16	P	36	ILE	CA-C-N	-7.26	111.51	121.23
16	P	36	ILE	C-N-CA	-7.26	111.51	121.23
2	B	12	GLU	N-CA-C	7.21	121.77	113.19
11	K	26	ASN	N-CA-C	7.15	122.17	113.38
12	L	121	GLY	N-CA-C	7.12	123.88	113.48
10	J	62	HIS	N-CA-C	7.08	121.20	109.95
8	H	125	ARG	N-CA-C	-7.05	103.64	111.82
2	B	9	GLU	N-CA-C	7.04	119.77	109.07
8	H	73	ASP	CA-C-N	7.00	126.61	119.19
8	H	73	ASP	C-N-CA	7.00	126.61	119.19
4	D	12	CYS	CA-CB-SG	6.99	130.48	114.40
16	P	9	PHE	N-CA-C	6.99	121.98	113.17
10	J	90	LEU	N-CA-C	6.98	125.24	109.81
15	O	7	GLU	N-CA-C	-6.95	103.78	111.36
16	P	19	ILE	CB-CA-C	-6.91	100.10	111.51
16	P	79	VAL	N-CA-C	6.78	116.88	110.30
8	H	80	ILE	CB-CA-C	-6.73	103.20	111.88
3	C	180	ALA	N-CA-C	6.72	120.45	112.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	T	92	LEU	CA-C-N	-6.71	112.83	122.77
20	T	92	LEU	C-N-CA	-6.71	112.83	122.77
19	S	10	PHE	N-CA-C	6.66	119.13	108.41
5	E	80	ILE	N-CA-C	6.64	118.35	108.46
5	E	15	ARG	N-CA-C	6.58	119.78	111.69
19	S	6	LYS	CB-CA-C	-6.58	108.28	117.23
12	L	22	SER	N-CA-C	6.55	119.22	109.59
7	G	118	VAL	CB-CA-C	-6.47	103.54	112.02
4	D	67	ILE	CB-CA-C	-6.47	103.60	111.88
8	H	107	LEU	N-CA-C	-6.42	105.20	113.16
5	E	17	ALA	N-CA-C	6.42	120.34	110.20
5	E	6	PHE	N-CA-C	6.38	118.81	108.41
5	E	109	ILE	N-CA-C	6.35	116.46	110.30
16	P	51	VAL	N-CA-C	6.33	122.51	109.34
18	R	35	ARG	CA-C-N	-6.30	114.09	122.85
18	R	35	ARG	C-N-CA	-6.30	114.09	122.85
11	K	120	ARG	CA-C-N	-6.29	111.97	119.84
11	K	120	ARG	C-N-CA	-6.29	111.97	119.84
3	C	25	GLY	N-CA-C	-6.29	101.92	111.10
7	G	56	GLN	N-CA-C	6.28	118.82	110.53
4	D	112	VAL	CB-CA-C	-6.26	103.95	111.97
4	D	194	LEU	N-CA-C	6.23	119.55	109.40
4	D	203	VAL	CB-CA-C	-6.20	103.95	111.88
2	B	197	VAL	CB-CA-C	-6.17	101.01	110.95
5	E	41	VAL	CB-CA-C	-6.16	101.01	110.50
2	B	21	ARG	N-CA-C	6.15	123.90	110.80
21	U	22	ARG	CA-C-N	-6.14	114.44	120.52
21	U	22	ARG	C-N-CA	-6.14	114.44	120.52
8	H	9	MET	N-CA-C	-6.13	104.52	111.14
18	R	51	LEU	CA-C-N	6.12	127.50	119.84
18	R	51	LEU	C-N-CA	6.12	127.50	119.84
8	H	81	HIS	N-CA-C	-6.11	104.73	111.82
7	G	6	ARG	N-CA-C	6.09	117.92	111.28
10	J	31	GLY	N-CA-C	6.04	123.50	112.27
8	H	32	LYS	N-CA-C	-6.03	104.63	111.14
12	L	25	PRO	N-CA-C	6.03	120.94	112.26
19	S	30	LEU	N-CA-C	6.01	120.38	109.32
2	B	8	LYS	N-CA-C	6.00	116.47	108.38
16	P	76	GLN	N-CA-C	-5.99	105.23	112.54
5	E	111	GLU	N-CA-C	-5.98	104.84	111.36
20	T	11	SER	N-CA-C	5.98	120.30	113.19
2	B	128	GLU	N-CA-C	5.97	117.48	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J	55	LYS	N-CA-C	5.96	119.04	109.02
4	D	88	VAL	N-CA-C	5.95	116.38	107.51
15	O	15	PHE	N-CA-C	5.93	120.52	113.16
13	M	11	ARG	N-CA-C	5.92	119.13	109.06
8	H	69	ARG	N-CA-C	5.90	118.44	109.95
15	O	11	VAL	CB-CA-C	-5.89	104.19	112.14
2	B	230	VAL	N-CA-C	5.89	116.78	108.36
15	O	36	ILE	CB-CA-C	-5.89	104.34	111.88
17	Q	26	GLN	N-CA-C	-5.88	100.21	109.50
2	B	103	THR	CB-CA-C	-5.87	101.62	110.90
7	G	75	VAL	N-CA-C	5.86	116.92	108.48
4	D	31	CYS	CA-C-N	5.85	132.71	121.54
4	D	31	CYS	C-N-CA	5.85	132.71	121.54
10	J	89	ASP	N-CA-C	5.85	118.11	109.69
1	A	1299	A	C4-N9-C1'	5.84	143.83	126.30
11	K	102	GLY	N-CA-C	-5.84	106.46	114.64
7	G	8	GLU	N-CA-C	5.83	118.07	110.43
17	Q	54	GLY	N-CA-C	-5.82	107.35	114.92
12	L	105	TYR	CB-CA-C	-5.79	108.23	116.34
1	A	1442	G	C4-N9-C1'	5.76	143.79	126.50
3	C	43	LEU	N-CA-C	5.75	117.63	111.36
4	D	141	ARG	CA-C-N	-5.74	114.02	119.76
4	D	141	ARG	C-N-CA	-5.74	114.02	119.76
7	G	155	ARG	N-CA-C	5.73	123.00	110.80
13	M	57	ARG	N-CA-C	-5.69	104.99	111.14
4	D	191	ARG	N-CA-C	-5.69	104.08	111.02
7	G	7	ALA	N-CA-C	-5.68	103.92	111.02
17	Q	72	ARG	CA-C-N	-5.68	115.28	122.37
17	Q	72	ARG	C-N-CA	-5.68	115.28	122.37
12	L	49	ASN	N-CA-C	5.67	118.64	109.79
4	D	135	LEU	N-CA-C	5.67	118.61	108.47
11	K	70	LYS	N-CA-C	-5.66	105.03	111.14
5	E	88	LYS	CA-C-N	-5.65	115.09	122.94
5	E	88	LYS	C-N-CA	-5.65	115.09	122.94
5	E	151	LEU	N-CA-C	5.64	117.51	111.36
11	K	65	ALA	N-CA-C	-5.62	105.06	111.07
5	E	80	ILE	CB-CA-C	-5.60	101.87	110.50
9	I	126	SER	N-CA-C	5.60	122.73	110.80
16	P	3	LYS	N-CA-C	5.60	119.03	110.36
2	B	105	PHE	N-CA-C	-5.54	106.56	113.38
13	M	15	VAL	N-CA-C	5.53	116.31	110.72
7	G	111	ARG	N-CA-C	5.48	118.07	110.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J	56	HIS	N-CA-C	-5.47	104.51	110.91
8	H	117	GLY	N-CA-C	5.45	117.60	112.04
18	R	83	GLU	N-CA-C	5.45	115.48	108.34
2	B	211	ILE	CB-CA-C	-5.45	104.90	111.88
5	E	39	GLY	CA-C-N	-5.44	115.33	123.00
5	E	39	GLY	C-N-CA	-5.44	115.33	123.00
20	T	81	LYS	N-CA-C	5.44	116.90	110.97
20	T	74	LYS	O-C-N	5.43	129.81	122.59
2	B	204	ASN	N-CA-C	5.42	117.74	108.90
6	F	78	GLU	N-CA-C	5.42	117.00	111.14
21	U	17	THR	N-CA-C	5.40	118.23	109.86
2	B	117	GLU	N-CA-C	5.38	116.95	111.14
17	Q	21	VAL	N-CA-C	5.38	115.71	108.17
1	A	1299	A	C8-N9-C1'	-5.38	111.57	127.70
3	C	127	ARG	N-CA-C	5.38	117.20	110.91
4	D	94	LEU	CA-CB-CG	-5.37	97.50	116.30
20	T	76	ALA	N-CA-C	-5.37	104.67	111.11
7	G	57	GLU	CA-C-N	5.36	126.53	119.84
7	G	57	GLU	C-N-CA	5.36	126.53	119.84
16	P	5	ARG	N-CA-C	5.35	115.42	107.88
2	B	239	VAL	N-CA-C	5.33	117.76	111.09
7	G	122	HIS	N-CA-C	5.33	116.78	111.07
4	D	93	PHE	CB-CA-C	-5.32	102.46	110.92
10	J	59	SER	N-CA-C	5.31	119.86	113.17
12	L	6	THR	CA-C-N	-5.30	113.77	120.56
12	L	6	THR	C-N-CA	-5.30	113.77	120.56
12	L	47	LYS	N-CA-C	5.28	120.74	113.77
5	E	119	LEU	CA-CB-CG	-5.27	97.85	116.30
12	L	43	VAL	CB-CA-C	-5.27	102.25	110.69
12	L	85	ILE	N-CA-C	5.27	115.89	108.36
1	A	1498	UR3	P-O3'-C3'	5.26	126.02	119.70
8	H	53	VAL	CB-CA-C	-5.25	103.31	110.77
4	D	135	LEU	CA-CB-CG	-5.25	97.94	116.30
16	P	72	ARG	N-CA-C	5.25	117.00	111.28
4	D	171	GLY	CA-C-N	5.24	126.39	119.84
4	D	171	GLY	C-N-CA	5.24	126.39	119.84
3	C	177	THR	CA-C-N	-5.24	115.42	123.07
3	C	177	THR	C-N-CA	-5.24	115.42	123.07
3	C	178	LEU	N-CA-C	5.21	117.14	108.02
9	I	26	VAL	N-CA-C	5.20	115.44	108.17
2	B	19	HIS	N-CA-C	5.19	115.90	108.74
13	M	10	PRO	CA-C-O	-5.18	115.26	121.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	222	ILE	CB-CA-C	-5.17	105.35	111.97
7	G	83	ALA	N-CA-C	5.17	117.53	110.24
9	I	20	ARG	CA-C-N	-5.17	114.91	120.03
9	I	20	ARG	C-N-CA	-5.17	114.91	120.03
12	L	115	LYS	CA-C-N	-5.17	115.49	123.14
12	L	115	LYS	C-N-CA	-5.17	115.49	123.14
3	C	130	VAL	N-CA-C	-5.17	105.56	110.42
1	A	1442	G	C8-N9-C1'	-5.17	111.50	127.00
5	E	105	VAL	CA-C-N	-5.16	113.72	119.19
5	E	105	VAL	C-N-CA	-5.16	113.72	119.19
5	E	95	ALA	CA-C-N	5.16	125.15	119.89
5	E	95	ALA	C-N-CA	5.16	125.15	119.89
17	Q	80	GLY	CA-C-N	-5.13	115.72	122.85
17	Q	80	GLY	C-N-CA	-5.13	115.72	122.85
16	P	55	ARG	N-CA-C	5.13	117.66	111.40
12	L	66	VAL	N-CA-C	5.11	117.38	108.90
15	O	18	PHE	CA-C-N	-5.09	114.53	119.78
15	O	18	PHE	C-N-CA	-5.09	114.53	119.78
15	O	11	VAL	N-CA-C	5.09	115.81	110.62
7	G	21	VAL	CB-CA-C	-5.08	105.38	112.04
2	B	148	TYR	N-CA-C	5.08	121.61	110.80
5	E	76	ILE	CA-C-N	5.07	124.68	119.56
5	E	76	ILE	C-N-CA	5.07	124.68	119.56
6	F	16	GLN	N-CA-C	5.06	116.48	110.97
14	N	31	ARG	CA-C-N	-5.06	115.82	122.85
14	N	31	ARG	C-N-CA	-5.06	115.82	122.85
12	L	55	VAL	CB-CA-C	-5.05	104.27	111.34
18	R	50	ILE	CB-CA-C	-5.05	103.09	111.32
12	L	20	LYS	CA-C-N	-5.04	115.39	122.94
12	L	20	LYS	C-N-CA	-5.04	115.39	122.94
14	N	49	HIS	N-CA-C	-5.04	105.26	111.40
11	K	111	ASP	N-CA-C	5.03	119.11	112.92
15	O	36	ILE	N-CA-C	5.02	115.63	110.36
4	D	7	PRO	CA-C-N	-5.02	118.05	122.97
4	D	7	PRO	C-N-CA	-5.02	118.05	122.97
18	R	36	ASN	N-CA-C	5.01	117.07	107.75
1	A	117	G	C4-N9-C1'	5.01	141.52	126.50
12	L	86	ARG	CA-C-N	-5.00	113.32	121.92
12	L	86	ARG	C-N-CA	-5.00	113.32	121.92

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	170	GLU	Peptide
4	D	195	ALA	Peptide
7	G	154	TYR	Peptide
8	H	90	GLY	Peptide
10	J	86	MET	Peptide
10	J	90	LEU	Peptide
12	L	27	LEU	Peptide
12	L	87	GLY	Peptide
13	M	105	THR	Peptide
15	O	2	PRO	Peptide
18	R	86	VAL	Peptide
20	T	12	ALA	Peptide
20	T	93	GLU	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	32645	0	16507	767	0
2	B	1900	0	1951	101	0
3	C	1612	0	1677	93	0
4	D	1703	0	1763	99	0
5	E	1146	0	1207	74	0
6	F	843	0	857	44	0
7	G	1257	0	1296	64	0
8	H	1116	0	1177	76	0
9	I	1010	0	1037	68	0
10	J	792	0	835	63	0
11	K	864	0	881	43	0
12	L	972	0	1058	60	0
13	M	937	0	995	53	0
14	N	492	0	529	30	0
15	O	729	0	768	50	0
16	P	700	0	720	38	0
17	Q	823	0	893	48	0
18	R	574	0	644	37	0
19	S	647	0	673	31	0
20	T	763	0	861	33	0
21	U	208	0	221	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	A	268	0	0	0	0
22	B	2	0	0	0	0
22	C	2	0	0	0	0
22	D	3	0	0	0	0
22	E	1	0	0	0	0
22	F	1	0	0	0	0
22	J	2	0	0	0	0
22	M	1	0	0	0	0
22	N	1	0	0	0	0
22	P	3	0	0	0	0
22	Q	2	0	0	0	0
22	S	1	0	0	0	0
23	D	1	0	0	0	0
23	N	1	0	0	0	0
24	A	383	0	0	11	0
24	E	3	0	0	0	0
24	G	2	0	0	2	0
24	I	1	0	0	1	0
24	J	3	0	0	3	0
24	L	1	0	0	0	0
24	M	7	0	0	1	0
24	N	2	0	0	0	0
24	P	8	0	0	1	0
24	Q	1	0	0	0	0
24	T	1	0	0	0	0
All	All	52434	0	36550	1702	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 20.

All (1702) 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)
18:R:39:VAL:HG13	18:R:40:LEU:HD23	1.46	0.98
8:H:9:MET:HG3	8:H:26:VAL:HG21	1.41	0.98
1:A:1399:C:H4'	1:A:1400:5MC:H5''	1.53	0.90
14:N:39:LEU:HD22	14:N:43:CYS:HB3	1.54	0.88
1:A:1309:G:OP2	13:M:99:ARG:NH1	2.07	0.87
3:C:131:ARG:HA	3:C:134:ILE:HD12	1.55	0.87
3:C:11:ARG:HH11	3:C:178:LEU:HD23	1.39	0.86
1:A:992:U:H3	1:A:1044:A:H62	1.23	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:10:ARG:HH11	21:U:10:ARG:HB2	1.40	0.85
1:A:21:G:N2	1:A:885:G:O3'	2.10	0.85
16:P:15:PRO:HD2	16:P:42:ARG:HD3	1.59	0.85
1:A:1368:G:H5''	9:I:112:LYS:HB3	1.59	0.84
2:B:9:GLU:OE1	2:B:10:LEU:N	2.09	0.84
1:A:692:U:OP1	11:K:124:LYS:NZ	2.11	0.83
6:F:68:PRO:HB2	6:F:71:ARG:HG3	1.60	0.83
18:R:36:ASN:HD22	18:R:39:VAL:HG12	1.43	0.83
5:E:11:ILE:HG22	5:E:31:LEU:HB3	1.60	0.83
6:F:70:ASP:OD1	6:F:70:ASP:N	2.10	0.83
1:A:427:U:OP1	4:D:13:ARG:NH2	2.11	0.82
11:K:110:ASP:HB2	18:R:88:LYS:HG2	1.62	0.82
1:A:310:G:OP2	16:P:27:LYS:NZ	2.10	0.82
12:L:27:LEU:C	12:L:29:GLY:H	1.87	0.82
1:A:481:G:HO2'	1:A:482:A:H8	1.27	0.82
1:A:532:A:O2'	1:A:533:A:OP1	1.98	0.82
1:A:1007:C:O2	1:A:1023:G:N1	2.11	0.81
1:A:836:G:OP1	18:R:61:LYS:NZ	2.14	0.81
1:A:869:G:N7	24:A:2164:HOH:O	2.14	0.81
8:H:4:ASP:OD2	8:H:85:ARG:NH1	2.13	0.80
12:L:87:GLY:HA2	12:L:98:TYR:HA	1.63	0.79
5:E:144:THR:HG22	5:E:146:ALA:H	1.47	0.79
1:A:1435:G:H2'	1:A:1436:U:C6	2.17	0.79
19:S:58:VAL:HG12	19:S:59:PRO:HD2	1.65	0.79
1:A:21:G:O2'	1:A:22:G:OP1	2.01	0.79
2:B:223:ILE:HG22	2:B:228:GLY:HA3	1.65	0.79
1:A:973:G:H3'	1:A:974:A:H5''	1.62	0.78
1:A:1369:C:H2'	1:A:1370:G:C8	2.19	0.78
2:B:12:GLU:HG3	2:B:213:LEU:HD21	1.62	0.78
12:L:41:ARG:HH12	12:L:43:VAL:HG13	1.47	0.78
1:A:1338:G:H2'	1:A:1339:A:C8	2.18	0.78
5:E:93:PRO:HD2	8:H:105:ARG:HH21	1.49	0.78
1:A:144:G:H1	1:A:178:C:H42	1.30	0.77
1:A:1195:C:H3'	1:A:1196:U:C5'	2.13	0.77
1:A:1195:C:H3'	1:A:1196:U:H5''	1.65	0.77
18:R:47:THR:HG22	18:R:83:GLU:H	1.49	0.77
1:A:1090:U:H2'	1:A:1091:U:H6	1.50	0.77
3:C:5:ILE:HD13	3:C:10:PHE:HB2	1.65	0.77
8:H:21:LYS:O	8:H:65:TYR:OH	2.02	0.76
4:D:11:LEU:HD13	4:D:66:ARG:HD3	1.67	0.76
1:A:656:C:O2'	15:O:28:GLN:NE2	2.19	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:982:U:OP2	14:N:23:ARG:NH2	2.20	0.75
2:B:15:VAL:HG13	2:B:209:ARG:HG3	1.69	0.75
1:A:407:G:OP1	4:D:115:ARG:NH1	2.20	0.75
12:L:20:LYS:H	12:L:20:LYS:HD3	1.51	0.75
8:H:29:SER:HB3	8:H:32:LYS:HD2	1.68	0.75
3:C:174:PRO:HB2	3:C:177:THR:HG23	1.69	0.74
15:O:87:ILE:HG22	15:O:88:ARG:H	1.50	0.74
17:Q:12:SER:HB3	17:Q:20:THR:HB	1.69	0.74
1:A:677:U:H3	1:A:713:G:H22	1.35	0.74
1:A:966:M2G:HM13	1:A:967:5MC:H1'	1.69	0.74
1:A:281:G:O2'	1:A:282:A:OP2	2.06	0.74
12:L:113:ARG:HH12	12:L:116:SER:H	1.36	0.74
7:G:40:ALA:HB3	9:I:41:VAL:HG21	1.70	0.73
1:A:1030(D):A:H62	1:A:1031:G:H21	1.34	0.73
9:I:26:VAL:HB	9:I:33:PHE:HB2	1.67	0.73
21:U:9:ARG:HH22	21:U:23:PRO:HD2	1.53	0.73
4:D:22:LYS:HB2	4:D:26:CYS:SG	2.29	0.73
5:E:142:LEU:O	5:E:143:ARG:NH1	2.20	0.73
3:C:91:LEU:HD21	3:C:99:VAL:HG22	1.68	0.73
1:A:600:C:H42	1:A:638:G:H1	1.35	0.73
4:D:78:LEU:HD21	4:D:96:LEU:HB3	1.71	0.73
8:H:111:ILE:HG22	8:H:134:ILE:HB	1.71	0.73
1:A:1497:G:H2'	1:A:1498:UR3:H5'	1.71	0.72
3:C:35:GLU:OE2	3:C:59:ARG:NH1	2.22	0.72
1:A:1124:G:H2'	1:A:1145:C:H41	1.55	0.72
1:A:758:G:N7	24:A:1965:HOH:O	2.21	0.72
3:C:11:ARG:HG2	3:C:178:LEU:HG	1.72	0.72
9:I:108:VAL:HG12	9:I:109:VAL:H	1.55	0.72
1:A:976:G:OP2	1:A:1358:U:H1'	1.90	0.72
1:A:1345:U:OP1	9:I:120:ARG:NH1	2.23	0.72
1:A:1127:G:O6	1:A:1144:G:N1	2.23	0.71
1:A:1064:G:N2	1:A:1190:G:H2'	2.05	0.71
4:D:187:ARG:CZ	4:D:188:LEU:H	2.02	0.71
1:A:298:A:N6	24:A:2036:HOH:O	2.13	0.71
1:A:660:G:H1	1:A:745:C:H42	1.38	0.71
1:A:838:G:H2'	1:A:839:U:H5''	1.71	0.71
16:P:21:VAL:HG12	16:P:33:ILE:HD12	1.72	0.71
1:A:1101:A:H4'	1:A:1102:A:O5'	1.90	0.71
17:Q:63:ARG:HG2	17:Q:64:PRO:HD2	1.73	0.71
1:A:977:A:H2'	1:A:978:A:H5''	1.73	0.71
9:I:50:LEU:HB3	9:I:55:ALA:HB3	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:10:PRO:HB2	13:M:18:ALA:HB1	1.73	0.71
13:M:11:ARG:HA	13:M:45:VAL:HG11	1.71	0.70
15:O:6:GLU:OE2	15:O:6:GLU:N	2.18	0.70
1:A:542:G:OP1	4:D:10:ARG:NH2	2.24	0.70
12:L:93:LEU:HD12	12:L:96:VAL:HG21	1.72	0.70
1:A:1241:G:H2'	1:A:1242:C:H6	1.56	0.70
13:M:34:LEU:HG	13:M:41:PRO:HB3	1.74	0.70
13:M:48:LEU:HB3	13:M:53:VAL:HG23	1.73	0.70
4:D:64:LEU:HA	4:D:67:ILE:HD12	1.72	0.70
1:A:1441:G:H4'	1:A:1442:G:C5	2.25	0.70
12:L:113:ARG:NH1	12:L:116:SER:H	1.89	0.70
17:Q:43:LEU:HB2	17:Q:68:ARG:O	1.91	0.70
1:A:31:G:N2	1:A:48:C:OP1	2.22	0.70
1:A:411:A:N7	1:A:413:G:N3	2.40	0.70
1:A:1442:G:N2	1:A:1447:G:N7	2.40	0.70
7:G:75:VAL:HG22	7:G:88:PRO:HA	1.72	0.70
1:A:1347:G:H3'	9:I:108:VAL:O	1.92	0.69
1:A:113:G:H1'	1:A:354:G:H5'	1.74	0.69
1:A:1243:C:OP1	21:U:10:ARG:NH1	2.24	0.69
5:E:147:ASP:OD1	5:E:147:ASP:N	2.19	0.69
1:A:1426:C:H42	1:A:1474:G:H1	1.41	0.68
1:A:719:C:H1'	18:R:49:LYS:HG2	1.75	0.68
1:A:953:G:N7	13:M:104:ARG:NH2	2.41	0.68
1:A:1314:C:H2'	1:A:1315:U:C6	2.29	0.68
4:D:61:LYS:NZ	4:D:62:GLN:OE1	2.27	0.68
1:A:509:A:C8	1:A:509:A:H3'	2.29	0.68
3:C:156:ARG:NE	3:C:160:ALA:O	2.24	0.68
11:K:124:LYS:HG3	11:K:125:PHE:CD1	2.29	0.68
3:C:180:ALA:HB3	3:C:203:PHE:CE1	2.28	0.68
7:G:69:VAL:HG21	7:G:104:LEU:HD21	1.76	0.68
8:H:9:MET:HE2	8:H:32:LYS:HG2	1.76	0.68
12:L:57:LYS:HD3	12:L:67:THR:HG23	1.76	0.68
1:A:452:A:O2'	1:A:453:A:O4'	2.11	0.68
12:L:10:LEU:HB3	17:Q:32:TYR:CE1	2.28	0.68
12:L:20:LYS:H	12:L:20:LYS:CD	2.07	0.68
1:A:536:C:H2'	1:A:537:G:C8	2.29	0.67
1:A:580:U:H2'	1:A:581:G:O4'	1.93	0.67
10:J:25:GLU:O	10:J:29:ARG:NE	2.27	0.67
10:J:48:THR:HA	10:J:62:HIS:HB3	1.76	0.67
21:U:10:ARG:HB2	21:U:10:ARG:NH1	2.09	0.67
2:B:208:ILE:HA	2:B:211:ILE:HD12	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:15:THR:HG23	10:J:94:VAL:HG22	1.77	0.67
3:C:71:ALA:HB1	3:C:109:PRO:HG3	1.76	0.67
4:D:107:ARG:HH21	4:D:194:LEU:HD11	1.59	0.67
7:G:16:LEU:H	7:G:16:LEU:HD22	1.58	0.67
14:N:8:GLU:HA	14:N:11:LYS:HD2	1.76	0.67
1:A:1004:A:H5''	1:A:1025:U:N3	2.10	0.67
6:F:50:TYR:CE1	18:R:77:GLY:HA2	2.29	0.67
7:G:70:LYS:O	7:G:72:ARG:NH1	2.28	0.67
12:L:10:LEU:HB3	17:Q:32:TYR:CD1	2.30	0.67
1:A:964:A:N6	24:A:2266:HOH:O	2.19	0.67
20:T:56:MET:HE2	20:T:85:MET:HA	1.75	0.67
1:A:1425:U:H3	1:A:1475:G:H1	1.42	0.67
1:A:1495:U:H2'	1:A:1496:C:C6	2.29	0.67
3:C:21:ARG:HG3	3:C:58:GLU:HG2	1.77	0.67
16:P:60:LEU:HD23	16:P:64:ALA:HB3	1.77	0.67
12:L:47:LYS:HG2	12:L:48:PRO:HD3	1.75	0.67
1:A:501:C:H2'	1:A:502:G:C8	2.30	0.66
4:D:200:GLU:CD	4:D:200:GLU:H	2.02	0.66
1:A:1147:C:H4'	9:I:5:TYR:HE1	1.59	0.66
1:A:1257:U:H4'	1:A:1258:G:O5'	1.95	0.66
1:A:1352:C:H42	1:A:1370:G:H1	1.43	0.66
1:A:1426:C:H2'	1:A:1427:U:H6	1.59	0.66
10:J:89:ASP:CG	10:J:91:PRO:HD3	2.20	0.66
3:C:37:GLN:HE22	14:N:47:LEU:HD11	1.60	0.66
17:Q:45:HIS:HD2	17:Q:65:ILE:HG12	1.60	0.66
1:A:1112:C:O2'	3:C:179:ARG:NH1	2.27	0.66
16:P:26:ARG:HG2	16:P:27:LYS:H	1.60	0.66
10:J:3:LYS:NZ	10:J:3:LYS:HB3	2.11	0.66
18:R:46:GLU:H	18:R:46:GLU:CD	2.03	0.66
20:T:60:GLU:HA	20:T:63:ILE:HD12	1.78	0.66
12:L:27:LEU:C	12:L:29:GLY:N	2.52	0.66
1:A:321:A:N7	1:A:328:C:H6	1.94	0.66
4:D:83:SER:HA	4:D:89:THR:HG23	1.77	0.66
5:E:19:MET:HE1	5:E:24:ARG:NH1	2.10	0.66
1:A:1305:G:N2	1:A:1331:G:H1'	2.11	0.66
1:A:1314:C:H5	19:S:6:LYS:HE2	1.60	0.66
1:A:1049:U:H4'	1:A:1050:G:O5'	1.96	0.65
1:A:972:C:H4'	10:J:57:LYS:HD3	1.78	0.65
1:A:1126:U:H3	1:A:1149:C:H1'	1.61	0.65
3:C:6:HIS:NE2	3:C:8:ILE:HB	2.11	0.65
1:A:1406:U:O2'	1:A:1517[B]:G:N2	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:163:GLU:HA	4:D:166:LYS:HD3	1.78	0.65
13:M:20:THR:HG22	24:M:307:HOH:O	1.96	0.65
11:K:57:THR:HG23	11:K:60:ALA:H	1.62	0.65
1:A:177:C:OP1	20:T:65:LYS:NZ	2.30	0.65
1:A:1065:U:H5''	1:A:1190:G:N2	2.11	0.65
1:A:519:C:OP2	12:L:50:SER:OG	2.08	0.65
1:A:1498:UR3:O2'	1:A:1499:A:OP2	2.13	0.65
2:B:97:TRP:HZ2	2:B:102:LEU:HD22	1.62	0.65
2:B:146:GLN:O	2:B:150:SER:OG	2.13	0.65
4:D:23:GLY:HA3	4:D:112:VAL:HG12	1.78	0.65
1:A:1301:U:O2'	1:A:1302:U:O5'	2.14	0.64
6:F:69:GLU:H	6:F:69:GLU:CD	2.05	0.64
10:J:50:ILE:H	10:J:50:ILE:HD12	1.62	0.64
2:B:42:ILE:HG21	2:B:202:PRO:HB2	1.79	0.64
14:N:47:LEU:HB3	14:N:53:LEU:HD21	1.79	0.64
1:A:1376:U:OP1	7:G:98:SER:OG	2.16	0.64
8:H:110:ALA:HB3	8:H:121:ASP:HB3	1.79	0.64
3:C:37:GLN:NE2	14:N:47:LEU:HD11	2.12	0.64
8:H:114:THR:HG22	8:H:130:GLY:O	1.98	0.64
9:I:8:GLY:HA3	9:I:79:LEU:HB3	1.79	0.64
17:Q:40:LYS:HD2	17:Q:42:TYR:CZ	2.32	0.64
1:A:80:G:O2'	1:A:81:U:OP1	2.12	0.64
1:A:1133:G:H2'	1:A:1134:G:H8	1.63	0.64
7:G:88:PRO:HB2	7:G:155:ARG:NH2	2.12	0.64
18:R:36:ASN:ND2	18:R:39:VAL:HG12	2.12	0.64
1:A:833:U:H2'	1:A:834:C:C6	2.32	0.63
2:B:223:ILE:HG21	2:B:230:VAL:HB	1.80	0.63
7:G:38:LEU:O	7:G:42:ILE:HG13	1.98	0.63
16:P:43:LYS:HG2	16:P:48:TRP:CG	2.33	0.63
2:B:84:GLU:OE2	2:B:233:SER:OG	2.11	0.63
10:J:42:THR:HG23	10:J:67:THR:O	1.97	0.63
1:A:411:A:H62	1:A:413:G:N2	1.97	0.63
1:A:1193:G:H2'	1:A:1194:U:H6	1.64	0.63
13:M:117:VAL:HG12	13:M:118:ALA:H	1.62	0.63
14:N:48:ALA:HB1	14:N:56:VAL:HG11	1.80	0.63
6:F:8:ILE:HB	6:F:61:LEU:HB2	1.81	0.63
16:P:4:ILE:HG12	16:P:21:VAL:HG22	1.80	0.63
1:A:1296:C:H4'	1:A:1302:U:C5	2.33	0.63
1:A:1314:C:C5	19:S:6:LYS:HE2	2.33	0.63
2:B:158:LEU:H	2:B:158:LEU:HD12	1.62	0.63
6:F:13:ASN:OD1	6:F:13:ASN:N	2.30	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:G:H2'	1:A:23:C:H6	1.64	0.63
9:I:118:LYS:O	9:I:120:ARG:N	2.31	0.63
1:A:755:G:H1'	8:H:1:MET:HE3	1.81	0.63
1:A:1366:C:H2'	1:A:1367:C:H6	1.64	0.63
16:P:10:GLY:HA3	16:P:14:ASN:O	1.99	0.63
13:M:12:ASN:H	13:M:45:VAL:HG12	1.64	0.62
1:A:1504:G:OP1	1:A:1507:A:H4'	1.99	0.62
3:C:179:ARG:HG2	3:C:206:GLU:HG3	1.80	0.62
6:F:10:LEU:HD11	6:F:59:TYR:HD2	1.64	0.62
8:H:85:ARG:NE	8:H:87:SER:O	2.31	0.62
13:M:4:ILE:HD13	13:M:56:LEU:HB3	1.80	0.62
1:A:536:C:H2'	1:A:537:G:H8	1.64	0.62
4:D:190:ASP:H	4:D:193:ASP:HB2	1.63	0.62
1:A:1412:C:H2'	1:A:1413:A:C8	2.33	0.62
10:J:7:LYS:HA	10:J:71:LEU:CD1	2.29	0.62
1:A:1144:G:N2	1:A:1145:C:O2	2.33	0.62
8:H:10:LEU:HD22	8:H:83:ILE:HD13	1.80	0.62
1:A:1241:G:H2'	1:A:1242:C:C6	2.34	0.62
15:O:55:GLY:O	15:O:59:MET:HG3	2.00	0.62
2:B:80:ILE:HD12	2:B:80:ILE:H	1.64	0.62
9:I:55:ALA:HB1	9:I:59:PHE:HB2	1.81	0.62
1:A:1372:U:H5''	9:I:71:SER:HB3	1.80	0.62
2:B:172:ILE:H	2:B:172:ILE:HD12	1.65	0.62
1:A:707:C:H4'	11:K:20:TYR:CD1	2.35	0.61
1:A:826:C:O2	8:H:15:ASN:ND2	2.33	0.61
10:J:61:GLU:HA	24:J:302:HOH:O	2.00	0.61
1:A:792:A:H4'	1:A:793:U:O5'	2.00	0.61
1:A:1124:G:N2	1:A:1127:G:H21	1.99	0.61
3:C:34:LEU:HD23	14:N:25:VAL:HG21	1.82	0.61
15:O:7:GLU:OE1	15:O:38:ARG:NH2	2.33	0.61
1:A:1392:G:H21	1:A:1502:A:H8	1.49	0.61
2:B:74:LYS:HE3	2:B:205:ASP:HB2	1.82	0.61
1:A:881:G:P	12:L:12:ARG:HH22	2.24	0.61
1:A:1086:U:H3	1:A:1099:G:H22	1.47	0.61
5:E:152:ARG:HB3	8:H:43:GLY:HA3	1.81	0.61
5:E:145:LYS:HG3	8:H:107:LEU:HD22	1.82	0.61
12:L:53:ARG:NH1	12:L:92:0TD:OD2	2.33	0.61
1:A:376:G:H5''	16:P:5:ARG:HD2	1.82	0.61
1:A:1518[B]:MA6:H93	1:A:1519[B]:MA6:N1	2.16	0.61
1:A:949:A:H5''	1:A:950:U:OP2	2.01	0.61
1:A:1064:G:H22	1:A:1190:G:H2'	1.63	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:5:PRO:HB2	8:H:6:ILE:HD12	1.83	0.61
8:H:114:THR:HG21	8:H:129:VAL:HG23	1.83	0.61
1:A:279:A:H5'	1:A:279:A:H8	1.66	0.61
1:A:1205:U:OP1	3:C:190:ARG:NH2	2.34	0.61
3:C:147:LYS:HE3	3:C:203:PHE:HE2	1.66	0.61
8:H:97:VAL:HG12	8:H:98:LYS:HG3	1.84	0.60
11:K:65:ALA:HB1	11:K:98:LEU:HB2	1.83	0.60
1:A:328:C:H4'	1:A:329:A:O5'	2.02	0.60
1:A:371:G:O2'	1:A:372:C:H5'	2.01	0.60
1:A:1465:C:H2'	1:A:1466:C:O4'	2.01	0.60
17:Q:15:MET:HE3	17:Q:18:THR:HB	1.84	0.60
1:A:1020:U:H2'	1:A:1021:G:H8	1.67	0.60
1:A:1290:G:H2'	1:A:1291:G:H8	1.65	0.60
10:J:62:HIS:N	24:J:301:HOH:O	2.12	0.60
2:B:53:ARG:HG2	2:B:54:THR:N	2.16	0.60
1:A:21:G:HO2'	1:A:22:G:P	2.23	0.60
1:A:1228:C:O3'	13:M:116:THR:HG23	2.02	0.60
1:A:1397:C:O2'	1:A:1398:A:OP1	2.14	0.60
1:A:436:C:H2'	1:A:437:U:H6	1.67	0.60
3:C:8:ILE:HG23	3:C:16:ARG:HE	1.67	0.60
1:A:419:C:H42	1:A:424:G:H1	1.48	0.60
1:A:518:C:H4'	1:A:519:C:O5'	2.02	0.60
1:A:1318:A:H2'	19:S:37:ARG:HD2	1.82	0.60
1:A:1356:G:H2'	1:A:1357:A:C8	2.37	0.60
1:A:1499:A:H1'	1:A:1520[A]:G:H5'	1.84	0.60
3:C:70:VAL:HG21	3:C:76:VAL:HG21	1.84	0.60
9:I:88:TYR:CD2	9:I:89:ASN:HB2	2.37	0.60
13:M:12:ASN:H	13:M:45:VAL:CG1	2.14	0.60
7:G:26:PHE:CD1	7:G:101:LEU:HD22	2.36	0.59
11:K:121:PRO:HD2	11:K:126:ARG:HD2	1.84	0.59
20:T:29:LYS:O	20:T:32:ALA:HB3	2.01	0.59
4:D:156:GLU:O	4:D:160:GLN:HB2	2.02	0.59
1:A:24:U:H2'	1:A:25:C:C6	2.37	0.59
1:A:372:C:H4'	1:A:373:A:O5'	2.01	0.59
1:A:1398:A:H5''	1:A:1401:G:H4'	1.84	0.59
1:A:1414:U:H2'	1:A:1415:G:H8	1.67	0.59
10:J:57:LYS:NZ	24:J:303:HOH:O	2.28	0.59
5:E:97:GLY:N	5:E:117:ASP:OD2	2.36	0.59
10:J:6:ILE:HB	10:J:72:VAL:HG21	1.84	0.59
14:N:27:CYS:SG	14:N:29:ARG:HB2	2.42	0.59
1:A:501:C:H2'	1:A:502:G:H8	1.64	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:7:LYS:HE2	10:J:9:ARG:HH21	1.67	0.59
1:A:413:G:H1	4:D:36:ARG:HH11	1.48	0.59
1:A:1130:A:O2'	9:I:3:GLN:NE2	2.32	0.59
9:I:113:LYS:H	9:I:119:ALA:HA	1.68	0.59
1:A:9:G:OP2	5:E:121:LYS:NZ	2.33	0.59
1:A:91:C:H2'	1:A:92:C:C6	2.37	0.59
1:A:864:A:H2'	1:A:865:A:C8	2.38	0.59
1:A:975:A:H4'	1:A:976:G:O5'	2.02	0.59
9:I:28:VAL:O	9:I:31:GLN:N	2.36	0.59
1:A:614:A:H2'	1:A:615:C:C6	2.37	0.59
1:A:738:C:OP2	6:F:92:LYS:NZ	2.31	0.59
1:A:1362:C:O2'	24:A:2162:HOH:O	2.17	0.59
7:G:89:MET:HA	7:G:155:ARG:HD3	1.84	0.59
1:A:563:A:H5''	1:A:564:C:OP1	2.03	0.59
1:A:1116:C:O2'	9:I:108:VAL:HG21	2.03	0.59
9:I:43:ALA:HA	9:I:74:ILE:HD13	1.85	0.59
3:C:11:ARG:NH2	3:C:175:LEU:O	2.33	0.58
11:K:120:ARG:HH11	11:K:120:ARG:HG2	1.67	0.58
15:O:35:ARG:HB3	15:O:59:MET:HE1	1.85	0.58
1:A:222:U:H2'	1:A:223:U:C6	2.38	0.58
1:A:778:G:H8	1:A:778:G:O5'	1.85	0.58
2:B:240:GLN:OE1	2:B:240:GLN:N	2.36	0.58
1:A:450:G:H4'	16:P:41:PRO:HB2	1.84	0.58
1:A:1004:A:O2'	1:A:1005:A:OP1	2.20	0.58
12:L:55:VAL:HG12	12:L:69:TYR:HA	1.84	0.58
19:S:39:THR:HG22	19:S:40:ILE:O	2.02	0.58
21:U:15:ARG:HH11	21:U:15:ARG:HB2	1.67	0.58
1:A:933:G:OP2	7:G:3:ARG:HB3	2.04	0.58
5:E:80:ILE:HD11	5:E:138:ALA:HB1	1.84	0.58
10:J:3:LYS:HA	10:J:75:ILE:HG12	1.85	0.58
10:J:32:ALA:O	10:J:34:VAL:HG23	2.03	0.58
20:T:39:LYS:O	20:T:43:LEU:HB2	2.03	0.58
1:A:937:A:N6	1:A:1345:U:O4	2.36	0.58
1:A:1111:A:H61	3:C:177:THR:HB	1.68	0.58
6:F:71:ARG:O	6:F:74:ASP:N	2.36	0.58
8:H:97:VAL:H	8:H:98:LYS:NZ	2.01	0.58
1:A:951:G:OP2	13:M:102:ARG:NH2	2.33	0.58
1:A:1147:C:H4'	9:I:5:TYR:CE1	2.38	0.58
1:A:1368:G:OP2	9:I:112:LYS:HD3	2.03	0.58
3:C:154:SER:OG	3:C:155:GLY:N	2.30	0.58
7:G:15:ASP:OD1	7:G:44:TYR:OH	2.20	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:84:LEU:HD23	12:L:101:VAL:HG21	1.85	0.58
1:A:1048:G:H1	1:A:1209:C:H42	1.49	0.58
1:A:1286:A:H2'	1:A:1287:A:H4'	1.85	0.58
1:A:1297:C:OP1	13:M:44:ARG:NH2	2.37	0.58
1:A:1426:C:H2'	1:A:1427:U:C6	2.38	0.58
7:G:37:ASN:ND2	24:G:202:HOH:O	2.21	0.58
10:J:3:LYS:N	10:J:75:ILE:HG23	2.19	0.58
1:A:1057:G:H5''	3:C:154:SER:HB2	1.85	0.57
10:J:50:ILE:HA	10:J:60:ARG:HG2	1.86	0.57
1:A:79:G:C2	1:A:80:G:C8	2.92	0.57
1:A:450:G:N7	1:A:481:G:O6	2.37	0.57
1:A:652:U:O4	1:A:752:G:O2'	2.19	0.57
1:A:1134:G:H1	1:A:1140:C:H42	1.50	0.57
5:E:92:LYS:O	5:E:118:ILE:HG13	2.04	0.57
1:A:1071:C:H42	1:A:1104:G:H1	1.51	0.57
4:D:9:CYS:O	4:D:12:CYS:HB2	2.04	0.57
15:O:60:VAL:HG12	15:O:61:GLY:N	2.19	0.57
1:A:1372:U:H2'	1:A:1373:G:O4'	2.04	0.57
2:B:213:LEU:HG	2:B:214:ILE:HD13	1.85	0.57
4:D:191:ARG:HH12	4:D:196:LEU:HB2	1.69	0.57
1:A:250:A:H4'	1:A:251:G:O5'	2.04	0.57
1:A:1055:A:N7	1:A:1200:C:N4	2.48	0.57
3:C:14:ILE:HG22	3:C:15:THR:HG23	1.85	0.57
7:G:18:TYR:CD2	7:G:59:LEU:HD13	2.38	0.57
8:H:6:ILE:HD12	8:H:6:ILE:N	2.19	0.57
18:R:36:ASN:HD22	18:R:39:VAL:H	1.52	0.57
1:A:685:G:H2'	1:A:686:U:H5''	1.85	0.57
17:Q:87:LYS:HA	17:Q:90:ILE:HD12	1.86	0.57
1:A:462:G:H21	16:P:82:GLN:HE21	1.52	0.57
1:A:572:A:H5'	1:A:573:A:OP2	2.04	0.57
1:A:1314:C:OP2	19:S:6:LYS:NZ	2.38	0.57
3:C:62:ASP:HA	3:C:97:LYS:HD3	1.86	0.57
1:A:451:A:N6	1:A:481:G:C4	2.73	0.57
1:A:673:G:H2'	1:A:674:G:C8	2.40	0.57
2:B:45:GLN:O	2:B:48:MET:HB2	2.04	0.57
2:B:76:GLN:HG3	2:B:206:ASP:OD1	2.05	0.57
12:L:48:PRO:HG2	12:L:92:0TD:H3	1.87	0.57
13:M:2:ALA:O	13:M:10:PRO:HD2	2.05	0.57
16:P:43:LYS:HG2	16:P:48:TRP:CD2	2.40	0.57
1:A:77:G:O2'	1:A:78:G:H5'	2.04	0.56
1:A:838:G:C2'	1:A:839:U:H5''	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:5:ILE:CD1	3:C:10:PHE:HB2	2.32	0.56
4:D:4:TYR:CE2	4:D:11:LEU:HD11	2.40	0.56
5:E:90:VAL:C	5:E:91:LEU:HD23	2.30	0.56
10:J:84:GLN:HG2	10:J:88:LEU:HD11	1.86	0.56
1:A:79:G:N1	1:A:80:G:C5	2.73	0.56
1:A:130:A:H1'	1:A:263:A:O2'	2.04	0.56
1:A:269:C:H2'	1:A:270:A:C8	2.40	0.56
1:A:518:C:H2'	1:A:530:G:C8	2.40	0.56
1:A:581:G:N7	24:A:1965:HOH:O	2.33	0.56
1:A:1145:C:HO2'	1:A:1146:A:P	2.28	0.56
1:A:1197:G:H5''	24:A:2043:HOH:O	2.04	0.56
1:A:1516[A]:G:N1	1:A:1519[A]:MA6:OP2	2.36	0.56
10:J:49:VAL:O	10:J:61:GLU:N	2.36	0.56
11:K:20:TYR:CD2	11:K:83:ILE:HB	2.40	0.56
1:A:22:G:H2'	1:A:23:C:C6	2.40	0.56
1:A:1152:A:OP1	10:J:68:HIS:NE2	2.38	0.56
1:A:1342:C:H2'	1:A:1343:G:C8	2.39	0.56
3:C:79:ARG:HB2	3:C:79:ARG:HH11	1.71	0.56
3:C:148:GLY:HA3	3:C:172:ARG:O	2.05	0.56
3:C:180:ALA:HB2	3:C:206:GLU:HA	1.87	0.56
9:I:49:PRO:HD3	9:I:101:PHE:CE2	2.40	0.56
12:L:24:VAL:HG13	12:L:98:TYR:HE2	1.69	0.56
12:L:30:ALA:HB1	12:L:31:PRO:HD2	1.87	0.56
16:P:39:TYR:HE2	16:P:41:PRO:HG3	1.71	0.56
1:A:481:G:O2'	1:A:482:A:H8	1.86	0.56
1:A:1256:A:H4'	1:A:1257:U:O5'	2.05	0.56
9:I:89:ASN:HB3	9:I:92:TYR:CD1	2.41	0.56
10:J:6:ILE:HG23	10:J:98:ILE:HG12	1.88	0.56
1:A:279:A:H5'	1:A:279:A:C8	2.40	0.56
1:A:975:A:H5'	1:A:975:A:H8	1.71	0.56
1:A:1006:C:N4	1:A:1022:G:H22	2.02	0.56
1:A:1493:A:O2'	1:A:1494:G:H8	1.88	0.56
10:J:49:VAL:HG13	14:N:41:ARG:HB2	1.87	0.56
12:L:25:PRO:HB3	12:L:27:LEU:HD22	1.86	0.56
1:A:1437:C:H2'	1:A:1438:G:H8	1.71	0.56
2:B:114:ARG:HH11	2:B:118:LEU:HD11	1.71	0.56
5:E:69:VAL:HG22	5:E:139:LEU:HB3	1.87	0.56
11:K:104:GLN:HG2	11:K:106:LYS:HE2	1.86	0.56
14:N:8:GLU:HA	14:N:11:LYS:CD	2.35	0.56
1:A:778:G:H2'	1:A:779:C:O4'	2.04	0.56
1:A:1290:G:H2'	1:A:1291:G:C8	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1435:G:H2'	1:A:1436:U:H6	1.69	0.56
3:C:6:HIS:HE2	3:C:8:ILE:HB	1.71	0.56
5:E:80:ILE:HG22	8:H:104:ARG:HH21	1.70	0.56
10:J:50:ILE:H	10:J:50:ILE:CD1	2.18	0.56
13:M:4:ILE:HG23	13:M:57:ARG:HA	1.87	0.56
1:A:1133:G:H1	1:A:1141:C:H42	1.54	0.56
1:A:1343:G:H2'	1:A:1344:C:C6	2.40	0.56
1:A:1419:G:H1	1:A:1481:U:H3	1.54	0.56
5:E:17:ALA:HA	5:E:26:PHE:HB3	1.87	0.56
12:L:70:ILE:HG21	12:L:75:HIS:HD2	1.71	0.56
1:A:1377:A:C5	7:G:7:ALA:HB1	2.41	0.56
4:D:28:SER:O	4:D:30:LYS:N	2.38	0.56
7:G:40:ALA:CB	9:I:41:VAL:HG21	2.36	0.56
19:S:71:LEU:HD22	19:S:72:GLY:N	2.20	0.56
1:A:707:C:OP1	11:K:85:ARG:NH1	2.39	0.56
1:A:1035:A:H2'	1:A:1036:G:C8	2.39	0.56
1:A:1420:C:H2'	1:A:1421:G:H8	1.70	0.56
1:A:1258:G:OP2	1:A:1258:G:H8	1.89	0.55
1:A:629:G:H2'	1:A:630:G:O4'	2.06	0.55
8:H:2:LEU:HD23	8:H:3:THR:N	2.21	0.55
10:J:91:PRO:HB2	10:J:94:VAL:HB	1.88	0.55
11:K:58:PRO:O	11:K:61:ALA:N	2.39	0.55
1:A:804:U:H5''	1:A:805:C:OP2	2.07	0.55
9:I:126:SER:OG	9:I:127:LYS:N	2.39	0.55
15:O:6:GLU:H	15:O:6:GLU:CD	2.06	0.55
20:T:81:LYS:O	20:T:85:MET:HG3	2.06	0.55
1:A:338:A:H2'	1:A:339:C:O4'	2.06	0.55
10:J:57:LYS:O	10:J:60:ARG:NH1	2.39	0.55
15:O:7:GLU:O	15:O:11:VAL:HG23	2.07	0.55
17:Q:4:LYS:HG3	17:Q:5:VAL:N	2.19	0.55
1:A:77:G:C4	1:A:93:G:N2	2.75	0.55
1:A:793:U:O2	1:A:1516[A]:G:O2'	2.24	0.55
1:A:942:G:H21	9:I:124:GLN:HE22	1.54	0.55
1:A:1349:A:OP2	9:I:118:LYS:HD3	2.07	0.55
1:A:1422:G:N2	1:A:1479:C:N3	2.55	0.55
2:B:17:PHE:HD1	2:B:18:GLY:N	2.04	0.55
2:B:20:GLU:HA	2:B:23:ARG:NH1	2.22	0.55
5:E:152:ARG:NE	8:H:44:PHE:HE1	2.03	0.55
1:A:89:C:O2'	1:A:90:U:H5'	2.07	0.55
1:A:513:C:H2'	1:A:514:C:O4'	2.06	0.55
1:A:881:G:OP2	12:L:12:ARG:NH2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:946:A:H2'	1:A:947:G:C8	2.42	0.55
13:M:15:VAL:HG21	13:M:48:LEU:HD21	1.87	0.55
17:Q:63:ARG:HG2	17:Q:64:PRO:CD	2.35	0.55
1:A:558:G:H5''	1:A:559:A:H3'	1.87	0.55
1:A:988:G:O2'	1:A:1015:A:N6	2.30	0.55
1:A:1511:G:H2'	1:A:1512:U:O4'	2.07	0.55
7:G:136:LYS:C	7:G:136:LYS:HE2	2.32	0.55
11:K:32:ILE:O	11:K:40:ILE:N	2.38	0.55
1:A:1349:A:C2	1:A:1374:A:C4	2.95	0.55
1:A:750:G:H1'	15:O:23:GLY:H	1.70	0.55
1:A:1145:C:O2'	1:A:1146:A:O5'	2.20	0.55
6:F:27:GLN:HA	6:F:30:LEU:HD12	1.88	0.55
10:J:79:ARG:HH22	10:J:82:ILE:HB	1.71	0.55
1:A:35:G:H2'	1:A:36:C:C6	2.42	0.55
1:A:411:A:C8	1:A:413:G:H1'	2.41	0.55
1:A:1315:U:O2'	1:A:1360:A:O2'	2.23	0.55
2:B:122:PHE:HA	2:B:127:ILE:HD11	1.88	0.55
3:C:167:TRP:HA	3:C:167:TRP:CE3	2.41	0.55
5:E:93:PRO:O	8:H:105:ARG:NH2	2.40	0.55
10:J:27:ALA:HB2	10:J:85:LEU:HD21	1.87	0.55
10:J:52:GLY:O	14:N:41:ARG:NH2	2.39	0.55
1:A:1497:G:C2'	1:A:1498:UR3:H5'	2.36	0.54
4:D:155:LEU:HB3	4:D:158:ILE:HG13	1.89	0.54
9:I:48:GLU:N	9:I:49:PRO:HD2	2.22	0.54
10:J:79:ARG:NH2	10:J:82:ILE:HB	2.22	0.54
12:L:70:ILE:HG21	12:L:75:HIS:CD2	2.42	0.54
1:A:276:G:O2'	17:Q:68:ARG:NH1	2.40	0.54
10:J:81:THR:O	10:J:85:LEU:HG	2.07	0.54
18:R:19:LYS:O	18:R:19:LYS:HD3	2.07	0.54
1:A:620:C:H2'	1:A:621:A:O4'	2.07	0.54
3:C:119:ARG:O	3:C:122:GLU:HB2	2.08	0.54
3:C:141:VAL:HG11	3:C:202:ILE:HG12	1.90	0.54
5:E:18:ARG:HG2	5:E:19:MET:N	2.22	0.54
16:P:19:ILE:HG22	16:P:36:ILE:HG13	1.90	0.54
1:A:1147:C:O2	9:I:16:ARG:NH2	2.40	0.54
1:A:1342:C:H2'	1:A:1343:G:H8	1.70	0.54
1:A:968:A:C8	1:A:1062:U:H4'	2.43	0.54
9:I:3:GLN:OE1	9:I:20:ARG:NH2	2.40	0.54
12:L:110:VAL:HG23	12:L:120:TYR:HB3	1.89	0.54
13:M:16:ASP:N	13:M:16:ASP:OD1	2.41	0.54
19:S:41:VAL:HG22	19:S:44:MET:HE3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:560:U:H5'	1:A:566:G:N2	2.23	0.54
6:F:29:ALA:HA	6:F:32:ASN:HB2	1.89	0.54
15:O:18:PHE:CZ	15:O:21:ASP:HB2	2.42	0.54
1:A:8:A:N6	4:D:209:ARG:HB2	2.23	0.54
1:A:1006:C:H2'	1:A:1007:C:H6	1.71	0.54
1:A:1236:A:H4'	1:A:1304:G:H4'	1.89	0.54
4:D:82:ALA:HB1	4:D:92:VAL:HG12	1.90	0.54
1:A:547:A:OP2	4:D:2:GLY:N	2.40	0.54
1:A:664:G:H22	1:A:741:G:H1	1.54	0.54
1:A:1197:G:H22	10:J:56:HIS:CE1	2.26	0.54
1:A:1291:G:H2'	1:A:1292:U:C6	2.42	0.54
20:T:49:ALA:HB3	20:T:99:LEU:HD12	1.90	0.54
1:A:644:G:C5	1:A:645:C:C5	2.95	0.54
1:A:1516[A]:G:H2'	1:A:1518[A]:MA6:OP2	2.08	0.54
2:B:9:GLU:HG3	2:B:12:GLU:HG2	1.90	0.54
3:C:174:PRO:HB2	3:C:177:THR:CG2	2.38	0.54
1:A:1285:A:H4'	1:A:1286:A:O5'	2.08	0.54
6:F:101:ALA:HA	18:R:28:GLU:HG2	1.90	0.54
1:A:113:G:H2'	1:A:114:U:C6	2.43	0.53
1:A:782:A:OP1	1:A:1521:G:N2	2.41	0.53
1:A:1111:A:N1	3:C:177:THR:HB	2.24	0.53
3:C:110:ASN:OD1	3:C:140:ARG:HB3	2.08	0.53
5:E:92:LYS:HB3	5:E:119:LEU:HB2	1.91	0.53
11:K:92:GLU:OE2	11:K:95:ILE:HD12	2.07	0.53
1:A:8:A:C6	4:D:209:ARG:HB2	2.43	0.53
1:A:186:C:H2'	1:A:187:C:C6	2.43	0.53
1:A:200:G:H2'	1:A:201:C:O4'	2.09	0.53
1:A:436:C:H2'	1:A:437:U:C6	2.42	0.53
1:A:1352:C:N3	1:A:1370:G:N2	2.44	0.53
9:I:103:THR:HG22	9:I:104:ARG:O	2.09	0.53
3:C:79:ARG:HB2	3:C:79:ARG:NH1	2.23	0.53
3:C:136:GLN:HG3	3:C:140:ARG:HH21	1.72	0.53
7:G:100:ALA:O	7:G:104:LEU:HG	2.09	0.53
18:R:36:ASN:ND2	18:R:39:VAL:H	2.06	0.53
20:T:61:SER:O	20:T:65:LYS:HG2	2.08	0.53
1:A:404:U:H2'	1:A:405:U:H6	1.74	0.53
1:A:1096:C:H2'	1:A:1097:C:H6	1.73	0.53
1:A:1373:G:H5''	7:G:36:LYS:HB2	1.89	0.53
2:B:162:ILE:O	2:B:185:ILE:HD12	2.09	0.53
8:H:120:THR:HG23	8:H:123:GLU:CD	2.34	0.53
2:B:60:ASP:O	2:B:64:ARG:HB2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:97:TRP:CZ2	2:B:101:MET:HB2	2.44	0.53
19:S:30:LEU:HA	19:S:48:THR:O	2.09	0.53
21:U:5:ASP:O	21:U:11:GLY:HA3	2.08	0.53
1:A:1225:A:H2'	1:A:1225:A:N3	2.23	0.53
1:A:1243:C:H5''	21:U:8:THR:HG22	1.89	0.53
1:A:1438:G:H2'	1:A:1439:C:H6	1.74	0.53
4:D:25:ARG:C	4:D:27:TYR:H	2.16	0.53
1:A:484:G:O2'	1:A:485:G:OP2	2.25	0.53
2:B:91:PRO:HG2	2:B:155:LEU:CD2	2.38	0.53
2:B:124:SER:HB3	2:B:126:GLU:OE2	2.09	0.53
4:D:18:LYS:HE2	4:D:20:TYR:HE2	1.73	0.53
13:M:89:GLY:O	13:M:93:ARG:HG2	2.09	0.53
18:R:30:ASP:OD1	18:R:32:ARG:N	2.37	0.53
1:A:88:A:H2'	1:A:89:C:O4'	2.09	0.53
1:A:1305:G:C8	1:A:1305:G:OP2	2.62	0.53
1:A:1417:G:O2'	1:A:1483:A:N6	2.42	0.53
2:B:36:ARG:O	2:B:39:ILE:HG22	2.09	0.53
4:D:102:ASP:OD1	4:D:103:ASN:N	2.40	0.53
5:E:88:LYS:HB3	5:E:123:LEU:HB2	1.91	0.53
6:F:8:ILE:HD13	6:F:26:ILE:HD13	1.90	0.53
5:E:100:VAL:O	5:E:107:ARG:NH2	2.42	0.53
6:F:3:ARG:HB3	6:F:93:SER:HB2	1.90	0.53
7:G:87:VAL:HG13	7:G:151:TYR:HB3	1.91	0.53
15:O:15:PHE:CZ	15:O:85:LEU:HD21	2.44	0.53
1:A:1053:G:HO2'	1:A:1199:U:H5	1.57	0.52
2:B:35:GLU:OE1	2:B:38:GLY:HA2	2.09	0.52
4:D:3:ARG:NH1	4:D:70:ILE:HA	2.24	0.52
8:H:114:THR:HB	8:H:116:LYS:H	1.74	0.52
14:N:21:TYR:HE2	14:N:23:ARG:HE	1.56	0.52
17:Q:37:LYS:O	17:Q:38:ARG:HD2	2.08	0.52
18:R:39:VAL:O	18:R:42:ARG:HB2	2.09	0.52
1:A:758:G:H8	1:A:758:G:O5'	1.92	0.52
1:A:966:M2G:H2'	1:A:967:5MC:H6	1.73	0.52
1:A:1498:UR3:O4'	1:A:1519[A]:MA6:H2	2.09	0.52
2:B:157:ARG:HG2	2:B:158:LEU:N	2.24	0.52
6:F:22:GLU:OE1	6:F:82:ARG:NH1	2.42	0.52
11:K:34:ASP:OD1	11:K:38:ASN:N	2.41	0.52
1:A:932:C:H5'	7:G:4:ARG:HG2	1.90	0.52
1:A:1367:C:O5'	9:I:112:LYS:NZ	2.42	0.52
4:D:155:LEU:HD23	4:D:156:GLU:H	1.73	0.52
12:L:42:THR:HG23	12:L:52:LEU:HB3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:G:C2	1:A:78:G:C4	2.97	0.52
1:A:373:A:H1'	1:A:481:G:N3	2.25	0.52
1:A:1240:U:H1'	7:G:38:LEU:HD21	1.92	0.52
4:D:101:LEU:O	4:D:105:VAL:HG23	2.09	0.52
1:A:560:U:H5'	1:A:566:G:C2	2.45	0.52
1:A:1178:G:N2	1:A:1181:G:OP2	2.43	0.52
7:G:47:CYS:HB3	7:G:58:PRO:HG2	1.91	0.52
15:O:5:LYS:O	15:O:8:LYS:HB2	2.09	0.52
1:A:378:G:H2'	1:A:379:C:C6	2.44	0.52
1:A:960:U:H1'	1:A:1223:C:H5'	1.92	0.52
1:A:1361(A):C:H2'	1:A:1362:C:H5''	1.92	0.52
11:K:33:THR:HA	11:K:39:PRO:HA	1.91	0.52
1:A:1004:A:H5''	1:A:1025:U:C2	2.44	0.52
4:D:177:ASP:OD2	4:D:179:GLU:HB2	2.09	0.52
11:K:59:TYR:O	11:K:62:GLN:HB3	2.09	0.52
1:A:409:G:H1	1:A:433:C:H42	1.56	0.52
1:A:476:G:H2'	1:A:477:G:C8	2.45	0.52
1:A:770:C:O2'	1:A:771:G:H5'	2.10	0.52
1:A:1283:G:H2'	1:A:1284:C:H6	1.75	0.52
8:H:4:ASP:OD1	8:H:6:ILE:N	2.38	0.52
20:T:13:LEU:HD12	20:T:14:LYS:N	2.24	0.52
1:A:75:G:N1	1:A:76:C:N3	2.58	0.52
1:A:999:C:H2'	1:A:1000:U:C6	2.45	0.52
4:D:3:ARG:HH11	4:D:70:ILE:HA	1.75	0.52
4:D:192:GLU:C	4:D:194:LEU:H	2.17	0.52
5:E:13:ILE:HG22	5:E:30:ALA:HA	1.92	0.52
7:G:18:TYR:CE2	7:G:59:LEU:HB2	2.45	0.52
8:H:9:MET:CG	8:H:26:VAL:HG21	2.28	0.52
10:J:10:GLY:HA3	10:J:16:LEU:HD21	1.91	0.52
12:L:25:PRO:HG3	12:L:27:LEU:HD13	1.92	0.52
4:D:57:ARG:HG3	4:D:202:LEU:HD13	1.90	0.51
9:I:25:LYS:HE2	9:I:60:ASP:OD2	2.09	0.51
15:O:18:PHE:HB2	15:O:19:PRO:HD2	1.91	0.51
21:U:15:ARG:HB2	21:U:15:ARG:NH1	2.26	0.51
1:A:1305:G:OP1	21:U:2:GLY:N	2.43	0.51
1:A:1305:G:O2'	1:A:1306:A:OP2	2.23	0.51
1:A:1376:U:O4	7:G:10:ARG:NH1	2.43	0.51
1:A:1488:G:H2'	1:A:1489:G:H8	1.75	0.51
2:B:47:THR:HG23	2:B:202:PRO:HG2	1.92	0.51
2:B:82:ARG:NE	2:B:92:TYR:OH	2.35	0.51
11:K:54:ARG:O	11:K:57:THR:HG22	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:7:THR:O	17:Q:23:VAL:HG13	2.10	0.51
1:A:176:C:O2'	1:A:177:C:H5'	2.09	0.51
1:A:518:C:H2'	1:A:530:G:H8	1.76	0.51
1:A:1008:C:O2	1:A:1023:G:N2	2.43	0.51
1:A:1009:G:H1	1:A:1020:U:H3	1.58	0.51
1:A:1414:U:H2'	1:A:1415:G:C8	2.44	0.51
2:B:114:ARG:NH1	2:B:118:LEU:HD21	2.25	0.51
4:D:3:ARG:NH2	4:D:74:GLN:OE1	2.43	0.51
7:G:106:GLN:O	7:G:110:GLN:HB2	2.10	0.51
10:J:3:LYS:HB3	10:J:3:LYS:HZ3	1.75	0.51
14:N:25:VAL:HG12	14:N:38:GLY:O	2.10	0.51
1:A:427:U:OP2	4:D:36:ARG:NH2	2.43	0.51
1:A:949:A:OP1	13:M:101:GLN:HB3	2.10	0.51
1:A:1313:U:O4	19:S:4:SER:OG	2.12	0.51
1:A:1392:G:N2	1:A:1502:A:H8	2.09	0.51
1:A:1415:G:H1	1:A:1485:U:H3	1.57	0.51
1:A:1510:U:H2'	1:A:1511:G:C8	2.46	0.51
3:C:108:ASN:C	3:C:110:ASN:N	2.68	0.51
12:L:46:LYS:HG2	12:L:47:LYS:HD3	1.92	0.51
14:N:8:GLU:O	14:N:11:LYS:HB2	2.10	0.51
17:Q:27:PHE:CZ	17:Q:36:ILE:HD11	2.45	0.51
1:A:28:G:O2'	1:A:296:U:OP1	2.28	0.51
1:A:383:A:C5	1:A:384:G:H1'	2.45	0.51
1:A:1009:G:N2	1:A:1010:G:N3	2.58	0.51
1:A:1427:U:H2'	1:A:1428:A:C8	2.46	0.51
3:C:6:HIS:HD2	14:N:49:HIS:HB3	1.74	0.51
1:A:243:A:C2	1:A:246:A:C8	2.99	0.51
1:A:474:G:H4'	16:P:81:ARG:NH2	2.26	0.51
5:E:43:LEU:HD21	5:E:133:TYR:CE2	2.45	0.51
12:L:41:ARG:NH1	12:L:43:VAL:HG13	2.22	0.51
1:A:836:G:C6	1:A:851:G:C6	2.99	0.51
1:A:1213:A:N6	1:A:1215:G:C4	2.78	0.51
1:A:1401:G:C2	1:A:1402:4OC:H1'	2.45	0.51
4:D:141:ARG:N	4:D:144:ASP:OD2	2.40	0.51
13:M:59:TYR:O	13:M:63:THR:OG1	2.28	0.51
15:O:3:ILE:CD1	15:O:35:ARG:HG3	2.41	0.51
18:R:26:LEU:HD12	18:R:27:GLY:H	1.75	0.51
1:A:76:C:H42	1:A:95:U:H3	1.57	0.51
1:A:428:G:H4'	1:A:429:U:O5'	2.11	0.51
1:A:566:G:H4'	1:A:567:G:OP1	2.11	0.51
1:A:757:U:H2'	1:A:758:G:O4'	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:828:A:H4'	1:A:828:A:OP1	2.11	0.51
2:B:24:TRP:CG	2:B:25:ASN:H	2.28	0.51
1:A:1301:U:HO2'	1:A:1302:U:P	2.33	0.51
2:B:98:LEU:HB2	2:B:101:MET:SD	2.51	0.51
5:E:102:ALA:H	5:E:107:ARG:HH12	1.59	0.51
5:E:122:GLU:O	5:E:123:LEU:HD23	2.11	0.51
7:G:68:ASN:O	7:G:138:LYS:HD3	2.11	0.51
8:H:97:VAL:N	8:H:98:LYS:NZ	2.59	0.51
20:T:65:LYS:O	20:T:68:LYS:HB3	2.11	0.51
1:A:31:G:O2'	1:A:48:C:N4	2.44	0.51
1:A:127:G:N2	1:A:234:C:O2	2.28	0.51
1:A:1305:G:H22	1:A:1331:G:H1'	1.76	0.51
1:A:1402:4OC:HM22	1:A:1403:C:H5'	1.92	0.51
15:O:39:LEU:HD13	15:O:56:LEU:HD13	1.93	0.51
19:S:11:VAL:HG13	19:S:15:LEU:HD11	1.92	0.51
1:A:91:C:C6	1:A:92:C:H5	2.29	0.50
1:A:335:C:H2'	1:A:336:C:C6	2.46	0.50
1:A:370:C:C2'	1:A:371:G:H5'	2.41	0.50
1:A:390:C:H2'	1:A:391:G:C8	2.46	0.50
1:A:476:G:H2'	1:A:477:G:H8	1.76	0.50
2:B:212:GLN:O	2:B:216:SER:HB3	2.11	0.50
3:C:178:LEU:HD22	3:C:179:ARG:N	2.26	0.50
6:F:36:ARG:NH1	6:F:66:GLU:OE1	2.44	0.50
9:I:118:LYS:C	9:I:120:ARG:H	2.19	0.50
1:A:115:G:H1'	1:A:116:A:N7	2.26	0.50
1:A:811:C:O2'	1:A:901:A:N1	2.42	0.50
1:A:1250:A:H5''	9:I:67:GLY:HA2	1.92	0.50
3:C:36:ASP:OD2	3:C:59:ARG:NH2	2.44	0.50
8:H:102:ARG:HH11	8:H:105:ARG:HD3	1.74	0.50
1:A:130:A:H5'	17:Q:63:ARG:HE	1.76	0.50
1:A:216:G:H2'	1:A:217:C:C6	2.46	0.50
1:A:321:A:H2'	1:A:322:C:C6	2.46	0.50
6:F:10:LEU:CD1	6:F:59:TYR:HB3	2.41	0.50
16:P:53:VAL:O	16:P:55:ARG:N	2.44	0.50
1:A:9:G:OP1	5:E:122:GLU:HG3	2.12	0.50
1:A:81:U:H5'	1:A:82:U:OP2	2.12	0.50
1:A:103:C:OP2	20:T:14:LYS:HD2	2.12	0.50
1:A:224:C:H2'	1:A:225:C:H6	1.76	0.50
1:A:344:A:H5'	1:A:345:C:C5	2.46	0.50
1:A:1313:U:H5	19:S:4:SER:HB2	1.76	0.50
1:A:1343:G:H2'	1:A:1344:C:H6	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1417:G:H2'	1:A:1482:G:H22	1.76	0.50
1:A:409:G:OP1	4:D:24:GLU:O	2.29	0.50
1:A:1222:G:OP2	1:A:1322:C:N4	2.43	0.50
2:B:17:PHE:HD1	2:B:18:GLY:H	1.59	0.50
2:B:115:LEU:HD11	2:B:146:GLN:HG3	1.94	0.50
1:A:108:G:C6	20:T:15:ARG:HD2	2.47	0.50
1:A:384:G:H2'	1:A:385:C:C6	2.46	0.50
1:A:588:G:H1	1:A:651:C:H42	1.60	0.50
1:A:1464:G:O2'	1:A:1465:C:H5'	2.11	0.50
3:C:11:ARG:NH1	3:C:178:LEU:HD23	2.19	0.50
3:C:15:THR:O	3:C:15:THR:OG1	2.25	0.50
1:A:1152:A:OP1	10:J:68:HIS:CD2	2.65	0.50
4:D:64:LEU:HD23	4:D:198:VAL:HG21	1.92	0.50
9:I:82:ALA:HB1	9:I:102:LEU:HD23	1.93	0.50
20:T:13:LEU:HD12	20:T:14:LYS:H	1.76	0.50
1:A:77:G:N2	1:A:78:G:C4	2.79	0.50
1:A:385:C:H2'	1:A:386:C:C6	2.47	0.50
1:A:875:C:O2'	8:H:14:ARG:NH1	2.45	0.50
3:C:87:LEU:O	3:C:91:LEU:HB3	2.12	0.50
4:D:25:ARG:C	4:D:27:TYR:N	2.69	0.50
15:O:3:ILE:HD11	15:O:35:ARG:HG3	1.94	0.50
16:P:34:GLU:OE1	16:P:55:ARG:NH1	2.42	0.50
19:S:80:TYR:CD1	19:S:81:ARG:N	2.78	0.50
1:A:374:A:H5''	1:A:375:U:OP2	2.12	0.50
1:A:532:A:HO2'	1:A:533:A:P	2.30	0.50
1:A:706:A:H1'	11:K:29:ILE:HD11	1.94	0.50
1:A:771:G:N2	1:A:808:C:O2	2.45	0.50
1:A:1251:A:H2'	1:A:1252:A:C8	2.47	0.50
4:D:12:CYS:SG	4:D:19:LEU:O	2.70	0.50
8:H:113:SER:HB2	8:H:134:ILE:HD11	1.93	0.50
19:S:50:ALA:HA	19:S:58:VAL:O	2.12	0.50
1:A:110:C:H2'	1:A:111:G:O4'	2.11	0.49
1:A:324:G:OP1	20:T:22:ARG:HD3	2.12	0.49
1:A:403:C:H2'	1:A:404:U:H6	1.76	0.49
1:A:993:G:H2'	1:A:995:C:H41	1.76	0.49
1:A:1201:A:H4'	1:A:1202:G:O5'	2.12	0.49
6:F:10:LEU:HD12	6:F:59:TYR:HB3	1.94	0.49
8:H:119:LEU:HD12	8:H:124:ALA:HB2	1.94	0.49
1:A:254:G:OP1	17:Q:67:LYS:O	2.29	0.49
4:D:62:GLN:O	4:D:66:ARG:HG3	2.13	0.49
1:A:130:A:C8	17:Q:63:ARG:HG3	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:457:C:H2'	1:A:458:C:H6	1.76	0.49
1:A:556:C:H2'	1:A:557:G:O4'	2.12	0.49
5:E:76:ILE:HB	5:E:77:PRO:HD2	1.93	0.49
7:G:146:GLU:OE2	7:G:149:ARG:HG3	2.12	0.49
13:M:23:TYR:HB3	13:M:67:GLU:H	1.77	0.49
1:A:62:U:O2'	1:A:63:C:H5'	2.12	0.49
1:A:81:U:H2'	1:A:83:U:OP2	2.12	0.49
1:A:337:C:H2'	1:A:338:A:H8	1.77	0.49
7:G:70:LYS:HG2	7:G:96:GLN:HB3	1.95	0.49
13:M:96:LEU:O	13:M:110:ARG:NH1	2.42	0.49
1:A:270:A:H2'	1:A:271:C:C6	2.48	0.49
1:A:353:A:H5'	1:A:353:A:H8	1.76	0.49
1:A:908:A:O2'	1:A:909:A:H5'	2.12	0.49
7:G:72:ARG:N	7:G:72:ARG:HH11	2.10	0.49
10:J:79:ARG:NE	10:J:79:ARG:HA	2.28	0.49
16:P:74:LEU:HD22	16:P:79:VAL:HG21	1.95	0.49
1:A:80:G:H2'	1:A:81:U:O5'	2.12	0.49
1:A:547:A:H4'	1:A:548:G:O5'	2.12	0.49
1:A:1124:G:C2	1:A:1127:G:N2	2.80	0.49
1:A:1329:A:P	13:M:28:ALA:HB3	2.52	0.49
1:A:1435:G:H8	1:A:1435:G:O5'	1.95	0.49
3:C:105:GLU:OE2	3:C:107:GLN:NE2	2.45	0.49
13:M:95:GLY:O	13:M:96:LEU:HD23	2.12	0.49
18:R:86:VAL:HG12	18:R:87:ARG:H	1.77	0.49
19:S:5:LEU:C	19:S:6:LYS:HD3	2.37	0.49
1:A:790:A:H2'	1:A:791:G:C8	2.48	0.49
1:A:908:A:C2	1:A:909:A:C4	3.00	0.49
13:M:11:ARG:HD2	13:M:45:VAL:CG1	2.43	0.49
18:R:58:LEU:HD13	18:R:62:GLU:HB3	1.94	0.49
1:A:409:G:OP2	4:D:22:LYS:HD2	2.13	0.49
1:A:646:U:H2'	1:A:647:C:C6	2.48	0.49
3:C:150:LYS:HB3	3:C:201:TYR:HB2	1.95	0.49
5:E:43:LEU:HD23	5:E:43:LEU:O	2.13	0.49
7:G:5:ARG:HH12	7:G:8:GLU:HG3	1.77	0.49
10:J:79:ARG:HH11	10:J:83:GLU:HB2	1.78	0.49
15:O:6:GLU:HA	15:O:9:GLN:HB2	1.95	0.49
21:U:15:ARG:HG2	21:U:17:THR:HG23	1.95	0.49
1:A:93:G:O2'	1:A:95:U:H5'	2.13	0.49
1:A:255:G:H1'	17:Q:16:GLN:OE1	2.13	0.49
1:A:337:C:H2'	1:A:338:A:C8	2.48	0.49
1:A:509:A:C8	1:A:509:A:C3'	2.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:522:C:H1'	1:A:536:C:H5''	1.95	0.49
1:A:687:A:H4'	1:A:688:G:O5'	2.13	0.49
4:D:8:VAL:O	4:D:11:LEU:N	2.32	0.49
4:D:32:ALA:O	4:D:36:ARG:N	2.41	0.49
6:F:10:LEU:HD12	6:F:10:LEU:H	1.77	0.49
16:P:15:PRO:CD	16:P:42:ARG:HD3	2.39	0.49
19:S:28:LYS:HG2	19:S:29:ARG:N	2.27	0.49
1:A:21:G:N2	1:A:886:G:P	2.86	0.49
1:A:448:A:C2	1:A:449:C:C4	3.01	0.49
1:A:674:G:O2'	1:A:675:A:H5'	2.13	0.49
8:H:86:ILE:HG21	8:H:133:LEU:HD13	1.95	0.49
15:O:17:ARG:HB2	15:O:18:PHE:CD2	2.48	0.49
1:A:679:C:H2'	1:A:680:C:C6	2.47	0.48
2:B:39:ILE:HG23	2:B:41:ILE:HD11	1.94	0.48
3:C:155:GLY:HA3	3:C:163:ALA:HB1	1.95	0.48
5:E:33:VAL:HG13	5:E:112:LEU:HD12	1.95	0.48
8:H:102:ARG:NH1	8:H:105:ARG:HD3	2.27	0.48
13:M:108:ARG:HD3	13:M:114:ARG:NH1	2.28	0.48
18:R:25:THR:O	18:R:26:LEU:HB2	2.12	0.48
2:B:87:ARG:HH21	2:B:219:VAL:HG12	1.78	0.48
3:C:156:ARG:H	3:C:163:ALA:HA	1.77	0.48
5:E:17:ALA:HB2	5:E:26:PHE:HD2	1.77	0.48
12:L:48:PRO:CG	12:L:92:OTD:H3	2.43	0.48
15:O:9:GLN:O	15:O:10:LYS:C	2.56	0.48
16:P:54:GLU:CD	16:P:54:GLU:C	2.81	0.48
18:R:74:ARG:HB3	18:R:81:PHE:CE1	2.47	0.48
1:A:197:A:N1	1:A:220:G:O2'	2.44	0.48
1:A:259:G:H2'	1:A:260:G:C8	2.48	0.48
1:A:858:G:O6	1:A:869:G:C8	2.66	0.48
1:A:926:G:N2	1:A:1542:U:OP1	2.34	0.48
1:A:1443:G:O5'	1:A:1443:G:H8	1.97	0.48
2:B:84:GLU:OE1	2:B:216:SER:HA	2.12	0.48
7:G:104:LEU:HA	7:G:104:LEU:HD23	1.52	0.48
8:H:98:LYS:H	8:H:98:LYS:HE2	1.77	0.48
1:A:438:G:H4'	4:D:123:HIS:CD2	2.48	0.48
1:A:628:G:H2'	1:A:629:G:H8	1.79	0.48
2:B:20:GLU:HA	2:B:23:ARG:HH11	1.79	0.48
5:E:19:MET:HE1	5:E:24:ARG:HH11	1.76	0.48
7:G:5:ARG:HG2	7:G:6:ARG:H	1.79	0.48
10:J:25:GLU:HA	10:J:28:ARG:HB2	1.96	0.48
11:K:80:VAL:HG21	11:K:103:LEU:HD13	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:91:ARG:HH12	18:R:88:LYS:HE2	1.78	0.48
12:L:93:LEU:O	12:L:96:VAL:HG23	2.13	0.48
13:M:8:GLU:CD	13:M:22:ILE:HA	2.37	0.48
1:A:113:G:H2'	1:A:114:U:H6	1.78	0.48
1:A:1117:G:H5''	9:I:104:ARG:NH2	2.28	0.48
3:C:20:SER:HA	3:C:57:ILE:O	2.13	0.48
13:M:62:ASN:OD1	13:M:62:ASN:N	2.40	0.48
15:O:12:ILE:O	15:O:15:PHE:N	2.46	0.48
18:R:22:VAL:HG23	18:R:55:ARG:O	2.14	0.48
1:A:393:A:OP2	16:P:12:LYS:NZ	2.44	0.48
1:A:1492:A:H3'	1:A:1493:A:O4'	2.14	0.48
4:D:30:LYS:C	4:D:32:ALA:H	2.21	0.48
5:E:131:ILE:O	5:E:134:ALA:N	2.45	0.48
7:G:135:VAL:O	7:G:139:GLU:HG3	2.14	0.48
9:I:5:TYR:CD2	9:I:6:GLY:N	2.82	0.48
9:I:25:LYS:HG3	9:I:60:ASP:OD1	2.14	0.48
10:J:7:LYS:HA	10:J:71:LEU:HD11	1.95	0.48
13:M:34:LEU:HD12	13:M:39:ILE:O	2.14	0.48
16:P:6:LEU:HD12	16:P:6:LEU:N	2.28	0.48
1:A:1488:G:H2'	1:A:1489:G:C8	2.49	0.48
2:B:170:GLU:O	2:B:172:ILE:N	2.46	0.48
4:D:31:CYS:O	4:D:31:CYS:SG	2.71	0.48
6:F:100:ASN:H	18:R:23:LYS:HZ1	1.60	0.48
7:G:94:ARG:O	7:G:97:GLN:HB3	2.14	0.48
8:H:69:ARG:NH1	8:H:75:ARG:O	2.46	0.48
14:N:16:PHE:HD1	14:N:19:ARG:HH11	1.61	0.48
20:T:56:MET:HG3	20:T:88:VAL:HG21	1.94	0.48
1:A:352:C:H6	1:A:352:C:H5''	1.78	0.48
1:A:841:U:H6	1:A:841:U:P	2.37	0.48
1:A:872:A:C8	1:A:874:G:C8	3.02	0.48
1:A:1004:A:HO2'	1:A:1005:A:P	2.36	0.48
1:A:1279:A:H5''	10:J:7:LYS:NZ	2.28	0.48
2:B:189:ASP:OD1	2:B:205:ASP:HB3	2.13	0.48
3:C:174:PRO:O	3:C:177:THR:HG23	2.13	0.48
4:D:200:GLU:CD	4:D:200:GLU:N	2.72	0.48
8:H:104:ARG:HD2	8:H:138:TRP:CD2	2.48	0.48
16:P:53:VAL:O	16:P:54:GLU:C	2.56	0.48
17:Q:95:TYR:HA	17:Q:98:LEU:CD1	2.44	0.48
1:A:1092:A:N3	1:A:1183:A:N6	2.62	0.48
1:A:1329:A:H5''	13:M:29:ARG:HD2	1.95	0.48
1:A:1409:C:H2'	1:A:1410:G:C8	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:236:TYR:O	2:B:239:VAL:HB	2.13	0.48
5:E:87:SER:HB3	5:E:131:ILE:HD13	1.94	0.48
8:H:113:SER:O	8:H:131:GLY:HA3	2.14	0.48
1:A:1437:C:H2'	1:A:1438:G:C8	2.48	0.48
8:H:98:LYS:H	8:H:98:LYS:CE	2.27	0.48
1:A:664:G:OP1	18:R:64:ARG:HD2	2.13	0.47
1:A:1347:G:O2'	1:A:1348:U:P	2.71	0.47
2:B:163:PHE:CD1	2:B:185:ILE:HB	2.49	0.47
3:C:108:ASN:HB3	3:C:111:LEU:H	1.79	0.47
4:D:36:ARG:HG2	4:D:38:TYR:OH	2.14	0.47
4:D:108:LEU:HD22	4:D:176:LEU:HB2	1.94	0.47
5:E:40:ARG:HG2	5:E:40:ARG:HH11	1.79	0.47
5:E:77:PRO:HD2	5:E:142:LEU:HD13	1.95	0.47
6:F:4:TYR:HE1	6:F:92:LYS:HG2	1.79	0.47
7:G:111:ARG:HG2	7:G:112:PRO:HD2	1.95	0.47
15:O:15:PHE:CZ	15:O:84:LYS:HD3	2.49	0.47
1:A:977:A:C2'	1:A:978:A:H5''	2.43	0.47
1:A:1031:G:H2'	1:A:1032:G:C8	2.49	0.47
1:A:1181:G:O2'	1:A:1182:G:H5'	2.14	0.47
1:A:1450:U:O2'	1:A:1451:A:H8	1.97	0.47
3:C:156:ARG:NH1	3:C:193:TYR:O	2.47	0.47
5:E:105:VAL:HG12	5:E:106:PRO:N	2.29	0.47
7:G:5:ARG:NH1	7:G:8:GLU:HG3	2.29	0.47
10:J:16:LEU:HD22	10:J:94:VAL:HG13	1.96	0.47
12:L:110:VAL:CG2	12:L:120:TYR:HB3	2.43	0.47
17:Q:11:VAL:HG12	17:Q:85:VAL:HG22	1.97	0.47
1:A:986:A:N3	19:S:52:TYR:OH	2.44	0.47
1:A:1530:G:H4'	1:A:1530:G:OP1	2.13	0.47
8:H:84:ARG:O	8:H:135:CYS:HB2	2.14	0.47
9:I:118:LYS:HG3	9:I:121:ARG:HB3	1.97	0.47
12:L:127:GLU:OE2	12:L:127:GLU:N	2.46	0.47
17:Q:90:ILE:O	17:Q:91:ARG:C	2.56	0.47
1:A:77:G:C5	1:A:93:G:N1	2.81	0.47
1:A:1474:G:H2'	1:A:1475:G:C8	2.49	0.47
6:F:8:ILE:HG21	6:F:61:LEU:HD12	1.96	0.47
10:J:38:ILE:H	10:J:38:ILE:HD13	1.79	0.47
11:K:122:LYS:HE2	11:K:122:LYS:HB3	1.48	0.47
20:T:59:ALA:O	20:T:63:ILE:HG13	2.14	0.47
1:A:95:U:H2'	1:A:96:G:H8	1.79	0.47
1:A:112:G:C2	1:A:113:G:C8	3.02	0.47
1:A:328:C:H1'	1:A:329:A:OP2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1409:C:H2'	1:A:1410:G:H8	1.78	0.47
4:D:187:ARG:NH1	4:D:187:ARG:HA	2.29	0.47
4:D:199:ASN:O	4:D:202:LEU:HB2	2.15	0.47
10:J:47:PHE:CZ	14:N:37:PHE:HE1	2.32	0.47
12:L:76:ASN:ND2	12:L:106:ASP:O	2.47	0.47
1:A:413:G:H1	4:D:36:ARG:NH1	2.11	0.47
1:A:1391:U:H2'	1:A:1392:G:C8	2.49	0.47
1:A:1517[B]:G:N7	1:A:1518[B]:MA6:H103	2.29	0.47
3:C:47:LEU:HB3	3:C:50:ALA:HB3	1.96	0.47
5:E:80:ILE:HG22	8:H:104:ARG:NH2	2.30	0.47
5:E:131:ILE:HD13	5:E:131:ILE:HA	1.66	0.47
7:G:17:VAL:HG12	7:G:18:TYR:CD1	2.49	0.47
10:J:40:LEU:HB3	10:J:41:PRO:HD2	1.96	0.47
1:A:7:G:H5'	1:A:298:A:H5'	1.96	0.47
1:A:80:G:HO2'	1:A:81:U:P	2.32	0.47
1:A:116:A:H2'	1:A:117:G:H8	1.79	0.47
1:A:840:C:H4'	1:A:841:U:OP1	2.13	0.47
1:A:925:G:C2	1:A:927:G:C8	3.03	0.47
1:A:1228:C:H4'	13:M:116:THR:HA	1.96	0.47
1:A:1228:C:OP1	13:M:108:ARG:NH2	2.48	0.47
1:A:1402:4OC:O2	1:A:1500:A:N1	2.48	0.47
3:C:6:HIS:CD2	14:N:49:HIS:HB3	2.50	0.47
5:E:96:PRO:HA	5:E:117:ASP:OD2	2.14	0.47
6:F:25:ILE:HD13	6:F:28:ARG:HD2	1.97	0.47
6:F:33:TYR:CD1	6:F:75:LEU:HD23	2.49	0.47
16:P:26:ARG:HD2	16:P:31:LYS:O	2.15	0.47
1:A:75:G:C2	1:A:76:C:C2	3.03	0.47
1:A:377:G:OP1	16:P:3:LYS:HD3	2.15	0.47
1:A:396:G:O2'	1:A:398:C:OP1	2.23	0.47
1:A:448:A:C4	1:A:487:A:C2	3.03	0.47
1:A:1133:G:H2'	1:A:1134:G:C8	2.48	0.47
17:Q:29:HIS:CE1	17:Q:30:PRO:HD2	2.50	0.47
1:A:321:A:H2'	1:A:322:C:H6	1.79	0.47
1:A:633:G:H2'	1:A:634:C:C6	2.49	0.47
1:A:707:C:H5''	11:K:85:ARG:HH12	1.79	0.47
1:A:922:G:C2	1:A:1396:A:C6	3.02	0.47
1:A:1080:A:O3'	5:E:16:THR:OG1	2.31	0.47
2:B:24:TRP:CG	2:B:25:ASN:N	2.83	0.47
4:D:190:ASP:HB2	4:D:193:ASP:OD2	2.15	0.47
7:G:26:PHE:HD1	7:G:101:LEU:HD22	1.78	0.47
10:J:48:THR:HG1	10:J:62:HIS:CG	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:40:LYS:HD2	17:Q:42:TYR:CE1	2.49	0.47
18:R:37:VAL:CG2	18:R:78:LEU:HB3	2.45	0.47
1:A:109:A:C4	1:A:327:A:C2	3.03	0.47
1:A:628:G:H2'	1:A:629:G:C8	2.50	0.47
1:A:841:U:H6	1:A:841:U:OP2	1.99	0.47
15:O:36:ILE:HG12	15:O:59:MET:HE2	1.97	0.47
1:A:1188:A:H5''	24:I:201:HOH:O	2.14	0.46
1:A:1330:U:H2'	1:A:1331:G:H5'	1.95	0.46
8:H:1:MET:HG2	8:H:2:LEU:O	2.15	0.46
9:I:28:VAL:HA	9:I:63:ILE:O	2.16	0.46
17:Q:29:HIS:HA	17:Q:30:PRO:HD3	1.77	0.46
1:A:344:A:H4'	1:A:345:C:OP2	2.15	0.46
1:A:706:A:C1'	11:K:29:ILE:HD11	2.45	0.46
1:A:1227:A:OP2	13:M:111:LYS:HE2	2.15	0.46
7:G:113:GLU:H	7:G:113:GLU:HG2	1.52	0.46
16:P:28:ARG:HG3	16:P:29:ASP:N	2.29	0.46
19:S:42:PRO:O	19:S:45:VAL:HG23	2.15	0.46
1:A:45:U:H2'	1:A:46:G:C8	2.50	0.46
1:A:77:G:C6	1:A:93:G:N1	2.83	0.46
1:A:224:C:H2'	1:A:225:C:C6	2.50	0.46
1:A:913:A:H4'	1:A:914:G:O5'	2.15	0.46
1:A:986:A:H2'	1:A:987:G:O4'	2.16	0.46
1:A:1345:U:H3'	24:A:2229:HOH:O	2.14	0.46
1:A:1438:G:H2'	1:A:1439:C:C6	2.49	0.46
2:B:187:LEU:HD11	2:B:203:GLY:HA3	1.97	0.46
7:G:41:ARG:HB3	7:G:41:ARG:HH11	1.80	0.46
12:L:53:ARG:HH11	12:L:53:ARG:HG3	1.80	0.46
1:A:190(D):U:O2'	1:A:190(E):U:H5'	2.15	0.46
1:A:419:C:N4	1:A:424:G:H1	2.12	0.46
1:A:509:A:H3'	1:A:509:A:H8	1.80	0.46
1:A:921:U:O2'	5:E:19:MET:O	2.29	0.46
2:B:88:ALA:HB2	2:B:219:VAL:HG13	1.98	0.46
5:E:144:THR:HB	5:E:147:ASP:OD1	2.15	0.46
12:L:46:LYS:HE2	12:L:94:PRO:HG2	1.97	0.46
12:L:46:LYS:HB2	12:L:92:OTD:O	2.15	0.46
20:T:68:LYS:HE3	20:T:68:LYS:HA	1.98	0.46
1:A:128:G:C6	1:A:129:U:N3	2.83	0.46
1:A:642:A:C8	8:H:115:SER:HA	2.51	0.46
1:A:877:C:O2'	8:H:3:THR:HG23	2.16	0.46
1:A:1068:G:OP1	1:A:1387:G:O2'	2.33	0.46
1:A:1225:A:H5'	1:A:1226:C:OP2	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1318:A:H4'	19:S:10:PHE:CD2	2.51	0.46
1:A:731:G:OP1	1:A:766:A:H1'	2.14	0.46
1:A:1006:C:H42	1:A:1022:G:H22	1.63	0.46
1:A:1442:G:C6	1:A:1446:A:N7	2.83	0.46
4:D:88:VAL:O	4:D:89:THR:C	2.57	0.46
8:H:20:TYR:HA	8:H:65:TYR:CE2	2.51	0.46
10:J:47:PHE:HB3	14:N:34:TYR:CE2	2.50	0.46
15:O:54:ARG:HG2	15:O:58:MET:HE2	1.96	0.46
1:A:24:U:H2'	1:A:25:C:H6	1.79	0.46
1:A:552:U:H4'	12:L:86:ARG:HG3	1.96	0.46
1:A:1361(A):C:HO2'	1:A:1362:C:H6	1.64	0.46
1:A:1498:UR3:C4'	1:A:1519[A]:MA6:H2	2.45	0.46
3:C:178:LEU:C	3:C:178:LEU:HD13	2.40	0.46
3:C:188:LEU:HD11	3:C:195:VAL:HG22	1.98	0.46
5:E:6:PHE:HE2	5:E:36:ASP:HB3	1.81	0.46
5:E:102:ALA:H	5:E:107:ARG:NH1	2.12	0.46
5:E:110:LEU:HD13	5:E:118:ILE:HD13	1.98	0.46
8:H:80:ILE:HG21	8:H:83:ILE:HG13	1.96	0.46
11:K:17:GLY:HA3	11:K:77:MET:HE1	1.97	0.46
20:T:64:ASP:O	20:T:67:ALA:HB3	2.15	0.46
1:A:78:G:N2	1:A:79:G:H1'	2.31	0.46
1:A:1320:C:N4	19:S:36:ARG:HG3	2.30	0.46
1:A:1405:G:O2'	1:A:1518[A]:MA6:O2'	2.32	0.46
17:Q:35:VAL:O	17:Q:35:VAL:HG12	2.11	0.46
17:Q:74:LEU:HA	17:Q:74:LEU:HD12	1.48	0.46
1:A:330:C:H2'	1:A:331:G:H5'	1.98	0.46
1:A:960:U:H4'	1:A:961:U:C5'	2.46	0.46
1:A:1250:A:H2'	1:A:1251:A:C8	2.51	0.46
2:B:187:LEU:HD22	2:B:201:ILE:HB	1.97	0.46
3:C:11:ARG:HD3	3:C:178:LEU:HD23	1.97	0.46
3:C:16:ARG:CZ	3:C:54:ARG:HH12	2.29	0.46
7:G:92:SER:HB3	7:G:95:ARG:HB2	1.97	0.46
11:K:33:THR:HG22	11:K:39:PRO:HA	1.98	0.46
15:O:26:GLU:OE1	15:O:70:LEU:HD11	2.16	0.46
20:T:50:GLU:HB2	20:T:99:LEU:HD13	1.96	0.46
1:A:75:G:C6	1:A:76:C:C4	3.04	0.46
1:A:204:U:H4'	1:A:216:G:O4'	2.16	0.46
1:A:1420:C:H2'	1:A:1421:G:C8	2.50	0.46
2:B:212:GLN:NE2	2:B:235:SER:OG	2.49	0.46
4:D:155:LEU:HD23	4:D:156:GLU:N	2.31	0.46
6:F:4:TYR:CE1	6:F:92:LYS:HG2	2.52	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:25:ASP:OD1	8:H:25:ASP:N	2.48	0.46
9:I:88:TYR:CE2	9:I:89:ASN:HB2	2.51	0.46
12:L:47:LYS:HD3	12:L:47:LYS:H	1.81	0.46
13:M:11:ARG:HD2	13:M:45:VAL:HG11	1.97	0.46
1:A:6:G:H2'	5:E:119:LEU:HD13	1.98	0.45
1:A:803:G:C6	1:A:804:U:C4	3.04	0.45
3:C:6:HIS:CD2	3:C:9:GLY:H	2.33	0.45
3:C:173:VAL:HG12	3:C:175:LEU:HD21	1.98	0.45
4:D:98:GLU:HG3	4:D:194:LEU:HD21	1.98	0.45
8:H:35:ILE:HD11	8:H:134:ILE:HD13	1.98	0.45
15:O:4:THR:HG23	15:O:7:GLU:OE2	2.16	0.45
15:O:39:LEU:HB3	15:O:56:LEU:HD13	1.97	0.45
16:P:51:VAL:HG12	16:P:53:VAL:N	2.31	0.45
1:A:413:G:H2'	1:A:428:G:N2	2.31	0.45
1:A:602:A:C2	1:A:637:G:C2	3.04	0.45
1:A:1030(A):G:H2'	1:A:1030(C):G:OP2	2.15	0.45
1:A:1074:G:O3'	2:B:103:THR:HG21	2.15	0.45
1:A:1223:C:H3'	1:A:1224:G:C5'	2.45	0.45
1:A:1413:A:H2'	1:A:1414:U:H6	1.82	0.45
2:B:158:LEU:HD12	2:B:158:LEU:N	2.29	0.45
3:C:134:ILE:O	3:C:138:VAL:HG23	2.16	0.45
7:G:26:PHE:HA	7:G:101:LEU:HD13	1.98	0.45
8:H:63:LEU:HD13	8:H:63:LEU:N	2.30	0.45
11:K:20:TYR:HD2	11:K:83:ILE:HB	1.81	0.45
11:K:95:ILE:HG21	11:K:108:ILE:HD13	1.98	0.45
12:L:77:LEU:HA	12:L:77:LEU:HD23	1.54	0.45
18:R:34:TYR:CE1	18:R:35:ARG:HG3	2.50	0.45
1:A:748:C:H4'	1:A:749:C:O5'	2.16	0.45
1:A:1122:U:H5	1:A:1123:A:C8	2.35	0.45
3:C:35:GLU:O	3:C:39:ILE:HG13	2.16	0.45
14:N:7:ILE:O	14:N:7:ILE:HG22	2.16	0.45
1:A:882:C:O2'	1:A:883:C:H5'	2.15	0.45
1:A:943:U:H2'	1:A:944:G:H5'	1.98	0.45
5:E:98:THR:HB	5:E:117:ASP:HB3	1.98	0.45
8:H:59:LEU:HA	8:H:59:LEU:HD23	1.74	0.45
12:L:35:GLY:HA3	12:L:60:LEU:HD13	1.98	0.45
1:A:91:C:H2'	1:A:92:C:H6	1.78	0.45
1:A:129:U:O3'	1:A:129(A):G:H3'	2.16	0.45
1:A:443:C:H42	1:A:491:G:H1	1.64	0.45
1:A:1063:C:H2'	1:A:1064:G:C8	2.52	0.45
1:A:1505:G:C8	1:A:1505:G:H3'	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:108:ASN:CB	3:C:111:LEU:H	2.29	0.45
3:C:150:LYS:HD2	3:C:173:VAL:HG11	1.98	0.45
8:H:80:ILE:CG2	8:H:83:ILE:HG13	2.47	0.45
1:A:918:A:H2'	1:A:919:A:C8	2.51	0.45
1:A:922:G:C6	1:A:923:A:C6	3.04	0.45
1:A:1071:C:N4	1:A:1104:G:H1	2.14	0.45
1:A:1300:G:C6	1:A:1335:C:C5	3.05	0.45
1:A:1314:C:H2'	1:A:1315:U:H6	1.77	0.45
1:A:1531:A:O5'	1:A:1531:A:H8	2.00	0.45
2:B:10:LEU:C	2:B:12:GLU:H	2.23	0.45
4:D:68:TYR:CE2	4:D:97:LEU:HB3	2.51	0.45
7:G:28:ASN:O	7:G:31:MET:HB3	2.17	0.45
8:H:86:ILE:HD13	8:H:86:ILE:HA	1.59	0.45
8:H:97:VAL:HG23	8:H:129:VAL:C	2.41	0.45
1:A:279:A:C4	17:Q:98:LEU:HD22	2.52	0.45
1:A:579:G:O3'	15:O:54:ARG:NH2	2.48	0.45
3:C:59:ARG:HD2	3:C:97:LYS:HZ3	1.81	0.45
13:M:37:THR:HG21	13:M:56:LEU:HD23	1.99	0.45
15:O:29:VAL:HG21	15:O:67:LEU:HD21	1.98	0.45
15:O:33:THR:HG23	15:O:63:ARG:NH1	2.32	0.45
1:A:1281:U:H5'	1:A:1282:C:H5	1.81	0.45
1:A:1502:A:H2	1:A:1505:G:H1	1.65	0.45
9:I:22:GLY:HA3	9:I:60:ASP:HB2	1.98	0.45
10:J:75:ILE:HG22	10:J:76:ASN:OD1	2.16	0.45
1:A:91:C:O2'	1:A:92:C:H5'	2.17	0.45
1:A:250:A:O5'	1:A:250:A:H8	2.00	0.45
1:A:1035:A:C6	1:A:1036:G:C6	3.04	0.45
1:A:1053:G:O2'	1:A:1199:U:H5	2.00	0.45
1:A:1185:G:C2	1:A:1186:G:C5	3.05	0.45
1:A:1222:G:N2	1:A:1223:C:O2	2.50	0.45
1:A:1443:G:H5''	1:A:1446:A:H5'	1.98	0.45
5:E:36:ASP:OD1	5:E:38:GLN:N	2.47	0.45
6:F:75:LEU:O	6:F:79:LEU:HD12	2.16	0.45
9:I:92:TYR:O	9:I:96:LEU:HB2	2.16	0.45
9:I:108:VAL:HG12	9:I:109:VAL:N	2.27	0.45
12:L:126:LYS:HE2	12:L:126:LYS:HB2	1.62	0.45
13:M:82:MET:HE3	13:M:93:ARG:HE	1.82	0.45
15:O:45:VAL:HG12	15:O:46:HIS:H	1.82	0.45
18:R:47:THR:CG2	18:R:83:GLU:H	2.26	0.45
19:S:63:THR:HG22	19:S:64:GLU:H	1.82	0.45
1:A:1203:C:O5'	1:A:1203:C:H6	2.00	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1316:G:N2	1:A:1319:A:OP2	2.50	0.45
2:B:47:THR:O	2:B:51:LEU:HB2	2.17	0.45
2:B:126:GLU:H	2:B:126:GLU:HG3	1.61	0.45
4:D:35:ARG:O	4:D:36:ARG:HG3	2.17	0.45
4:D:187:ARG:HA	4:D:187:ARG:HD2	1.50	0.45
6:F:2:ARG:NE	6:F:69:GLU:HG2	2.32	0.45
6:F:75:LEU:HD13	6:F:79:LEU:HD11	1.99	0.45
9:I:50:LEU:O	9:I:54:ASP:N	2.49	0.45
11:K:73:MET:HE1	11:K:103:LEU:HG	1.99	0.45
1:A:14:U:O2	1:A:16:A:C8	2.71	0.44
1:A:35:G:H2'	1:A:36:C:H6	1.82	0.44
1:A:317:G:N2	1:A:336:C:O2	2.48	0.44
1:A:567:G:H2'	1:A:568:G:O4'	2.16	0.44
1:A:695:A:H61	1:A:797:C:H1'	1.82	0.44
1:A:1003:G:N2	1:A:1039:C:O2	2.50	0.44
1:A:1120:G:C2	1:A:1154:G:N3	2.85	0.44
1:A:1355:G:C6	1:A:1368:G:C6	3.04	0.44
2:B:18:GLY:HA3	2:B:42:ILE:H	1.81	0.44
2:B:69:LEU:HD21	2:B:93:VAL:HG23	1.99	0.44
4:D:4:TYR:HE2	4:D:11:LEU:HD11	1.78	0.44
4:D:80:GLU:O	4:D:84:LYS:HD2	2.17	0.44
5:E:84:PHE:CE1	5:E:133:TYR:HB3	2.52	0.44
7:G:77:SER:HA	7:G:86:GLN:HA	2.00	0.44
11:K:52:GLY:O	11:K:55:LYS:HB2	2.16	0.44
16:P:74:LEU:O	16:P:77:ALA:HB3	2.18	0.44
19:S:51:VAL:HG21	19:S:71:LEU:HD21	1.98	0.44
1:A:1054:C:OP1	1:A:1197:G:OP1	2.35	0.44
1:A:1199:U:H5''	1:A:1200:C:OP2	2.17	0.44
1:A:1281:U:H5'	1:A:1282:C:C5	2.52	0.44
1:A:1338:G:H2'	1:A:1339:A:H8	1.75	0.44
1:A:1338:G:C6	1:A:1339:A:C6	3.05	0.44
2:B:17:PHE:HA	2:B:44:LEU:HD11	1.99	0.44
12:L:7:ILE:HA	12:L:7:ILE:HD13	1.72	0.44
20:T:20:LEU:N	20:T:20:LEU:HD23	2.32	0.44
1:A:117:G:P	24:A:1912:HOH:O	2.75	0.44
1:A:191:G:O2'	20:T:102:GLY:O	2.23	0.44
1:A:236:G:H2'	1:A:237:C:O4'	2.18	0.44
9:I:8:GLY:N	9:I:83:ARG:HD2	2.33	0.44
13:M:97:PRO:HA	13:M:110:ARG:HD3	1.98	0.44
17:Q:5:VAL:HA	17:Q:59:ILE:O	2.17	0.44
17:Q:45:HIS:ND1	17:Q:45:HIS:C	2.75	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:434:U:C4	1:A:435:C:C4	3.06	0.44
1:A:1020:U:H2'	1:A:1021:G:C8	2.50	0.44
1:A:1028:C:N3	1:A:1034:G:N2	2.66	0.44
1:A:1318:A:O2'	19:S:37:ARG:HB3	2.17	0.44
1:A:1361(A):C:O2'	1:A:1362:C:H6	2.00	0.44
2:B:186:ALA:HB3	2:B:197:VAL:HG11	2.00	0.44
3:C:15:THR:OG1	3:C:178:LEU:HD11	2.18	0.44
5:E:90:VAL:O	5:E:91:LEU:HD23	2.18	0.44
7:G:72:ARG:HB3	7:G:73:MET:HE3	1.98	0.44
8:H:86:ILE:HG23	8:H:86:ILE:HD12	1.59	0.44
9:I:17:VAL:HG21	9:I:80:GLY:HA3	2.00	0.44
12:L:7:ILE:O	12:L:10:LEU:N	2.46	0.44
15:O:68:ARG:HE	15:O:68:ARG:HB2	1.22	0.44
15:O:85:LEU:HD23	15:O:85:LEU:N	2.32	0.44
1:A:690:G:H2'	1:A:691:G:O4'	2.16	0.44
1:A:865:A:H1'	1:A:918:A:O2'	2.18	0.44
1:A:1190:G:OP1	3:C:4:LYS:HA	2.17	0.44
1:A:1234:C:H2'	1:A:1235:U:H6	1.82	0.44
1:A:1245:A:N1	1:A:1293:G:C2	2.85	0.44
1:A:1370:G:C2	1:A:1371:G:N7	2.85	0.44
1:A:1424:C:H2'	1:A:1425:U:C6	2.52	0.44
2:B:16:HIS:CD2	2:B:17:PHE:O	2.70	0.44
2:B:54:THR:OG1	2:B:199:TYR:HB3	2.18	0.44
3:C:112:SER:O	3:C:115:LEU:HB2	2.17	0.44
4:D:186:LEU:O	4:D:187:ARG:HD2	2.17	0.44
6:F:77:ARG:O	6:F:81:ILE:HG13	2.18	0.44
7:G:156:TRP:CD1	7:G:156:TRP:O	2.71	0.44
1:A:17:U:H2'	1:A:18:C:C6	2.52	0.44
1:A:329:A:H3'	1:A:330:C:C5'	2.47	0.44
1:A:521:G:OP1	12:L:54:LYS:HE2	2.17	0.44
1:A:660:G:H1	1:A:745:C:N4	2.10	0.44
1:A:949:A:C2	1:A:1233:G:N3	2.86	0.44
1:A:1048:G:H1	1:A:1209:C:N4	2.13	0.44
1:A:1258:G:OP2	1:A:1258:G:C8	2.69	0.44
2:B:162:ILE:C	2:B:185:ILE:HD12	2.43	0.44
5:E:119:LEU:HD23	5:E:119:LEU:HA	1.41	0.44
5:E:142:LEU:HA	5:E:142:LEU:HD23	1.70	0.44
10:J:5:ARG:HD2	10:J:99:LYS:O	2.18	0.44
19:S:70:LYS:NZ	19:S:70:LYS:HB3	2.33	0.44
1:A:50:A:N6	1:A:361:G:H4'	2.33	0.44
1:A:407:G:C6	1:A:408:A:C6	3.05	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:665:A:H1'	1:A:733:A:O4'	2.16	0.44
1:A:793:U:H4'	1:A:794:A:OP2	2.18	0.44
1:A:1065:U:H4'	1:A:1066:C:O5'	2.17	0.44
1:A:1095:U:H2'	1:A:1096:C:C6	2.53	0.44
3:C:58:GLU:HB3	10:J:92:THR:HG21	1.99	0.44
5:E:112:LEU:HD23	5:E:112:LEU:HA	1.72	0.44
11:K:122:LYS:H	11:K:122:LYS:HG2	1.49	0.44
16:P:65:GLN:HA	16:P:66:PRO:HD2	1.80	0.44
17:Q:51:TYR:CE1	17:Q:73:VAL:HB	2.53	0.44
1:A:475:G:H2'	1:A:476:G:C8	2.52	0.44
1:A:1026:G:C8	1:A:1027:C:C5	3.06	0.44
1:A:1486:G:H2'	1:A:1487:G:O4'	2.17	0.44
3:C:114:PRO:O	3:C:118:GLN:HG3	2.18	0.44
4:D:19:LEU:HD11	4:D:67:ILE:HG13	1.99	0.44
17:Q:15:MET:HE3	17:Q:15:MET:HB2	1.46	0.44
20:T:75:ASN:O	20:T:76:ALA:C	2.61	0.44
1:A:192:U:H5'	20:T:102:GLY:C	2.43	0.44
1:A:279:A:OP2	17:Q:95:TYR:OH	2.24	0.44
1:A:299:G:H2'	1:A:300:A:C8	2.53	0.44
1:A:503:C:OP2	12:L:116:SER:HB3	2.18	0.44
1:A:594:G:H1	1:A:645:C:H42	1.66	0.44
1:A:1078:U:H5''	1:A:1079:G:OP2	2.18	0.44
1:A:1251:A:H4'	9:I:12:GLU:CD	2.43	0.44
1:A:1304:G:O3'	21:U:2:GLY:N	2.51	0.44
2:B:17:PHE:CD1	2:B:18:GLY:N	2.84	0.44
2:B:97:TRP:CH2	2:B:176:GLU:CD	2.96	0.44
2:B:131:PRO:HD2	2:B:134:GLU:CD	2.43	0.44
4:D:67:ILE:HG22	4:D:114:ARG:HH12	1.83	0.44
6:F:21:LEU:O	6:F:21:LEU:HG	2.18	0.44
12:L:84:LEU:HG	12:L:85:ILE:N	2.32	0.44
13:M:51:ALA:HA	13:M:54:VAL:HG12	1.99	0.44
16:P:19:ILE:H	16:P:19:ILE:HG13	1.59	0.44
1:A:1284:C:OP2	1:A:1285:A:O2'	2.30	0.43
1:A:1349:A:P	9:I:118:LYS:HD3	2.58	0.43
3:C:69:HIS:HA	3:C:104:GLN:O	2.18	0.43
4:D:163:GLU:O	4:D:166:LYS:HG2	2.18	0.43
4:D:187:ARG:HH22	4:D:188:LEU:HG	1.82	0.43
9:I:112:LYS:HE2	9:I:113:LYS:O	2.18	0.43
9:I:116:LYS:HB3	9:I:121:ARG:O	2.18	0.43
15:O:31:LEU:HD12	15:O:31:LEU:HA	1.89	0.43
1:A:46:G:H2'	1:A:366:C:C5	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1111:A:C5	1:A:1112:C:C5	3.06	0.43
1:A:1111:A:N6	3:C:177:THR:HB	2.33	0.43
1:A:1519[B]:MA6:H5'	1:A:1520[B]:G:OP2	2.17	0.43
4:D:30:LYS:O	4:D:32:ALA:N	2.51	0.43
5:E:10:MET:SD	5:E:13:ILE:HG23	2.58	0.43
5:E:80:ILE:HG13	5:E:80:ILE:O	2.17	0.43
7:G:138:LYS:HG2	7:G:139:GLU:CG	2.48	0.43
8:H:10:LEU:HD23	8:H:10:LEU:HA	1.58	0.43
13:M:65:LYS:C	13:M:66:LEU:HG	2.43	0.43
15:O:29:VAL:HG21	15:O:67:LEU:CD2	2.49	0.43
17:Q:65:ILE:HG21	17:Q:69:LYS:HE2	2.00	0.43
18:R:79:LEU:HA	18:R:80:PRO:HD3	1.67	0.43
20:T:36:LEU:HD23	20:T:36:LEU:HA	1.53	0.43
1:A:109:A:C6	1:A:326:G:C6	3.07	0.43
1:A:391:G:C6	1:A:392:G:C5	3.06	0.43
1:A:779:C:H2'	1:A:780:A:O4'	2.18	0.43
1:A:1347:G:C2'	1:A:1348:U:OP2	2.66	0.43
1:A:1480:G:C6	1:A:1481:U:C4	3.06	0.43
2:B:88:ALA:C	2:B:90:MET:H	2.27	0.43
3:C:43:LEU:HD23	3:C:43:LEU:HA	1.67	0.43
5:E:35:GLY:HA3	5:E:112:LEU:HB3	1.99	0.43
5:E:121:LYS:HG3	5:E:122:GLU:N	2.33	0.43
6:F:11:ASN:ND2	6:F:13:ASN:OD1	2.29	0.43
7:G:138:LYS:HG2	7:G:139:GLU:HG2	1.99	0.43
15:O:39:LEU:HD13	15:O:56:LEU:HB2	1.99	0.43
1:A:115:G:H4'	1:A:116:A:O5'	2.18	0.43
1:A:912:C:H5''	12:L:46:LYS:HE3	2.01	0.43
1:A:940:C:H5''	1:A:941:G:OP2	2.18	0.43
1:A:1241:G:C4	1:A:1242:C:C5	3.06	0.43
3:C:39:ILE:HD12	3:C:57:ILE:HD13	2.00	0.43
12:L:11:VAL:H	12:L:11:VAL:HG23	1.52	0.43
12:L:120:TYR:N	12:L:120:TYR:CD2	2.86	0.43
13:M:22:ILE:N	13:M:22:ILE:HD12	2.34	0.43
13:M:82:MET:HA	13:M:89:GLY:HA3	2.01	0.43
17:Q:22:LEU:HD12	17:Q:22:LEU:HA	1.44	0.43
17:Q:59:ILE:HD13	17:Q:59:ILE:HA	1.49	0.43
1:A:1001:A:H2'	1:A:1002:G:H8	1.83	0.43
1:A:1392:G:O2'	1:A:1393:U:H5'	2.19	0.43
2:B:29:ALA:HA	2:B:32:ILE:HG13	2.00	0.43
2:B:73:THR:HG21	2:B:96:ARG:HD2	1.99	0.43
5:E:103:GLY:O	5:E:107:ARG:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:42:THR:CG2	12:L:52:LEU:HB3	2.48	0.43
13:M:37:THR:CG2	13:M:55:ARG:HB3	2.49	0.43
15:O:70:LEU:HD23	15:O:78:TYR:HB2	2.00	0.43
17:Q:32:TYR:N	17:Q:32:TYR:CD2	2.82	0.43
1:A:315:A:O2'	1:A:330:C:O2'	2.29	0.43
1:A:990:C:C2	1:A:1216:G:N2	2.87	0.43
1:A:1179:A:H2'	1:A:1180:A:O4'	2.18	0.43
1:A:1284:C:H3'	1:A:1285:A:H2'	2.00	0.43
2:B:46:LYS:HA	2:B:49:GLU:OE2	2.19	0.43
2:B:187:LEU:HD22	2:B:187:LEU:HA	1.56	0.43
7:G:71:PRO:HD3	7:G:103:TRP:HZ3	1.83	0.43
8:H:20:TYR:CE1	8:H:76:PRO:HD2	2.54	0.43
9:I:79:LEU:HD23	9:I:79:LEU:HA	1.91	0.43
1:A:118:U:H3'	1:A:288:A:H61	1.83	0.43
1:A:269:C:H2'	1:A:270:A:H8	1.84	0.43
1:A:299:G:N1	24:A:2036:HOH:O	2.36	0.43
1:A:1012:U:H2'	1:A:1013:G:O4'	2.19	0.43
1:A:1268:A:H2'	1:A:1269:A:C8	2.54	0.43
1:A:1296:C:H4'	1:A:1302:U:H5	1.78	0.43
1:A:1313:U:C5	19:S:4:SER:HB2	2.54	0.43
1:A:1505:G:H3'	1:A:1505:G:H8	1.84	0.43
2:B:84:GLU:OE2	2:B:235:SER:OG	2.29	0.43
2:B:233:SER:HA	2:B:234:PRO:HD3	1.87	0.43
3:C:69:HIS:HB3	3:C:106:VAL:HG23	2.01	0.43
4:D:19:LEU:HD21	4:D:67:ILE:HG12	2.00	0.43
5:E:146:ALA:HB3	5:E:147:ASP:OD1	2.19	0.43
8:H:103:VAL:HG12	8:H:108:GLY:HA3	2.00	0.43
9:I:8:GLY:HA2	9:I:79:LEU:HD13	2.01	0.43
10:J:6:ILE:HB	10:J:72:VAL:CG2	2.49	0.43
11:K:54:ARG:H	11:K:54:ARG:HG2	1.71	0.43
17:Q:43:LEU:HD12	17:Q:68:ARG:HB3	2.00	0.43
18:R:22:VAL:O	18:R:25:THR:N	2.52	0.43
1:A:106:C:C2'	1:A:107:G:H5'	2.48	0.43
1:A:144:G:H1	1:A:178:C:N4	2.09	0.43
1:A:241:C:H42	1:A:285:G:H1	1.66	0.43
1:A:524:G:H2'	1:A:525:C:C6	2.53	0.43
1:A:1021:G:C6	1:A:1022:G:C8	3.07	0.43
1:A:1286:A:H5'	21:U:25:LYS:HD3	2.01	0.43
2:B:16:HIS:HD2	2:B:17:PHE:O	2.02	0.43
2:B:163:PHE:HD1	2:B:163:PHE:HA	1.63	0.43
3:C:130:VAL:O	3:C:134:ILE:HG13	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:37:ASN:HB3	24:G:202:HOH:O	2.19	0.43
8:H:69:ARG:HH11	8:H:69:ARG:HG3	1.84	0.43
13:M:39:ILE:HG22	13:M:40:ASN:O	2.18	0.43
19:S:17:GLU:HA	19:S:20:LEU:HG	2.00	0.43
1:A:909:A:H2'	1:A:910:C:O4'	2.18	0.43
1:A:1114:C:H2'	1:A:1115:C:H6	1.83	0.43
1:A:1311:G:H1	1:A:1326:C:H42	1.66	0.43
2:B:87:ARG:HH21	2:B:219:VAL:CG1	2.32	0.43
4:D:19:LEU:HD23	4:D:20:TYR:H	1.83	0.43
4:D:96:LEU:HA	4:D:96:LEU:HD12	1.71	0.43
4:D:201:GLN:NE2	5:E:117:ASP:OD1	2.52	0.43
7:G:59:LEU:O	7:G:62:PHE:HB3	2.19	0.43
9:I:9:ARG:HB3	9:I:14:VAL:HG13	1.99	0.43
12:L:27:LEU:CA	12:L:29:GLY:H	2.32	0.43
13:M:95:GLY:C	13:M:96:LEU:HD23	2.44	0.43
17:Q:6:LEU:HD13	17:Q:23:VAL:HG11	2.01	0.43
17:Q:29:HIS:CG	17:Q:30:PRO:HD2	2.54	0.43
1:A:652:U:C2	1:A:752:G:N2	2.87	0.43
3:C:8:ILE:HG23	3:C:16:ARG:HG2	2.00	0.43
6:F:6:VAL:HG22	6:F:90:VAL:HG22	2.01	0.43
18:R:47:THR:HA	18:R:83:GLU:HB2	2.01	0.43
1:A:277:C:H5'	17:Q:68:ARG:NH1	2.34	0.42
1:A:491:G:H2'	1:A:492:G:H8	1.84	0.42
1:A:714:G:H2'	1:A:715:A:C8	2.54	0.42
1:A:1157:A:H4'	1:A:1158:C:O5'	2.19	0.42
1:A:1258:G:H2'	1:A:1259:C:C6	2.54	0.42
1:A:1305:G:H4'	1:A:1306:A:O5'	2.19	0.42
1:A:1513:A:H2'	1:A:1514:C:C6	2.53	0.42
2:B:74:LYS:NZ	2:B:74:LYS:HB3	2.33	0.42
4:D:125:HIS:C	4:D:126:ILE:HD12	2.44	0.42
6:F:6:VAL:HG13	6:F:90:VAL:CG2	2.49	0.42
9:I:127:LYS:HD3	9:I:127:LYS:HA	1.64	0.42
10:J:50:ILE:HD13	14:N:41:ARG:HD2	2.01	0.42
20:T:43:LEU:HD22	20:T:43:LEU:HA	1.62	0.42
1:A:83:U:C4	1:A:84:U:C5	3.07	0.42
1:A:455:C:O5'	1:A:455:C:H6	2.02	0.42
1:A:459:G:H1'	1:A:463:A:N6	2.35	0.42
1:A:707:C:H4'	11:K:20:TYR:CE1	2.54	0.42
1:A:825:G:H21	8:H:11:THR:HG21	1.83	0.42
4:D:108:LEU:HD23	4:D:108:LEU:HA	1.77	0.42
11:K:95:ILE:H	11:K:95:ILE:HG13	1.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:41:ILE:HG22	20:T:42:GLN:N	2.34	0.42
1:A:1092:A:H5''	7:G:4:ARG:CZ	2.49	0.42
1:A:1367:C:H5'	10:J:60:ARG:HE	1.85	0.42
1:A:1478:C:H5	1:A:1479:C:C5	2.37	0.42
2:B:87:ARG:NH1	2:B:233:SER:HB2	2.35	0.42
3:C:56:ASP:N	3:C:56:ASP:OD1	2.52	0.42
3:C:113:ALA:N	3:C:114:PRO:HD2	2.35	0.42
3:C:182:ILE:HA	3:C:202:ILE:O	2.19	0.42
5:E:44:GLY:N	5:E:62:ALA:HB2	2.34	0.42
7:G:88:PRO:HB2	7:G:155:ARG:CZ	2.49	0.42
9:I:112:LYS:HA	9:I:119:ALA:HB2	2.01	0.42
11:K:46:GLY:HA2	11:K:50:TYR:O	2.19	0.42
11:K:106:LYS:HD3	11:K:106:LYS:HA	1.84	0.42
13:M:9:ILE:HD12	13:M:9:ILE:N	2.34	0.42
17:Q:24:GLU:CD	17:Q:37:LYS:HD2	2.43	0.42
17:Q:41:LYS:HB2	17:Q:41:LYS:HE2	1.89	0.42
1:A:345:C:OP2	1:A:345:C:H6	2.03	0.42
1:A:507:C:OP2	1:A:508:C:O2'	2.29	0.42
1:A:597:G:H2'	1:A:598:U:H5'	2.01	0.42
1:A:1004:A:H5''	1:A:1025:U:C4	2.54	0.42
1:A:1151:A:O2'	1:A:1152:A:OP2	2.28	0.42
1:A:1287:A:H2	1:A:1353:G:N3	2.18	0.42
4:D:13:ARG:HD2	4:D:38:TYR:O	2.20	0.42
4:D:70:ILE:HG22	4:D:71:SER:O	2.18	0.42
4:D:187:ARG:HA	4:D:187:ARG:HH11	1.84	0.42
9:I:46:ALA:O	9:I:81:ILE:HD12	2.20	0.42
9:I:55:ALA:HA	9:I:58:HIS:HB3	2.02	0.42
10:J:86:MET:HE3	10:J:86:MET:HB3	1.73	0.42
15:O:57:LEU:HA	15:O:57:LEU:HD12	1.83	0.42
1:A:115:G:O2'	1:A:116:A:OP2	2.23	0.42
1:A:260:G:H2'	1:A:261:U:C6	2.54	0.42
1:A:803:G:H2'	1:A:804:U:O4'	2.19	0.42
1:A:827:U:H5''	1:A:828:A:OP2	2.19	0.42
6:F:99:ALA:C	6:F:101:ALA:H	2.27	0.42
11:K:40:ILE:HG22	11:K:75:TYR:CE1	2.54	0.42
18:R:59:SER:H	18:R:62:GLU:HB2	1.84	0.42
19:S:16:LEU:HG	19:S:20:LEU:HD23	2.02	0.42
1:A:321:A:N7	1:A:328:C:C6	2.81	0.42
1:A:413:G:O6	4:D:36:ARG:HD2	2.19	0.42
1:A:722:A:O3'	1:A:723:U:C6	2.71	0.42
1:A:770:C:C2'	1:A:771:G:H5'	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:778:G:O5'	1:A:778:G:C8	2.71	0.42
1:A:1011:G:H2'	1:A:1012:U:O4'	2.19	0.42
1:A:1096:C:H2'	1:A:1097:C:C6	2.54	0.42
1:A:1343:G:C5	1:A:1344:C:C4	3.08	0.42
1:A:1527:C:H2'	1:A:1528:U:C6	2.55	0.42
2:B:223:ILE:O	2:B:228:GLY:N	2.52	0.42
4:D:9:CYS:SG	4:D:31:CYS:O	2.77	0.42
4:D:79:PHE:O	4:D:82:ALA:N	2.53	0.42
7:G:92:SER:HB3	7:G:95:ARG:H	1.84	0.42
8:H:69:ARG:NH1	8:H:69:ARG:HG3	2.34	0.42
10:J:86:MET:SD	10:J:87:THR:N	2.92	0.42
15:O:12:ILE:C	15:O:14:GLU:N	2.76	0.42
1:A:22:G:C4	1:A:23:C:C5	3.08	0.42
1:A:22:G:C5	1:A:914:G:O6	2.71	0.42
1:A:815:A:N6	1:A:1509:C:H1'	2.35	0.42
1:A:998:G:C2	1:A:1044:A:C5	3.08	0.42
1:A:1009:G:N2	1:A:1010:G:H1'	2.35	0.42
1:A:1058:G:C6	1:A:1059:C:N3	2.87	0.42
2:B:49:GLU:H	2:B:49:GLU:HG3	1.59	0.42
2:B:187:LEU:HD22	2:B:201:ILE:O	2.20	0.42
2:B:215:LEU:HD23	2:B:215:LEU:HA	1.67	0.42
6:F:10:LEU:HD11	6:F:59:TYR:CD2	2.48	0.42
6:F:25:ILE:HD13	6:F:25:ILE:HA	1.96	0.42
6:F:41:GLU:OE1	18:R:35:ARG:NH1	2.49	0.42
8:H:6:ILE:N	8:H:6:ILE:CD1	2.81	0.42
15:O:29:VAL:O	15:O:33:THR:OG1	2.34	0.42
15:O:67:LEU:HD13	15:O:82:ILE:HD11	2.02	0.42
1:A:430:A:OP1	4:D:8:VAL:N	2.50	0.42
1:A:976:G:C8	1:A:1358:U:C2	3.08	0.42
2:B:169:LYS:HE3	2:B:169:LYS:HB3	1.91	0.42
5:E:6:PHE:HD2	5:E:6:PHE:HA	1.68	0.42
8:H:116:LYS:CD	8:H:127:LEU:HD12	2.50	0.42
10:J:14:LYS:NZ	10:J:14:LYS:HB2	2.35	0.42
11:K:59:TYR:CE1	11:K:63:LEU:HD21	2.55	0.42
18:R:76:LEU:HD23	18:R:76:LEU:HA	1.70	0.42
1:A:9:G:C2	1:A:26:A:N1	2.87	0.42
1:A:109:A:H2'	1:A:326:G:N2	2.33	0.42
1:A:179:A:H2'	1:A:180:U:C6	2.55	0.42
1:A:794:A:N6	1:A:795:C:N4	2.67	0.42
1:A:839:U:H5'	1:A:840:C:C5	2.55	0.42
1:A:1010:G:N2	1:A:1019:C:N3	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:13:ARG:HA	4:D:33:MET:SD	2.60	0.42
4:D:63:LYS:HE3	4:D:198:VAL:HG23	2.00	0.42
4:D:94:LEU:HA	4:D:94:LEU:HD23	1.46	0.42
5:E:66:MET:HE3	5:E:66:MET:HB3	1.78	0.42
5:E:88:LYS:HD2	5:E:123:LEU:HD12	2.02	0.42
8:H:87:SER:HA	8:H:93:VAL:HG12	2.02	0.42
9:I:16:ARG:HH11	9:I:64:THR:HG23	1.84	0.42
12:L:60:LEU:HD13	12:L:60:LEU:HA	1.80	0.42
16:P:60:LEU:HD23	16:P:60:LEU:HA	1.53	0.42
17:Q:22:LEU:HD12	17:Q:23:VAL:N	2.35	0.42
19:S:22:LEU:HD12	19:S:31:ILE:HD11	2.02	0.42
1:A:152:A:N6	1:A:170:U:C2	2.87	0.42
1:A:329:A:H3'	1:A:330:C:H5'	2.01	0.42
1:A:355:C:C4	1:A:356:A:N7	2.88	0.42
1:A:837:G:C2	1:A:850:U:O2	2.73	0.42
1:A:1474:G:N1	1:A:1475:G:C6	2.88	0.42
1:A:1499:A:C1'	1:A:1520[A]:G:H5'	2.47	0.42
4:D:192:GLU:C	4:D:194:LEU:N	2.77	0.42
8:H:29:SER:HB3	8:H:32:LYS:CD	2.43	0.42
10:J:19:SER:O	10:J:23:ILE:HD12	2.20	0.42
13:M:72:ALA:HA	13:M:75:ALA:HB3	2.02	0.42
14:N:40:CYS:H	14:N:43:CYS:HB2	1.84	0.42
15:O:81:LEU:HA	15:O:81:LEU:HD23	1.63	0.42
16:P:75:ARG:HA	24:P:206:HOH:O	2.20	0.42
1:A:16:A:C2	1:A:920:U:O2	2.73	0.41
1:A:135:C:H5''	1:A:136:C:OP2	2.20	0.41
1:A:309:G:H2'	1:A:310:G:H8	1.85	0.41
1:A:405:U:O4	4:D:2:GLY:HA3	2.20	0.41
1:A:570:G:C6	1:A:873:A:C2	3.07	0.41
1:A:1497:G:O2'	1:A:1518[A]:MA6:H92	2.19	0.41
2:B:53:ARG:HH11	2:B:199:TYR:HD2	1.68	0.41
3:C:136:GLN:HG3	3:C:140:ARG:NH2	2.35	0.41
6:F:67:MET:HB2	6:F:68:PRO:HD2	2.02	0.41
8:H:97:VAL:H	8:H:98:LYS:HZ3	1.65	0.41
14:N:26:ARG:HH11	14:N:47:LEU:HD21	1.85	0.41
17:Q:45:HIS:CD2	17:Q:65:ILE:HG12	2.47	0.41
18:R:59:SER:N	18:R:62:GLU:OE1	2.52	0.41
19:S:67:VAL:C	19:S:69:HIS:H	2.28	0.41
1:A:463:A:C8	1:A:474:G:N7	2.89	0.41
1:A:571:U:H5''	1:A:572:A:OP2	2.19	0.41
1:A:597:G:C5	1:A:598:U:C6	3.08	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:854:G:H3'	1:A:871:U:O4	2.20	0.41
1:A:1124:G:H5'	10:J:35:SER:O	2.20	0.41
1:A:1185:G:N2	1:A:1186:G:C4	2.88	0.41
2:B:30:ARG:HG2	2:B:31:TYR:CD1	2.55	0.41
2:B:92:TYR:CD1	2:B:151:GLY:HA3	2.55	0.41
5:E:31:LEU:HD23	5:E:31:LEU:HA	1.67	0.41
9:I:6:GLY:CA	9:I:83:ARG:HB2	2.50	0.41
10:J:52:GLY:HA2	10:J:53:PRO:HD2	1.73	0.41
10:J:79:ARG:NH2	10:J:82:ILE:HD12	2.35	0.41
13:M:18:ALA:O	13:M:21:TYR:HB2	2.20	0.41
1:A:5:U:H4'	1:A:6:G:O5'	2.20	0.41
1:A:41:G:H2'	1:A:42:G:C8	2.55	0.41
1:A:77:G:C6	1:A:93:G:C6	3.08	0.41
1:A:115:G:O2'	1:A:289:G:H5''	2.20	0.41
1:A:264:U:H2'	1:A:265:G:O4'	2.20	0.41
1:A:299:G:C6	1:A:300:A:C6	3.08	0.41
1:A:509:A:H5'	4:D:54:TYR:HD2	1.85	0.41
1:A:1090:U:H2'	1:A:1091:U:C6	2.40	0.41
1:A:1167:A:N6	1:A:1168:A:N1	2.68	0.41
1:A:1255:G:O2'	1:A:1258:G:H1'	2.19	0.41
1:A:1371:G:C6	1:A:1372:U:C4	3.09	0.41
1:A:1399:C:O2	1:A:1401:G:C5	2.73	0.41
2:B:30:ARG:HD2	2:B:31:TYR:CZ	2.55	0.41
2:B:143:GLU:HA	2:B:146:GLN:OE1	2.20	0.41
3:C:127:ARG:HG2	3:C:193:TYR:OH	2.21	0.41
4:D:100:ARG:CZ	4:D:137:SER:HA	2.50	0.41
5:E:11:ILE:O	5:E:11:ILE:HD13	2.21	0.41
5:E:151:LEU:HD23	5:E:151:LEU:HA	1.52	0.41
7:G:44:TYR:HD2	7:G:44:TYR:HA	1.76	0.41
7:G:59:LEU:HG	7:G:63:LYS:HE2	2.01	0.41
16:P:28:ARG:HG3	16:P:29:ASP:OD2	2.20	0.41
17:Q:29:HIS:CG	17:Q:30:PRO:CD	3.04	0.41
20:T:46:GLU:H	20:T:46:GLU:CD	2.27	0.41
1:A:378:G:H2'	1:A:379:C:H6	1.83	0.41
1:A:481:G:O2'	1:A:482:A:C8	2.64	0.41
1:A:795:C:H5''	1:A:796:C:OP2	2.20	0.41
1:A:1425:U:H2'	1:A:1426:C:C6	2.55	0.41
2:B:98:LEU:HB2	2:B:101:MET:HG3	2.02	0.41
2:B:158:LEU:H	2:B:158:LEU:CD1	2.20	0.41
7:G:22:LEU:HA	7:G:22:LEU:HD12	1.80	0.41
8:H:27:PRO:HA	8:H:58:TYR:CD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:126:LYS:HE2	8:H:126:LYS:HB3	1.77	0.41
11:K:33:THR:HG22	11:K:39:PRO:CA	2.51	0.41
16:P:39:TYR:CE2	16:P:41:PRO:HG3	2.55	0.41
20:T:55:ILE:HD13	20:T:55:ILE:HA	1.69	0.41
1:A:190:C:H42	1:A:190(I):G:H1	1.68	0.41
1:A:374:A:N3	1:A:374:A:H2'	2.35	0.41
1:A:403:C:H2'	1:A:404:U:C6	2.55	0.41
1:A:1105:A:H2'	1:A:1106:G:C8	2.56	0.41
1:A:1180:A:OP1	9:I:103:THR:HG23	2.21	0.41
1:A:1222:G:C2	1:A:1223:C:C2	3.08	0.41
1:A:1435:G:H1	1:A:1466:C:H42	1.67	0.41
1:A:1518[A]:MA6:H93	1:A:1519[A]:MA6:C9	2.50	0.41
5:E:92:LYS:HA	5:E:93:PRO:HD3	1.90	0.41
5:E:105:VAL:HG11	5:E:131:ILE:HG22	2.02	0.41
9:I:9:ARG:HD3	9:I:14:VAL:HG13	2.02	0.41
12:L:6:THR:HG1	12:L:9:GLN:H	1.60	0.41
1:A:116:A:H2'	1:A:117:G:C8	2.55	0.41
1:A:244:U:H4'	1:A:245:C:H5''	2.02	0.41
1:A:266:G:H5''	1:A:266:G:H8	1.86	0.41
1:A:490:G:C6	1:A:491:G:N7	2.89	0.41
1:A:730:G:N2	1:A:765:G:H5''	2.35	0.41
1:A:865:A:H2'	1:A:866:C:C6	2.54	0.41
1:A:953:G:H2'	1:A:954:G:O4'	2.20	0.41
1:A:976:G:H4'	1:A:977:A:OP1	2.21	0.41
1:A:1027:C:H2'	1:A:1028:C:C6	2.56	0.41
1:A:1518[B]:MA6:H93	1:A:1519[B]:MA6:C6	2.50	0.41
2:B:57:PHE:O	2:B:58:ILE:C	2.62	0.41
3:C:153:VAL:HG13	3:C:198:VAL:HG22	2.03	0.41
4:D:57:ARG:HG3	4:D:202:LEU:CD1	2.50	0.41
4:D:207:TYR:HD2	4:D:207:TYR:HA	1.65	0.41
6:F:46:ARG:NH1	6:F:46:ARG:HB3	2.35	0.41
14:N:24:CYS:HB3	14:N:29:ARG:HB3	2.03	0.41
16:P:18:ARG:O	16:P:20:VAL:HG23	2.20	0.41
16:P:82:GLN:H	16:P:82:GLN:HG2	1.76	0.41
18:R:29:PHE:CD1	18:R:39:VAL:HG21	2.56	0.41
1:A:21:G:N2	1:A:886:G:OP1	2.53	0.41
1:A:767:A:H2'	1:A:768:A:C8	2.55	0.41
1:A:1267:C:O2	1:A:1327:C:H4'	2.21	0.41
1:A:1354:C:O5'	1:A:1354:C:H6	2.03	0.41
3:C:20:SER:O	14:N:54:PRO:HB3	2.20	0.41
4:D:25:ARG:O	4:D:25:ARG:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:142:PRO:HB3	4:D:187:ARG:NH1	2.36	0.41
5:E:82:VAL:HG21	5:E:138:ALA:HA	2.03	0.41
16:P:3:LYS:HG3	16:P:24:ALA:HB2	2.02	0.41
1:A:1124:G:C8	1:A:1145:C:C5	3.08	0.41
2:B:40:HIS:O	2:B:41:ILE:HD13	2.20	0.41
2:B:210:SER:O	2:B:214:ILE:HG12	2.21	0.41
10:J:47:PHE:CZ	14:N:37:PHE:CE1	3.09	0.41
11:K:69:ALA:O	11:K:73:MET:HE2	2.21	0.41
14:N:31:ARG:O	14:N:33:VAL:HG23	2.20	0.41
18:R:70:ILE:HG22	18:R:71:LYS:N	2.36	0.41
1:A:128:G:C2	1:A:234:C:C2	3.09	0.41
1:A:227:G:H1'	24:A:2159:HOH:O	2.20	0.41
1:A:261:U:O2	1:A:263:A:C8	2.74	0.41
1:A:452:A:HO2'	1:A:453:A:H8	1.59	0.41
1:A:508:C:O5'	1:A:508:C:H6	2.04	0.41
1:A:665:A:N3	1:A:732:C:H2'	2.35	0.41
1:A:791:G:H2'	1:A:792:A:H5'	2.01	0.41
1:A:1073:U:O2	2:B:104:ASN:ND2	2.54	0.41
1:A:1221:G:OP1	19:S:36:ARG:HD3	2.20	0.41
1:A:1279:A:H5''	10:J:7:LYS:HZ3	1.86	0.41
1:A:1343:G:H4'	9:I:122:ALA:HB3	2.03	0.41
1:A:1406:U:H3'	1:A:1407:5MC:HM53	2.02	0.41
1:A:1515[B]:C:H42	1:A:1520[B]:G:H1	1.68	0.41
3:C:3:ASN:OD1	3:C:3:ASN:N	2.54	0.41
3:C:23:TYR:OH	10:J:9:ARG:NH1	2.54	0.41
3:C:88:ARG:HH21	3:C:100:ALA:HB1	1.86	0.41
5:E:107:ARG:O	5:E:111:GLU:HB2	2.21	0.41
6:F:35:ALA:HA	6:F:67:MET:HB3	2.02	0.41
7:G:99:LEU:HA	7:G:99:LEU:HD23	1.60	0.41
7:G:101:LEU:HD23	7:G:101:LEU:HA	1.93	0.41
7:G:116:ALA:O	7:G:120:ILE:HG12	2.21	0.41
8:H:70:GLN:HA	8:H:70:GLN:OE1	2.20	0.41
8:H:75:ARG:HA	8:H:76:PRO:HD3	1.64	0.41
8:H:97:VAL:N	8:H:98:LYS:HZ1	2.18	0.41
8:H:102:ARG:HG3	8:H:102:ARG:O	2.21	0.41
9:I:96:LEU:HD23	9:I:102:LEU:HD21	2.03	0.41
11:K:29:ILE:HD13	11:K:29:ILE:HG21	1.83	0.41
11:K:111:ASP:O	11:K:112:THR:C	2.63	0.41
12:L:59:ARG:HE	12:L:65:GLU:HG3	1.86	0.41
15:O:45:VAL:HB	15:O:46:HIS:ND1	2.36	0.41
15:O:64:ARG:HH21	15:O:68:ARG:HH22	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:67:LEU:O	15:O:68:ARG:C	2.64	0.41
20:T:84:LEU:HD22	20:T:84:LEU:HA	1.64	0.41
1:A:53:A:C2	1:A:54:C:H1'	2.57	0.41
1:A:721:G:OP2	18:R:53:ARG:HG3	2.20	0.41
1:A:738:C:OP1	6:F:92:LYS:HD3	2.21	0.41
4:D:5:ILE:H	4:D:5:ILE:HG13	1.70	0.41
5:E:84:PHE:CD2	5:E:84:PHE:C	2.99	0.41
6:F:28:ARG:O	6:F:31:GLU:HG3	2.21	0.41
6:F:45:LEU:O	6:F:46:ARG:HG2	2.20	0.41
8:H:36:LEU:O	8:H:37:ARG:C	2.62	0.41
9:I:47:LEU:HB3	9:I:50:LEU:HD12	2.02	0.41
9:I:93:ARG:HB3	9:I:93:ARG:NH1	2.36	0.41
12:L:39:VAL:HG12	12:L:57:LYS:HG2	2.03	0.41
15:O:18:PHE:HD1	15:O:19:PRO:O	2.04	0.41
15:O:26:GLU:OE1	15:O:77:ARG:HD2	2.21	0.41
15:O:67:LEU:HD23	15:O:67:LEU:HA	1.82	0.41
19:S:63:THR:HG22	19:S:64:GLU:N	2.36	0.41
1:A:77:G:C5	1:A:93:G:C2	3.09	0.40
1:A:316:G:OP2	1:A:351:G:O2'	2.39	0.40
1:A:376:G:C4	1:A:389:A:C2	3.09	0.40
1:A:451:A:N7	1:A:481:G:C2	2.89	0.40
1:A:515:G:C6	1:A:516:PSU:C2	3.09	0.40
1:A:651:C:O2'	1:A:652:U:H5'	2.21	0.40
1:A:794:A:C6	1:A:795:C:C4	3.08	0.40
1:A:797:C:H2'	1:A:798:G:H8	1.86	0.40
1:A:831:U:OP2	2:B:22:LYS:NZ	2.47	0.40
1:A:833:U:H2'	1:A:834:C:H6	1.82	0.40
1:A:942:G:N2	1:A:943:U:C2	2.89	0.40
1:A:947:G:H2'	1:A:948:C:O4'	2.21	0.40
1:A:987:G:N2	1:A:1219:U:O2	2.54	0.40
1:A:1422:G:H2'	1:A:1423:G:H8	1.86	0.40
2:B:155:LEU:HD23	2:B:155:LEU:HA	1.72	0.40
4:D:127:THR:HB	4:D:147:ALA:HB3	2.03	0.40
5:E:43:LEU:HD21	5:E:133:TYR:CD2	2.56	0.40
7:G:16:LEU:HG	9:I:42:ARG:HA	2.02	0.40
7:G:26:PHE:CE1	7:G:105:VAL:HG23	2.56	0.40
12:L:11:VAL:HG13	17:Q:29:HIS:CD2	2.57	0.40
13:M:56:LEU:HD23	13:M:56:LEU:HA	1.75	0.40
15:O:64:ARG:HG2	15:O:88:ARG:HH11	1.85	0.40
1:A:44:G:N2	1:A:399:G:C4	2.89	0.40
1:A:59:A:H3'	1:A:331:G:H22	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:C:O2	1:A:93:G:C8	2.74	0.40
1:A:523:A:O5'	1:A:523:A:H8	2.04	0.40
1:A:825:G:N2	8:H:11:THR:HG21	2.36	0.40
1:A:838:G:N2	1:A:849:C:C2	2.88	0.40
1:A:858:G:O6	1:A:869:G:H3'	2.21	0.40
1:A:1143:G:H2'	1:A:1144:G:C8	2.57	0.40
1:A:1148:U:O3'	9:I:14:VAL:HG11	2.22	0.40
1:A:1430:C:C2	1:A:1471:G:N2	2.89	0.40
2:B:21:ARG:HA	2:B:39:ILE:HA	2.02	0.40
2:B:180:LEU:HD23	2:B:180:LEU:HA	1.86	0.40
8:H:9:MET:HE3	8:H:9:MET:HB3	1.84	0.40
13:M:34:LEU:CD1	13:M:39:ILE:HB	2.50	0.40
13:M:67:GLU:O	13:M:71:ARG:HB2	2.21	0.40
20:T:22:ARG:O	20:T:23:ARG:C	2.62	0.40
20:T:73:HIS:O	20:T:76:ALA:HB3	2.21	0.40
1:A:90:U:H6	1:A:90:U:H2'	1.80	0.40
1:A:115:G:H8	1:A:115:G:O5'	2.04	0.40
1:A:475:G:H2'	1:A:476:G:H8	1.86	0.40
1:A:765:G:C6	1:A:812:C:C2	3.09	0.40
1:A:1177:G:H8	1:A:1177:G:O5'	2.04	0.40
1:A:1265:G:C6	1:A:1266:G:C6	3.10	0.40
2:B:166:ASP:O	2:B:170:GLU:HG2	2.22	0.40
3:C:167:TRP:HB3	3:C:168:ALA:H	1.65	0.40
4:D:131:ARG:HD3	4:D:131:ARG:HA	1.88	0.40
7:G:65:ALA:HB1	7:G:127:ALA:HB3	2.03	0.40
8:H:23:SER:HA	8:H:63:LEU:HD22	2.02	0.40
12:L:89:ARG:HE	12:L:89:ARG:HB3	1.36	0.40
13:M:15:VAL:O	13:M:19:LEU:HG	2.22	0.40
1:A:156:G:N1	1:A:166:G:C6	2.90	0.40
1:A:186:C:H2'	1:A:187:C:H6	1.86	0.40
1:A:852:G:N1	1:A:853:G:N7	2.70	0.40
1:A:1089:G:C6	1:A:1090:U:N3	2.89	0.40
1:A:1124:G:H2'	1:A:1145:C:N4	2.30	0.40
1:A:1345:U:C2	1:A:1377:A:C2	3.09	0.40
1:A:1424:C:H2'	1:A:1425:U:H6	1.85	0.40
1:A:1533:C:O2	1:A:1533:C:H2'	2.20	0.40
3:C:180:ALA:HB3	3:C:203:PHE:HE1	1.83	0.40
6:F:41:GLU:HB2	6:F:62:TRP:HB3	2.02	0.40
11:K:53:SER:O	11:K:55:LYS:N	2.55	0.40
12:L:89:ARG:HH21	12:L:97:ARG:CG	2.34	0.40
13:M:29:ARG:HB3	13:M:64:TRP:CH2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:74:LYS:HB3	20:T:75:ASN:H	1.14	0.40
1:A:41:G:C2	1:A:42:G:C5	3.09	0.40
1:A:771:G:H2'	1:A:772:U:C6	2.56	0.40
1:A:1059:C:O3'	14:N:45:ARG:NH2	2.55	0.40
1:A:1505:G:H2'	1:A:1541:PSU:OP2	2.22	0.40
3:C:88:ARG:HA	3:C:91:LEU:HD22	2.03	0.40
4:D:80:GLU:H	4:D:80:GLU:HG2	1.67	0.40
10:J:51:ARG:HG3	10:J:59:SER:O	2.21	0.40
14:N:23:ARG:O	14:N:24:CYS:C	2.64	0.40
15:O:17:ARG:HD3	15:O:26:GLU:OE2	2.21	0.40
16:P:19:ILE:CG2	16:P:36:ILE:HG13	2.51	0.40
17:Q:95:TYR:HA	17:Q:98:LEU:HD13	2.03	0.40
20:T:53:LEU:HD22	20:T:53:LEU:HA	1.70	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	232/256 (91%)	201 (87%)	28 (12%)	3 (1%)	9	36
3	C	204/239 (85%)	173 (85%)	31 (15%)	0	100	100
4	D	206/209 (99%)	194 (94%)	12 (6%)	0	100	100
5	E	148/162 (91%)	139 (94%)	9 (6%)	0	100	100
6	F	99/101 (98%)	93 (94%)	6 (6%)	0	100	100
7	G	153/156 (98%)	141 (92%)	12 (8%)	0	100	100
8	H	136/138 (99%)	129 (95%)	7 (5%)	0	100	100
9	I	125/128 (98%)	112 (90%)	12 (10%)	1 (1%)	16	45
10	J	96/105 (91%)	76 (79%)	17 (18%)	3 (3%)	3	22
11	K	114/129 (88%)	99 (87%)	14 (12%)	1 (1%)	14	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	L	121/135 (90%)	108 (89%)	12 (10%)	1 (1%)	16	45
13	M	116/126 (92%)	99 (85%)	16 (14%)	1 (1%)	14	43
14	N	58/61 (95%)	49 (84%)	9 (16%)	0	100	100
15	O	85/89 (96%)	78 (92%)	7 (8%)	0	100	100
16	P	81/88 (92%)	73 (90%)	8 (10%)	0	100	100
17	Q	97/105 (92%)	87 (90%)	10 (10%)	0	100	100
18	R	68/88 (77%)	58 (85%)	9 (13%)	1 (2%)	8	33
19	S	78/93 (84%)	73 (94%)	4 (5%)	1 (1%)	9	36
20	T	97/106 (92%)	83 (86%)	12 (12%)	2 (2%)	5	28
21	U	22/27 (82%)	21 (96%)	0	1 (4%)	2	15
All	All	2336/2541 (92%)	2086 (89%)	235 (10%)	15 (1%)	21	51

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	21	ARG
19	S	31	ILE
20	T	99	LEU
9	I	119	ALA
10	J	86	MET
12	L	28	LYS
20	T	73	HIS
10	J	81	THR
11	K	117	ASN
18	R	26	LEU
2	B	87	ARG
2	B	95	GLN
21	U	24	ARG
10	J	34	VAL
13	M	84	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	202/220 (92%)	147 (73%)	55 (27%)	0	3
3	C	160/188 (85%)	123 (77%)	37 (23%)	1	5
4	D	180/181 (99%)	137 (76%)	43 (24%)	1	5
5	E	115/123 (94%)	82 (71%)	33 (29%)	0	2
6	F	90/90 (100%)	68 (76%)	22 (24%)	1	4
7	G	126/127 (99%)	101 (80%)	25 (20%)	1	8
8	H	119/119 (100%)	89 (75%)	30 (25%)	0	4
9	I	98/99 (99%)	78 (80%)	20 (20%)	1	7
10	J	87/92 (95%)	68 (78%)	19 (22%)	1	6
11	K	88/99 (89%)	75 (85%)	13 (15%)	3	16
12	L	103/110 (94%)	76 (74%)	27 (26%)	0	4
13	M	94/101 (93%)	74 (79%)	20 (21%)	1	7
14	N	49/50 (98%)	35 (71%)	14 (29%)	0	2
15	O	79/80 (99%)	61 (77%)	18 (23%)	1	6
16	P	72/74 (97%)	55 (76%)	17 (24%)	1	5
17	Q	94/97 (97%)	74 (79%)	20 (21%)	1	7
18	R	61/77 (79%)	45 (74%)	16 (26%)	0	4
19	S	71/80 (89%)	56 (79%)	15 (21%)	1	7
20	T	76/82 (93%)	53 (70%)	23 (30%)	0	2
21	U	19/22 (86%)	15 (79%)	4 (21%)	1	7
All	All	1983/2111 (94%)	1512 (76%)	471 (24%)	1	5

All (471) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	7	VAL
2	B	8	LYS
2	B	9	GLU
2	B	11	LEU
2	B	12	GLU
2	B	19	HIS
2	B	22	LYS
2	B	30	ARG
2	B	32	ILE
2	B	47	THR
2	B	49	GLU

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Mol	Chain	Res	Type
2	B	51	LEU
2	B	52	GLU
2	B	53	ARG
2	B	55	PHE
2	B	63	MET
2	B	64	ARG
2	B	69	LEU
2	B	74	LYS
2	B	75	LYS
2	B	79	ASP
2	B	92	TYR
2	B	98	LEU
2	B	102	LEU
2	B	106	LYS
2	B	114	ARG
2	B	121	LEU
2	B	126	GLU
2	B	128	GLU
2	B	135	GLN
2	B	141	GLU
2	B	144	ARG
2	B	149	LEU
2	B	157	ARG
2	B	158	LEU
2	B	162	ILE
2	B	164	VAL
2	B	169	LYS
2	B	175	ARG
2	B	178	ARG
2	B	184	VAL
2	B	185	ILE
2	B	187	LEU
2	B	190	THR
2	B	192	SER
2	B	196	LEU
2	B	197	VAL
2	B	200	ILE
2	B	204	ASN
2	B	206	ASP
2	B	209	ARG
2	B	215	LEU
2	B	216	SER

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Mol	Chain	Res	Type
2	B	236	TYR
2	B	239	VAL
3	C	3	ASN
3	C	5	ILE
3	C	15	THR
3	C	19	GLU
3	C	26	LYS
3	C	32	LEU
3	C	34	LEU
3	C	47	LEU
3	C	56	ASP
3	C	63	ASN
3	C	64	VAL
3	C	70	VAL
3	C	75	VAL
3	C	84	ILE
3	C	91	LEU
3	C	95	THR
3	C	99	VAL
3	C	102	ASN
3	C	111	LEU
3	C	120	VAL
3	C	130	VAL
3	C	153	VAL
3	C	154	SER
3	C	156	ARG
3	C	162	GLN
3	C	166	GLU
3	C	167	TRP
3	C	172	ARG
3	C	173	VAL
3	C	175	LEU
3	C	177	THR
3	C	179	ARG
3	C	188	LEU
3	C	191	THR
3	C	192	THR
3	C	195	VAL
3	C	204	LEU
4	D	5	ILE
4	D	9	CYS
4	D	10	ARG

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Mol	Chain	Res	Type
4	D	17	VAL
4	D	19	LEU
4	D	21	LEU
4	D	25	ARG
4	D	26	CYS
4	D	34	GLU
4	D	52	SER
4	D	59	ARG
4	D	64	LEU
4	D	76	ARG
4	D	80	GLU
4	D	83	SER
4	D	84	LYS
4	D	96	LEU
4	D	119	GLN
4	D	122	ARG
4	D	127	THR
4	D	132	ARG
4	D	135	LEU
4	D	137	SER
4	D	145	GLU
4	D	150	GLU
4	D	155	LEU
4	D	157	LEU
4	D	158	ILE
4	D	160	GLN
4	D	162	LEU
4	D	163	GLU
4	D	166	LYS
4	D	170	VAL
4	D	177	ASP
4	D	178	VAL
4	D	186	LEU
4	D	187	ARG
4	D	190	ASP
4	D	192	GLU
4	D	194	LEU
4	D	196	LEU
4	D	198	VAL
4	D	202	LEU
5	E	6	PHE
5	E	11	ILE

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Mol	Chain	Res	Type
5	E	12	LEU
5	E	13	ILE
5	E	14	ARG
5	E	20	GLN
5	E	26	PHE
5	E	31	LEU
5	E	32	VAL
5	E	33	VAL
5	E	41	VAL
5	E	43	LEU
5	E	51	VAL
5	E	55	VAL
5	E	63	ARG
5	E	64	ARG
5	E	68	GLU
5	E	75	THR
5	E	79	GLU
5	E	100	VAL
5	E	105	VAL
5	E	111	GLU
5	E	112	LEU
5	E	116	THR
5	E	120	THR
5	E	131	ILE
5	E	137	GLU
5	E	140	ARG
5	E	147	ASP
5	E	148	VAL
5	E	149	GLU
5	E	150	ARG
5	E	151	LEU
6	F	9	VAL
6	F	10	LEU
6	F	11	ASN
6	F	13	ASN
6	F	14	LEU
6	F	21	LEU
6	F	24	GLU
6	F	25	ILE
6	F	32	ASN
6	F	40	VAL
6	F	43	LEU

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Mol	Chain	Res	Type
6	F	47	ARG
6	F	65	VAL
6	F	69	GLU
6	F	70	ASP
6	F	72	VAL
6	F	75	LEU
6	F	82	ARG
6	F	88	VAL
6	F	89	MET
6	F	91	VAL
6	F	93	SER
7	G	8	GLU
7	G	9	VAL
7	G	10	ARG
7	G	11	GLN
7	G	16	LEU
7	G	17	VAL
7	G	21	VAL
7	G	23	VAL
7	G	27	ILE
7	G	38	LEU
7	G	53	LYS
7	G	66	VAL
7	G	69	VAL
7	G	72	ARG
7	G	77	SER
7	G	87	VAL
7	G	94	ARG
7	G	95	ARG
7	G	106	GLN
7	G	110	GLN
7	G	113	GLU
7	G	136	LYS
7	G	141	VAL
7	G	144	MET
7	G	149	ARG
8	H	3	THR
8	H	9	MET
8	H	11	THR
8	H	14	ARG
8	H	19	VAL
8	H	22	GLU

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Mol	Chain	Res	Type
8	H	24	THR
8	H	26	VAL
8	H	29	SER
8	H	35	ILE
8	H	45	ILE
8	H	46	LYS
8	H	50	ARG
8	H	63	LEU
8	H	83	ILE
8	H	85	ARG
8	H	87	SER
8	H	88	LYS
8	H	91	ARG
8	H	92	ARG
8	H	93	VAL
8	H	95	VAL
8	H	97	VAL
8	H	98	LYS
8	H	102	ARG
8	H	111	ILE
8	H	112	LEU
8	H	114	THR
8	H	120	THR
8	H	133	LEU
9	I	3	GLN
9	I	10	ARG
9	I	14	VAL
9	I	16	ARG
9	I	19	LEU
9	I	26	VAL
9	I	35	GLU
9	I	40	LEU
9	I	47	LEU
9	I	56	LEU
9	I	64	THR
9	I	70	LYS
9	I	78	LYS
9	I	79	LEU
9	I	83	ARG
9	I	85	LEU
9	I	91	ASP
9	I	96	LEU

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Mol	Chain	Res	Type
9	I	109	VAL
9	I	121	ARG
10	J	3	LYS
10	J	6	ILE
10	J	9	ARG
10	J	15	THR
10	J	16	LEU
10	J	29	ARG
10	J	30	SER
10	J	33	GLN
10	J	38	ILE
10	J	46	ARG
10	J	50	ILE
10	J	65	LEU
10	J	67	THR
10	J	79	ARG
10	J	81	THR
10	J	82	ILE
10	J	92	THR
10	J	95	GLU
10	J	96	ILE
11	K	11	LYS
11	K	14	VAL
11	K	29	ILE
11	K	47	VAL
11	K	48	ILE
11	K	62	GLN
11	K	70	LYS
11	K	78	GLN
11	K	79	SER
11	K	83	ILE
11	K	95	ILE
11	K	98	LEU
11	K	122	LYS
12	L	7	ILE
12	L	18	VAL
12	L	20	LYS
12	L	33	ARG
12	L	36	VAL
12	L	39	VAL
12	L	42	THR
12	L	43	VAL

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Mol	Chain	Res	Type
12	L	47	LYS
12	L	60	LEU
12	L	62	SER
12	L	66	VAL
12	L	67	THR
12	L	78	GLN
12	L	80	HIS
12	L	85	ILE
12	L	89	ARG
12	L	93	LEU
12	L	96	VAL
12	L	100	ILE
12	L	101	VAL
12	L	102	ARG
12	L	104	VAL
12	L	116	SER
12	L	119	LYS
12	L	120	TYR
12	L	122	THR
13	M	14	ARG
13	M	17	VAL
13	M	27	LYS
13	M	45	VAL
13	M	48	LEU
13	M	54	VAL
13	M	56	LEU
13	M	61	GLU
13	M	63	THR
13	M	66	LEU
13	M	67	GLU
13	M	74	VAL
13	M	80	ARG
13	M	81	LEU
13	M	82	MET
13	M	105	THR
13	M	108	ARG
13	M	109	THR
13	M	110	ARG
13	M	117	VAL
14	N	4	LYS
14	N	6	LEU
14	N	9	LYS

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Mol	Chain	Res	Type
14	N	22	THR
14	N	24	CYS
14	N	25	VAL
14	N	29	ARG
14	N	31	ARG
14	N	42	ILE
14	N	47	LEU
14	N	50	LYS
14	N	53	LEU
14	N	57	ARG
14	N	58	LYS
15	O	8	LYS
15	O	9	GLN
15	O	14	GLU
15	O	31	LEU
15	O	32	LEU
15	O	36	ILE
15	O	39	LEU
15	O	40	SER
15	O	57	LEU
15	O	60	VAL
15	O	62	GLN
15	O	65	ARG
15	O	66	LEU
15	O	68	ARG
15	O	71	GLN
15	O	73	GLU
15	O	81	LEU
15	O	87	ILE
16	P	1	MET
16	P	2	VAL
16	P	20	VAL
16	P	25	ARG
16	P	28	ARG
16	P	33	ILE
16	P	42	ARG
16	P	44	THR
16	P	45	THR
16	P	51	VAL
16	P	53	VAL
16	P	54	GLU
16	P	55	ARG

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Mol	Chain	Res	Type
16	P	62	VAL
16	P	67	THR
16	P	80	PHE
16	P	82	GLN
17	Q	9	VAL
17	Q	13	ASP
17	Q	23	VAL
17	Q	24	GLU
17	Q	34	LYS
17	Q	35	VAL
17	Q	36	ILE
17	Q	37	LYS
17	Q	41	LYS
17	Q	45	HIS
17	Q	53	LEU
17	Q	59	ILE
17	Q	60	ILE
17	Q	66	SER
17	Q	67	LYS
17	Q	75	ARG
17	Q	86	GLU
17	Q	90	ILE
17	Q	92	ARG
17	Q	100	LYS
18	R	19	LYS
18	R	25	THR
18	R	37	VAL
18	R	38	GLU
18	R	40	LEU
18	R	46	GLU
18	R	47	THR
18	R	49	LYS
18	R	50	ILE
18	R	52	PRO
18	R	54	ARG
18	R	65	ILE
18	R	69	THR
18	R	78	LEU
18	R	82	THR
18	R	87	ARG
19	S	5	LEU
19	S	6	LYS

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Mol	Chain	Res	Type
19	S	7	LYS
19	S	13	ASP
19	S	20	LEU
19	S	29	ARG
19	S	31	ILE
19	S	37	ARG
19	S	38	SER
19	S	58	VAL
19	S	60	VAL
19	S	65	ASN
19	S	70	LYS
19	S	71	LEU
19	S	81	ARG
20	T	10	LEU
20	T	11	SER
20	T	13	LEU
20	T	19	SER
20	T	20	LEU
20	T	24	LEU
20	T	41	ILE
20	T	42	GLN
20	T	43	LEU
20	T	53	LEU
20	T	56	MET
20	T	62	LEU
20	T	68	LYS
20	T	72	LEU
20	T	75	ASN
20	T	83	ARG
20	T	84	LEU
20	T	86	ARG
20	T	87	LYS
20	T	90	GLN
20	T	91	LEU
20	T	93	GLU
20	T	99	LEU
21	U	8	THR
21	U	10	ARG
21	U	13	ILE
21	U	14	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	140	HIS
3	C	6	HIS
3	C	37	GLN
3	C	98	ASN
3	C	104	GLN
3	C	136	GLN
4	D	42	GLN
4	D	161	ASN
4	D	201	GLN
9	I	124	GLN
12	L	80	HIS
15	O	13	GLN
15	O	28	GLN
15	O	53	HIS
16	P	82	GLN
17	Q	45	HIS
18	R	36	ASN
19	S	23	ASN
19	S	57	HIS
20	T	90	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1505/1522 (98%)	360 (23%)	45 (2%)

All (360) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	G
1	A	9	G
1	A	21	G
1	A	22	G
1	A	31	G
1	A	32	A
1	A	39	G
1	A	47	C
1	A	48	C
1	A	49	U
1	A	50	A
1	A	51	A
1	A	54	C

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Mol	Chain	Res	Type
1	A	59	A
1	A	74	C
1	A	75	G
1	A	80	G
1	A	81	U
1	A	91	C
1	A	95	U
1	A	99	C
1	A	101	A
1	A	108	G
1	A	115	G
1	A	116	A
1	A	117	G
1	A	121	C
1	A	129(A)	G
1	A	130	A
1	A	131	C
1	A	135	C
1	A	163	C
1	A	166	G
1	A	178	C
1	A	181	G
1	A	182	U
1	A	183	G
1	A	190(D)	U
1	A	190(E)	U
1	A	195	A
1	A	197	A
1	A	202	U
1	A	203	U
1	A	204	U
1	A	216	G
1	A	217	C
1	A	221	C
1	A	227	G
1	A	231	G
1	A	245	C
1	A	247	G
1	A	251	G
1	A	254	G
1	A	258	G
1	A	266	G

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Mol	Chain	Res	Type
1	A	267	C
1	A	281	G
1	A	282	A
1	A	289	G
1	A	299	G
1	A	301	G
1	A	319	G
1	A	321	A
1	A	325	A
1	A	328	C
1	A	329	A
1	A	330	C
1	A	331	G
1	A	332	G
1	A	344	A
1	A	345	C
1	A	346	G
1	A	349	A
1	A	351	G
1	A	352	C
1	A	353	A
1	A	354	G
1	A	367	U
1	A	372	C
1	A	373	A
1	A	374	A
1	A	382	A
1	A	384	G
1	A	390	C
1	A	397	A
1	A	398	C
1	A	406	G
1	A	409	G
1	A	412	A
1	A	413	G
1	A	419	C
1	A	421	U
1	A	422	C
1	A	429	U
1	A	430	A
1	A	435	C
1	A	439	A

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Mol	Chain	Res	Type
1	A	450	G
1	A	453	A
1	A	460	A
1	A	461	C
1	A	475	G
1	A	481	G
1	A	482	A
1	A	484	G
1	A	485	G
1	A	486	U
1	A	497	A
1	A	498	U
1	A	505	G
1	A	509	A
1	A	510	A
1	A	511	C
1	A	513	C
1	A	518	C
1	A	519	C
1	A	526	C
1	A	527	7MG
1	A	531	U
1	A	532	A
1	A	533	A
1	A	535	A
1	A	536	C
1	A	547	A
1	A	558	G
1	A	559	A
1	A	560	U
1	A	562	C
1	A	563	A
1	A	564	C
1	A	566	G
1	A	568	G
1	A	572	A
1	A	573	A
1	A	576	G
1	A	577	G
1	A	579	G
1	A	581	G
1	A	584	G

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Mol	Chain	Res	Type
1	A	588	G
1	A	607	A
1	A	624	C
1	A	651	C
1	A	653	A
1	A	665	A
1	A	671	G
1	A	686	U
1	A	687	A
1	A	688	G
1	A	701	C
1	A	702	A
1	A	703	G
1	A	718	G
1	A	719	C
1	A	721	G
1	A	722	A
1	A	723	U
1	A	724	G
1	A	731	G
1	A	740	U
1	A	749	C
1	A	755	G
1	A	771	G
1	A	777	A
1	A	780	A
1	A	781	A
1	A	782	A
1	A	785	G
1	A	791	G
1	A	792	A
1	A	793	U
1	A	794	A
1	A	813	U
1	A	817	C
1	A	818	G
1	A	821	G
1	A	826	C
1	A	828	A
1	A	839	U
1	A	840	C
1	A	841	U

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Mol	Chain	Res	Type
1	A	848	C
1	A	851	G
1	A	858	G
1	A	872	A
1	A	873	A
1	A	885	G
1	A	889	A
1	A	902	G
1	A	913	A
1	A	914	G
1	A	916	G
1	A	922	G
1	A	926	G
1	A	927	G
1	A	934	C
1	A	935	A
1	A	936	C
1	A	940	C
1	A	941	G
1	A	942	G
1	A	949	A
1	A	950	U
1	A	960	U
1	A	961	U
1	A	963	G
1	A	964	A
1	A	966	M2G
1	A	967	5MC
1	A	968	A
1	A	969	A
1	A	971	G
1	A	974	A
1	A	975	A
1	A	976	G
1	A	977	A
1	A	981	U
1	A	982	U
1	A	991	U
1	A	992	U
1	A	993	G
1	A	994	A
1	A	1003(A)	G

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Mol	Chain	Res	Type
1	A	1004	A
1	A	1005	A
1	A	1006	C
1	A	1012	U
1	A	1015	A
1	A	1020	U
1	A	1023	G
1	A	1024	G
1	A	1034	G
1	A	1045	C
1	A	1050	G
1	A	1053	G
1	A	1054	C
1	A	1065	U
1	A	1066	C
1	A	1068	G
1	A	1078	U
1	A	1094	G
1	A	1095	U
1	A	1101	A
1	A	1104	G
1	A	1124	G
1	A	1125	U
1	A	1126	U
1	A	1127	G
1	A	1129	C
1	A	1130	A
1	A	1132	C
1	A	1137	C
1	A	1138	G
1	A	1139	G
1	A	1140	C
1	A	1143	G
1	A	1145	C
1	A	1146	A
1	A	1152	A
1	A	1159	U
1	A	1160	G
1	A	1169	A
1	A	1171	G
1	A	1174	G
1	A	1176	A

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Mol	Chain	Res	Type
1	A	1182	G
1	A	1183	A
1	A	1190	G
1	A	1191	A
1	A	1193	G
1	A	1196	U
1	A	1197	G
1	A	1198	G
1	A	1200	C
1	A	1201	A
1	A	1202	G
1	A	1207	2MG
1	A	1209	C
1	A	1212	U
1	A	1213	A
1	A	1214	C
1	A	1215	G
1	A	1224	G
1	A	1225	A
1	A	1226	C
1	A	1227	A
1	A	1228	C
1	A	1233	G
1	A	1238	A
1	A	1241	G
1	A	1256	A
1	A	1257	U
1	A	1258	G
1	A	1260	C
1	A	1263	C
1	A	1268	A
1	A	1278	U
1	A	1280	A
1	A	1281	U
1	A	1282	C
1	A	1286	A
1	A	1287	A
1	A	1288	A
1	A	1297	C
1	A	1299	A
1	A	1300	G
1	A	1301	U

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Mol	Chain	Res	Type
1	A	1302	U
1	A	1303	C
1	A	1304	G
1	A	1305	G
1	A	1306	A
1	A	1310	G
1	A	1318	A
1	A	1319	A
1	A	1320	C
1	A	1323	G
1	A	1335	C
1	A	1336	C
1	A	1338	G
1	A	1339	A
1	A	1340	A
1	A	1347	G
1	A	1348	U
1	A	1353	G
1	A	1362	C
1	A	1364	U
1	A	1365	G
1	A	1370	G
1	A	1381	U
1	A	1398	A
1	A	1399	C
1	A	1400	5MC
1	A	1402	4OC
1	A	1406	U
1	A	1407	5MC
1	A	1412	C
1	A	1442	G
1	A	1446	A
1	A	1447	G
1	A	1451	A
1	A	1454	G
1	A	1485	U
1	A	1487	G
1	A	1490	C
1	A	1493	A
1	A	1497	G
1	A	1498	UR3
1	A	1499	A

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Mol	Chain	Res	Type
1	A	1503	A
1	A	1504	G
1	A	1505	G
1	A	1506	U
1	A	1507	A
1	A	1529	G
1	A	1530	G
1	A	1531	A
1	A	1541	PSU
1	A	1542	U
1	A	1543	C

All (45) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	5	U
1	A	21	G
1	A	80	G
1	A	115	G
1	A	129(A)	G
1	A	181	G
1	A	250	A
1	A	281	G
1	A	328	C
1	A	372	C
1	A	428	G
1	A	429	U
1	A	484	G
1	A	509	A
1	A	518	C
1	A	532	A
1	A	559	A
1	A	686	U
1	A	687	A
1	A	701	C
1	A	748	C
1	A	792	A
1	A	812	C
1	A	913	A
1	A	960	U
1	A	965	A
1	A	975	A

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Mol	Chain	Res	Type
1	A	992	U
1	A	1004	A
1	A	1049	U
1	A	1065	U
1	A	1139	G
1	A	1145	C
1	A	1182	G
1	A	1190	G
1	A	1201	A
1	A	1256	A
1	A	1257	U
1	A	1285	A
1	A	1300	G
1	A	1301	U
1	A	1305	G
1	A	1347	G
1	A	1380	U
1	A	1505	G

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MA6	A	1519[A]	1	23,26,27	0.98	1 (4%)	33,38,41	1.12	4 (12%)
1	5MC	A	1407	1	19,22,23	1.44	3 (15%)	26,32,35	1.37	3 (11%)
1	MA6	A	1519[B]	1	23,26,27	1.54	7 (30%)	33,38,41	1.03	3 (9%)
1	5MC	A	1400	1	19,22,23	1.61	4 (21%)	26,32,35	1.03	2 (7%)
1	PSU	A	1541	1	18,21,22	1.04	1 (5%)	21,30,33	1.70	4 (19%)
1	M2G	A	966	1	24,27,28	1.13	2 (8%)	33,40,43	0.97	3 (9%)
1	MA6	A	1518[A]	1	23,26,27	1.01	2 (8%)	33,38,41	0.93	1 (3%)
1	7MG	A	527	1,22	23,26,27	4.56	8 (34%)	27,39,42	2.76	9 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MA6	A	1518[B]	1	23,26,27	1.24	3 (13%)	33,38,41	0.98	1 (3%)
12	0TD	L	92	12	8,9,10	2.13	1 (12%)	6,11,13	3.25	5 (83%)
1	PSU	A	516	1,22	18,21,22	1.31	1 (5%)	21,30,33	1.46	4 (19%)
1	PSU	A	1540	1	18,21,22	1.18	1 (5%)	21,30,33	1.45	3 (14%)
1	5MC	A	967	1	19,22,23	1.52	5 (26%)	26,32,35	0.82	0
1	UR3	A	1498	1	19,22,23	1.14	2 (10%)	26,32,35	1.52	3 (11%)
1	2MG	A	1207	1	23,26,27	1.73	5 (21%)	33,38,41	1.13	5 (15%)
1	5MC	A	1404	1	19,22,23	1.48	3 (15%)	26,32,35	1.56	4 (15%)
1	4OC	A	1402	1	20,23,24	1.29	1 (5%)	25,32,35	0.74	0

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	MA6	A	1519[A]	1	-	2/11/29/30	0/3/3/3
1	5MC	A	1407	1	-	2/7/25/26	0/2/2/2
1	MA6	A	1519[B]	1	-	3/11/29/30	0/3/3/3
1	5MC	A	1400	1	-	2/7/25/26	0/2/2/2
1	PSU	A	1541	1	-	2/7/25/26	0/2/2/2
1	M2G	A	966	1	-	3/11/29/30	0/3/3/3
1	MA6	A	1518[A]	1	-	0/11/29/30	0/3/3/3
1	7MG	A	527	1,22	-	2/7/37/38	0/3/3/3
1	MA6	A	1518[B]	1	-	0/11/29/30	0/3/3/3
12	0TD	L	92	12	-	4/7/12/14	-
1	PSU	A	516	1,22	-	0/7/25/26	0/2/2/2
1	PSU	A	1540	1	-	0/7/25/26	0/2/2/2
1	5MC	A	967	1	-	4/7/25/26	0/2/2/2
1	UR3	A	1498	1	-	2/7/25/26	0/2/2/2
1	2MG	A	1207	1	-	2/9/27/28	0/3/3/3
1	5MC	A	1404	1	-	0/7/25/26	0/2/2/2
1	4OC	A	1402	1	-	3/9/29/30	0/2/2/2

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	527	7MG	C8-N9	-20.19	1.32	1.45
1	A	1404	5MC	C5-C4	5.39	1.48	1.44
12	L	92	0TD	CB-CA	5.36	1.56	1.54
1	A	516	PSU	C6-C5	4.51	1.40	1.35
1	A	1540	PSU	C6-C5	4.20	1.39	1.35
1	A	527	7MG	C5-N7	4.11	1.40	1.35
1	A	1207	2MG	C2-N1	4.01	1.43	1.36
1	A	527	7MG	C2-N2	3.70	1.42	1.34
1	A	1400	5MC	C5-C4	-3.67	1.41	1.44
1	A	1407	5MC	C5-C4	3.67	1.46	1.44
1	A	1402	4OC	C2-N1	3.49	1.47	1.40
1	A	1207	2MG	C6-N1	3.48	1.45	1.38
1	A	1400	5MC	C2-N1	3.46	1.47	1.40
1	A	1541	PSU	C6-C5	3.39	1.39	1.35
1	A	967	5MC	C2-N3	3.36	1.43	1.36
1	A	1207	2MG	C8-N9	3.21	1.44	1.37
1	A	1519[B]	MA6	C5-C4	3.19	1.44	1.39
1	A	1519[B]	MA6	C4-N3	3.12	1.40	1.34
1	A	1207	2MG	C2-N2	3.09	1.39	1.33
1	A	527	7MG	C4-N3	3.08	1.41	1.34
1	A	966	M2G	C2-N2	3.03	1.40	1.35
1	A	1407	5MC	C2-N1	3.01	1.46	1.40
1	A	967	5MC	C6-C5	2.97	1.39	1.34
1	A	1518[B]	MA6	C8-N9	2.94	1.42	1.37
1	A	1519[B]	MA6	C2-N1	2.81	1.38	1.33
1	A	1519[B]	MA6	C4-N9	2.73	1.43	1.37
1	A	1207	2MG	C4-N3	2.72	1.40	1.34
1	A	527	7MG	O6-C6	-2.72	1.18	1.23
1	A	966	M2G	C4-N3	2.67	1.40	1.34
1	A	1407	5MC	C2-N3	2.59	1.41	1.36
1	A	1400	5MC	C2-N3	2.59	1.41	1.36
1	A	1518[A]	MA6	C2-N3	-2.48	1.29	1.33
1	A	967	5MC	C4-N4	2.45	1.40	1.34
1	A	527	7MG	C2-N1	-2.41	1.31	1.37
1	A	1519[B]	MA6	C8-N9	2.41	1.41	1.37
1	A	1518[B]	MA6	C5-C4	2.27	1.43	1.39
1	A	1404	5MC	C2-N1	2.20	1.44	1.40
1	A	1498	UR3	O3'-C3'	2.19	1.48	1.43
1	A	527	7MG	C6-N1	-2.16	1.34	1.38
1	A	527	7MG	C8-N7	-2.14	1.31	1.42
1	A	1404	5MC	C2-N3	2.11	1.40	1.36
1	A	967	5MC	C4-N3	2.09	1.37	1.34
1	A	1400	5MC	C6-C5	2.09	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1519[B]	MA6	C6-N1	2.07	1.38	1.34
1	A	1518[A]	MA6	C5-C4	2.05	1.42	1.39
1	A	1519[B]	MA6	C8-N7	2.04	1.35	1.31
1	A	1498	UR3	C3U-N3	-2.04	1.43	1.47
1	A	967	5MC	C2-N1	2.03	1.44	1.40
1	A	1518[B]	MA6	C4-N9	2.03	1.41	1.37
1	A	1519[A]	MA6	C5-C4	2.02	1.42	1.39

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	527	7MG	C5-C6-N1	6.87	123.04	110.94
1	A	527	7MG	N9-C4-N3	6.49	134.96	125.46
12	L	92	0TD	CSB-SB-CB	-5.97	91.63	102.36
1	A	527	7MG	C5-C4-N3	-5.29	118.21	128.13
1	A	527	7MG	C2-N3-C4	4.88	120.70	112.30
1	A	1541	PSU	C4-N3-C2	-4.37	120.35	126.37
1	A	1404	5MC	N4-C4-N3	-4.31	110.70	118.51
1	A	527	7MG	C2-N1-C6	-4.18	117.52	125.11
1	A	1498	UR3	C6-N1-C2	-3.82	118.68	121.80
1	A	1404	5MC	C5-C4-N3	3.77	125.62	121.75
1	A	1541	PSU	N1-C2-N3	3.68	119.05	115.17
1	A	516	PSU	C4-N3-C2	-3.67	121.31	126.37
1	A	1540	PSU	C4-N3-C2	-3.36	121.74	126.37
1	A	516	PSU	N1-C2-N3	3.35	118.70	115.17
1	A	527	7MG	N9-C8-N7	3.35	108.11	103.37
1	A	1407	5MC	C1'-N1-C6	-3.25	115.80	121.15
12	L	92	0TD	OD1-CG-CB	-3.16	115.82	122.44
1	A	527	7MG	O6-C6-C5	-3.07	120.07	127.62
1	A	1404	5MC	C5-C6-N1	-2.94	120.11	123.31
1	A	1407	5MC	N4-C4-N3	-2.93	113.21	118.51
1	A	1540	PSU	O2-C2-N1	-2.90	119.80	122.79
1	A	1540	PSU	N1-C2-N3	2.86	118.18	115.17
1	A	527	7MG	C6-C5-N7	2.85	136.34	131.93
1	A	527	7MG	C6-C5-C4	-2.80	117.48	122.40
1	A	1498	UR3	C5-C4-N3	-2.70	111.48	115.04
1	A	1404	5MC	C4-N3-C2	-2.68	117.08	120.81
12	L	92	0TD	CB-CA-N	-2.68	103.67	109.10
1	A	1518[A]	MA6	C2-N1-C6	2.61	118.22	111.83
1	A	1541	PSU	O4'-C1'-C2'	2.57	108.70	105.15
1	A	1519[A]	MA6	C4-C5-C6	2.56	118.56	115.91
1	A	1541	PSU	O2-C2-N1	-2.53	120.18	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1207	2MG	N2-C2-N3	-2.50	117.32	120.51
1	A	966	M2G	C5-C4-N3	-2.50	124.41	128.39
1	A	1207	2MG	O6-C6-N1	-2.45	115.51	120.11
1	A	1519[B]	MA6	C4-C5-C6	2.42	118.41	115.91
1	A	1519[B]	MA6	C5-C4-N3	-2.35	123.48	126.72
1	A	1400	5MC	O2-C2-N1	2.29	123.39	118.90
1	A	516	PSU	C6-N1-C2	-2.27	120.58	122.69
1	A	1519[A]	MA6	C5-C4-N9	2.26	108.28	105.81
1	A	1207	2MG	C5-C4-N3	-2.25	124.81	128.39
12	L	92	0TD	OD2-CG-CB	2.22	117.95	113.15
1	A	1400	5MC	C5-C4-N3	2.20	124.01	121.75
12	L	92	0TD	O-C-CA	-2.20	119.12	124.77
1	A	516	PSU	O4'-C1'-C2'	2.19	108.19	105.15
1	A	1407	5MC	C5-C4-N3	2.14	123.95	121.75
1	A	1207	2MG	C2-N1-C6	-2.13	121.97	124.55
1	A	1519[A]	MA6	C2-N1-C6	2.10	116.96	111.83
1	A	1519[B]	MA6	C5-C6-N6	-2.08	122.05	125.33
1	A	1519[A]	MA6	C4-C5-N7	-2.06	108.22	110.58
1	A	1518[B]	MA6	C5-C4-N3	-2.06	123.88	126.72
1	A	966	M2G	O6-C6-N1	-2.04	116.28	120.11
1	A	1498	UR3	C3U-N3-C2	-2.03	113.79	117.33
1	A	966	M2G	N9-C4-N3	2.02	130.00	125.95
1	A	1207	2MG	C2-N3-C4	2.00	114.51	112.00

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	527	7MG	O4'-C4'-C5'-O5'
1	A	967	5MC	O4'-C4'-C5'-O5'
1	A	967	5MC	C3'-C4'-C5'-O5'
1	A	1207	2MG	O4'-C4'-C5'-O5'
1	A	1400	5MC	O4'-C4'-C5'-O5'
1	A	1402	4OC	O4'-C4'-C5'-O5'
1	A	1407	5MC	O4'-C4'-C5'-O5'
1	A	1519[B]	MA6	C5-C6-N6-C9
1	A	1519[B]	MA6	N1-C6-N6-C9
12	L	92	0TD	CG-CB-SB-CSB
1	A	527	7MG	C3'-C4'-C5'-O5'
1	A	1402	4OC	C3'-C4'-C5'-O5'
1	A	1407	5MC	C3'-C4'-C5'-O5'
1	A	966	M2G	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	A	966	M2G	C3'-C4'-C5'-O5'
1	A	1207	2MG	C3'-C4'-C5'-O5'
1	A	1400	5MC	C3'-C4'-C5'-O5'
1	A	1519[A]	MA6	C5-C6-N6-C9
1	A	1498	UR3	O4'-C4'-C5'-O5'
1	A	1519[B]	MA6	C5-C6-N6-C10
1	A	1498	UR3	C3'-C4'-C5'-O5'
12	L	92	0TD	SB-CB-CG-OD1
1	A	966	M2G	C4'-C5'-O5'-P
1	A	1541	PSU	O4'-C1'-C5-C4
1	A	1519[A]	MA6	O4'-C4'-C5'-O5'
12	L	92	0TD	CA-CB-SB-CSB
12	L	92	0TD	SB-CB-CG-OD2
1	A	1541	PSU	O4'-C1'-C5-C6
1	A	967	5MC	C2'-C1'-N1-C6
1	A	967	5MC	C2'-C1'-N1-C2
1	A	1402	4OC	C2'-C1'-N1-C2

There are no ring outliers.

13 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1519[A]	MA6	4	0
1	A	1407	5MC	1	0
1	A	1519[B]	MA6	3	0
1	A	1400	5MC	1	0
1	A	1541	PSU	1	0
1	A	966	M2G	2	0
1	A	1518[A]	MA6	4	0
1	A	1518[B]	MA6	3	0
12	L	92	0TD	4	0
1	A	516	PSU	1	0
1	A	967	5MC	2	0
1	A	1498	UR3	5	0
1	A	1402	4OC	3	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 289 ligands modelled in this entry, 289 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1498/1522 (98%)	-0.55	5 (0%) 90 75	59, 150, 286, 387	4 (0%)
2	B	234/256 (91%)	-0.56	0 100 100	110, 168, 268, 286	0
3	C	206/239 (86%)	-0.42	0 100 100	162, 213, 261, 290	0
4	D	208/209 (99%)	-0.38	5 (2%) 59 35	108, 155, 199, 234	0
5	E	150/162 (92%)	-0.73	0 100 100	86, 126, 170, 198	0
6	F	101/101 (100%)	-0.67	0 100 100	121, 179, 212, 250	0
7	G	155/156 (99%)	-0.45	1 (0%) 85 64	143, 190, 248, 259	0
8	H	138/138 (100%)	-0.75	1 (0%) 84 61	82, 115, 151, 197	0
9	I	127/128 (99%)	-0.34	2 (1%) 70 43	157, 217, 260, 283	0
10	J	98/105 (93%)	-0.17	2 (2%) 65 39	188, 246, 325, 368	0
11	K	116/129 (89%)	-0.54	1 (0%) 81 57	116, 151, 201, 215	0
12	L	123/135 (91%)	-0.45	1 (0%) 82 59	95, 157, 200, 225	0
13	M	118/126 (93%)	-0.43	2 (1%) 69 41	151, 183, 216, 272	0
14	N	60/61 (98%)	-0.09	0 100 100	166, 205, 258, 282	0
15	O	87/89 (97%)	-0.68	0 100 100	94, 140, 184, 196	0
16	P	83/88 (94%)	-0.47	0 100 100	103, 146, 190, 220	0
17	Q	99/105 (94%)	-0.53	0 100 100	84, 126, 176, 199	0
18	R	70/88 (79%)	-0.61	0 100 100	106, 150, 201, 227	0
19	S	80/93 (86%)	-0.00	3 (3%) 44 27	185, 234, 275, 291	0
20	T	99/106 (93%)	-0.35	1 (1%) 79 54	115, 152, 198, 234	0
21	U	24/27 (88%)	-0.05	0 100 100	165, 177, 208, 219	0
All	All	3874/4063 (95%)	-0.50	24 (0%) 85 64	59, 163, 261, 387	4 (0%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
19	S	3	ARG	7.1
1	A	1129	C	5.7
20	T	106	ALA	5.3
4	D	31	CYS	4.6
19	S	2	PRO	4.4
1	A	1417	G	3.6
11	K	56	GLY	3.3
1	A	1517[A]	G	3.1
4	D	26	CYS	3.1
4	D	9	CYS	3.1
10	J	58	ASP	3.0
4	D	2	GLY	2.9
8	H	18	ARG	2.8
19	S	5	LEU	2.6
4	D	3	ARG	2.5
1	A	1220	G	2.5
7	G	74	GLU	2.5
10	J	39	PRO	2.4
13	M	106	ASN	2.3
9	I	128	ARG	2.3
9	I	110	GLU	2.2
12	L	73	GLU	2.1
1	A	985	C	2.1
13	M	8	GLU	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	1541	20/21	0.92	0.10	220,227,234,235	0
1	PSU	A	1540	20/21	0.93	0.12	212,224,250,256	0
1	M2G	A	966	25/26	0.93	0.09	167,195,202,204	0
1	PSU	A	516	20/21	0.95	0.06	130,162,189,195	0
1	2MG	A	1207	24/25	0.95	0.09	201,225,261,267	0
1	UR3	A	1498	21/22	0.96	0.10	132,143,155,163	0
1	5MC	A	1400	21/22	0.96	0.07	117,141,147,151	0
1	5MC	A	1407	21/22	0.96	0.10	155,176,182,195	0
1	MA6	A	1518[A]	24/25	0.97	0.11	121,138,144,149	24
1	MA6	A	1518[B]	24/25	0.97	0.11	123,140,152,155	24

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	7MG	A	527	24/25	0.97	0.08	125,139,158,159	0
1	5MC	A	967	21/22	0.97	0.06	158,165,199,200	0
1	5MC	A	1404	21/22	0.98	0.06	127,137,174,177	0
12	0TD	L	92	10/11	0.98	0.13	144,153,175,322	0
1	4OC	A	1402	22/23	0.99	0.08	130,141,155,213	0
1	MA6	A	1519[A]	24/25	0.99	0.09	114,123,128,180	24
1	MA6	A	1519[B]	24/25	0.99	0.09	115,125,129,130	24

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

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	1783	1/1	0.45	0.18	179,179,179,179	0
22	MG	A	1706	1/1	0.49	0.29	207,207,207,207	0
22	MG	A	1832	1/1	0.49	0.11	390,390,390,390	0
22	MG	A	1833	1/1	0.56	0.11	230,230,230,230	0
22	MG	A	1773	1/1	0.60	0.10	142,142,142,142	0
22	MG	A	1670	1/1	0.63	0.26	109,109,109,109	0
22	MG	A	1830	1/1	0.68	0.12	512,512,512,512	0
22	MG	A	1728	1/1	0.70	0.18	128,128,128,128	0
22	MG	Q	201	1/1	0.71	0.08	136,136,136,136	0
22	MG	A	1857	1/1	0.73	0.19	141,141,141,141	0
22	MG	A	1744	1/1	0.73	0.26	150,150,150,150	0
22	MG	A	1767	1/1	0.74	0.29	167,167,167,167	0
22	MG	A	1769	1/1	0.76	0.14	134,134,134,134	0
22	MG	A	1686	1/1	0.76	0.10	166,166,166,166	0
22	MG	A	1777	1/1	0.76	0.34	144,144,144,144	0
22	MG	E	201	1/1	0.77	0.14	163,163,163,163	0
22	MG	A	1845	1/1	0.78	0.12	157,157,157,157	0
22	MG	A	1737	1/1	0.78	0.19	133,133,133,133	0
22	MG	A	1714	1/1	0.80	0.72	124,124,124,124	0
22	MG	A	1699	1/1	0.80	0.28	171,171,171,171	0
22	MG	A	1605	1/1	0.81	0.19	105,105,105,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	MG	Q	202	1/1	0.81	0.15	146,146,146,146	0
22	MG	A	1861	1/1	0.82	0.16	163,163,163,163	0
22	MG	A	1778	1/1	0.82	0.33	132,132,132,132	0
22	MG	C	302	1/1	0.83	0.14	181,181,181,181	0
22	MG	A	1851	1/1	0.83	0.11	136,136,136,136	0
22	MG	P	102	1/1	0.83	0.08	141,141,141,141	0
22	MG	A	1754	1/1	0.83	0.27	134,134,134,134	0
22	MG	A	1821	1/1	0.83	0.21	119,119,119,119	0
22	MG	A	1705	1/1	0.84	0.14	156,156,156,156	0
22	MG	A	1601	1/1	0.84	0.19	122,122,122,122	0
22	MG	A	1792	1/1	0.84	0.12	145,145,145,145	0
22	MG	F	201	1/1	0.84	0.10	144,144,144,144	0
22	MG	A	1809	1/1	0.84	0.07	466,466,466,466	0
22	MG	A	1818	1/1	0.84	0.57	126,126,126,126	0
22	MG	A	1713	1/1	0.84	0.12	92,92,92,92	0
22	MG	A	1666	1/1	0.85	0.29	118,118,118,118	0
22	MG	A	1758	1/1	0.85	0.09	150,150,150,150	0
22	MG	A	1822	1/1	0.85	0.16	147,147,147,147	0
22	MG	J	201	1/1	0.85	0.18	127,127,127,127	0
22	MG	A	1837	1/1	0.85	0.10	150,150,150,150	0
22	MG	A	1863	1/1	0.85	0.25	121,121,121,121	0
22	MG	A	1864	1/1	0.85	0.07	129,129,129,129	0
22	MG	A	1676	1/1	0.86	0.34	151,151,151,151	0
22	MG	A	1709	1/1	0.86	0.56	118,118,118,118	0
22	MG	A	1788	1/1	0.86	0.29	420,420,420,420	0
22	MG	A	1756	1/1	0.86	0.24	127,127,127,127	0
22	MG	A	1637	1/1	0.86	0.33	127,127,127,127	0
22	MG	B	301	1/1	0.87	0.16	138,138,138,138	0
22	MG	A	1725	1/1	0.88	0.41	126,126,126,126	0
22	MG	A	1812	1/1	0.88	0.08	429,429,429,429	0
22	MG	A	1816	1/1	0.88	0.07	422,422,422,422	0
22	MG	A	1662	1/1	0.88	0.17	128,128,128,128	0
22	MG	A	1735	1/1	0.88	0.18	122,122,122,122	0
22	MG	A	1618	1/1	0.88	0.20	147,147,147,147	0
22	MG	A	1669	1/1	0.88	0.28	144,144,144,144	0
22	MG	A	1623	1/1	0.88	0.13	148,148,148,148	0
22	MG	A	1607	1/1	0.88	0.10	183,183,183,183	0
22	MG	A	1834	1/1	0.88	0.11	157,157,157,157	0
22	MG	A	1642	1/1	0.88	0.14	158,158,158,158	0
22	MG	A	1841	1/1	0.88	0.17	149,149,149,149	0
22	MG	A	1794	1/1	0.88	0.15	211,211,211,211	0
22	MG	A	1826	1/1	0.89	0.08	225,225,225,225	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	MG	A	1656	1/1	0.89	0.29	110,110,110,110	0
22	MG	A	1621	1/1	0.89	0.11	111,111,111,111	0
22	MG	A	1745	1/1	0.89	0.12	155,155,155,155	0
22	MG	A	1810	1/1	0.89	0.20	386,386,386,386	0
22	MG	A	1746	1/1	0.89	0.08	181,181,181,181	0
22	MG	A	1675	1/1	0.89	0.49	123,123,123,123	0
22	MG	A	1780	1/1	0.89	0.18	154,154,154,154	0
22	MG	N	102	1/1	0.89	0.10	184,184,184,184	0
22	MG	A	1625	1/1	0.89	0.24	124,124,124,124	0
22	MG	A	1854	1/1	0.89	0.15	112,112,112,112	0
22	MG	A	1685	1/1	0.89	0.46	109,109,109,109	0
22	MG	A	1813	1/1	0.90	0.18	105,105,105,105	0
22	MG	A	1848	1/1	0.90	0.22	144,144,144,144	0
22	MG	A	1751	1/1	0.90	0.19	139,139,139,139	0
22	MG	A	1696	1/1	0.90	0.10	399,399,399,399	0
22	MG	A	1782	1/1	0.90	0.12	244,244,244,244	0
22	MG	A	1860	1/1	0.90	0.12	167,167,167,167	0
22	MG	A	1836	1/1	0.90	0.35	98,98,98,98	0
22	MG	A	1722	1/1	0.90	0.40	115,115,115,115	0
22	MG	A	1671	1/1	0.90	0.33	120,120,120,120	0
22	MG	A	1850	1/1	0.91	0.48	150,150,150,150	0
22	MG	A	1753	1/1	0.91	0.10	128,128,128,128	0
22	MG	A	1717	1/1	0.91	0.21	120,120,120,120	0
22	MG	A	1738	1/1	0.91	0.34	115,115,115,115	0
22	MG	A	1858	1/1	0.91	0.43	115,115,115,115	0
22	MG	A	1790	1/1	0.91	0.17	356,356,356,356	0
22	MG	A	1739	1/1	0.91	0.61	132,132,132,132	0
22	MG	A	1628	1/1	0.91	0.29	110,110,110,110	0
22	MG	A	1796	1/1	0.91	0.19	168,168,168,168	0
22	MG	A	1799	1/1	0.91	0.27	466,466,466,466	0
22	MG	A	1663	1/1	0.91	0.13	102,102,102,102	0
22	MG	A	1682	1/1	0.91	0.28	126,126,126,126	0
22	MG	A	1839	1/1	0.91	0.07	170,170,170,170	0
22	MG	A	1748	1/1	0.91	0.21	136,136,136,136	0
22	MG	A	1843	1/1	0.91	0.14	186,186,186,186	0
22	MG	A	1750	1/1	0.91	0.10	102,102,102,102	0
22	MG	P	103	1/1	0.91	0.27	132,132,132,132	0
22	MG	A	1659	1/1	0.91	0.29	148,148,148,148	0
22	MG	A	1849	1/1	0.91	0.10	133,133,133,133	0
22	MG	A	1859	1/1	0.92	0.36	143,143,143,143	0
22	MG	A	1653	1/1	0.92	0.12	127,127,127,127	0
22	MG	A	1664	1/1	0.92	0.12	129,129,129,129	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	MG	A	1814	1/1	0.92	0.21	113,113,113,113	0
22	MG	A	1608	1/1	0.92	0.17	99,99,99,99	0
22	MG	A	1718	1/1	0.92	0.06	103,103,103,103	0
22	MG	A	1820	1/1	0.92	0.09	459,459,459,459	0
22	MG	A	1759	1/1	0.92	0.17	155,155,155,155	0
22	MG	A	1702	1/1	0.92	0.50	124,124,124,124	0
22	MG	A	1677	1/1	0.92	0.13	130,130,130,130	0
22	MG	A	1771	1/1	0.92	0.06	114,114,114,114	0
22	MG	A	1853	1/1	0.92	0.14	161,161,161,161	0
22	MG	A	1641	1/1	0.92	0.08	188,188,188,188	0
22	MG	A	1731	1/1	0.92	0.21	109,109,109,109	0
22	MG	A	1619	1/1	0.92	0.19	178,178,178,178	0
22	MG	A	1617	1/1	0.93	0.14	113,113,113,113	0
22	MG	A	1727	1/1	0.93	0.09	91,91,91,91	0
22	MG	A	1755	1/1	0.93	0.09	118,118,118,118	0
22	MG	A	1781	1/1	0.93	0.05	174,174,174,174	0
22	MG	A	1632	1/1	0.93	0.21	90,90,90,90	0
22	MG	A	1866	1/1	0.93	0.46	123,123,123,123	0
22	MG	A	1729	1/1	0.93	0.06	105,105,105,105	0
22	MG	A	1787	1/1	0.93	0.38	175,175,175,175	0
22	MG	A	1819	1/1	0.93	0.09	294,294,294,294	0
22	MG	A	1673	1/1	0.93	0.13	211,211,211,211	0
22	MG	A	1747	1/1	0.93	0.23	118,118,118,118	0
22	MG	A	1791	1/1	0.93	0.16	244,244,244,244	0
22	MG	A	1636	1/1	0.93	0.12	127,127,127,127	0
22	MG	A	1736	1/1	0.93	0.10	156,156,156,156	0
22	MG	A	1772	1/1	0.93	0.10	115,115,115,115	0
22	MG	A	1652	1/1	0.93	0.24	150,150,150,150	0
22	MG	A	1774	1/1	0.94	0.32	142,142,142,142	0
22	MG	A	1808	1/1	0.94	0.06	265,265,265,265	0
22	MG	A	1665	1/1	0.94	0.20	271,271,271,271	0
22	MG	A	1862	1/1	0.94	0.22	155,155,155,155	0
22	MG	A	1604	1/1	0.94	0.16	151,151,151,151	0
22	MG	A	1734	1/1	0.94	0.28	94,94,94,94	0
22	MG	A	1757	1/1	0.94	0.46	105,105,105,105	0
22	MG	A	1667	1/1	0.94	0.36	123,123,123,123	0
22	MG	A	1603	1/1	0.94	0.10	117,117,117,117	0
22	MG	A	1785	1/1	0.94	0.08	364,364,364,364	0
22	MG	A	1765	1/1	0.94	0.24	127,127,127,127	0
22	MG	A	1749	1/1	0.94	0.13	114,114,114,114	0
22	MG	A	1638	1/1	0.94	0.06	95,95,95,95	0
22	MG	A	1770	1/1	0.94	0.08	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	MG	A	1634	1/1	0.94	0.08	290,290,290,290	0
22	MG	A	1752	1/1	0.94	0.09	108,108,108,108	0
22	MG	A	1672	1/1	0.94	0.07	166,166,166,166	0
22	MG	S	101	1/1	0.94	0.11	156,156,156,156	0
22	MG	A	1795	1/1	0.95	0.19	247,247,247,247	0
22	MG	A	1779	1/1	0.95	0.19	374,374,374,374	0
22	MG	A	1798	1/1	0.95	0.15	212,212,212,212	0
22	MG	A	1622	1/1	0.95	0.27	67,67,67,67	0
22	MG	A	1803	1/1	0.95	0.26	386,386,386,386	0
22	MG	A	1716	1/1	0.95	0.41	139,139,139,139	0
22	MG	A	1611	1/1	0.95	0.14	171,171,171,171	0
22	MG	A	1624	1/1	0.95	0.09	113,113,113,113	0
22	MG	A	1840	1/1	0.95	0.18	136,136,136,136	0
22	MG	A	1784	1/1	0.95	0.10	153,153,153,153	0
22	MG	A	1721	1/1	0.95	0.07	127,127,127,127	0
22	MG	D	304	1/1	0.95	0.12	111,111,111,111	0
22	MG	A	1704	1/1	0.95	0.07	95,95,95,95	0
22	MG	A	1846	1/1	0.95	0.11	150,150,150,150	0
22	MG	A	1684	1/1	0.95	0.09	158,158,158,158	0
22	MG	M	201	1/1	0.95	0.19	375,375,375,375	0
22	MG	A	1789	1/1	0.95	0.10	215,215,215,215	0
22	MG	A	1674	1/1	0.95	0.23	171,171,171,171	0
22	MG	A	1650	1/1	0.95	0.06	112,112,112,112	0
22	MG	A	1852	1/1	0.95	0.26	102,102,102,102	0
22	MG	A	1689	1/1	0.95	0.41	124,124,124,124	0
22	MG	A	1730	1/1	0.95	0.18	129,129,129,129	0
22	MG	A	1644	1/1	0.96	0.09	126,126,126,126	0
22	MG	A	1691	1/1	0.96	0.06	128,128,128,128	0
22	MG	A	1775	1/1	0.96	0.31	110,110,110,110	0
22	MG	A	1776	1/1	0.96	0.14	135,135,135,135	0
22	MG	A	1692	1/1	0.96	0.09	175,175,175,175	0
22	MG	A	1723	1/1	0.96	0.08	151,151,151,151	0
22	MG	A	1645	1/1	0.96	0.07	76,76,76,76	0
22	MG	A	1855	1/1	0.96	0.06	114,114,114,114	0
22	MG	A	1856	1/1	0.96	0.20	136,136,136,136	0
22	MG	A	1726	1/1	0.96	0.17	130,130,130,130	0
22	MG	A	1646	1/1	0.96	0.32	134,134,134,134	0
22	MG	A	1700	1/1	0.96	0.20	110,110,110,110	0
22	MG	A	1649	1/1	0.96	0.12	130,130,130,130	0
22	MG	A	1630	1/1	0.96	0.09	139,139,139,139	0
22	MG	A	1651	1/1	0.96	0.08	184,184,184,184	0
22	MG	A	1825	1/1	0.96	0.07	470,470,470,470	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	MG	A	1733	1/1	0.96	0.21	102,102,102,102	0
22	MG	A	1678	1/1	0.96	0.07	182,182,182,182	0
22	MG	A	1867	1/1	0.96	0.05	139,139,139,139	0
22	MG	A	1626	1/1	0.96	0.32	112,112,112,112	0
22	MG	A	1763	1/1	0.96	0.25	362,362,362,362	0
22	MG	D	303	1/1	0.96	0.10	119,119,119,119	0
22	MG	A	1710	1/1	0.96	0.20	111,111,111,111	0
22	MG	A	1766	1/1	0.96	0.11	131,131,131,131	0
22	MG	A	1793	1/1	0.96	0.18	134,134,134,134	0
22	MG	A	1711	1/1	0.96	0.07	139,139,139,139	0
22	MG	A	1609	1/1	0.96	0.07	115,115,115,115	0
22	MG	A	1655	1/1	0.96	0.09	113,113,113,113	0
22	MG	P	101	1/1	0.96	0.14	90,90,90,90	0
22	MG	A	1629	1/1	0.96	0.08	147,147,147,147	0
22	MG	A	1844	1/1	0.96	0.34	123,123,123,123	0
22	MG	A	1688	1/1	0.96	0.10	121,121,121,121	0
22	MG	A	1802	1/1	0.96	0.06	250,250,250,250	0
22	MG	A	1847	1/1	0.96	0.28	155,155,155,155	0
22	MG	A	1720	1/1	0.97	0.03	114,114,114,114	0
22	MG	A	1640	1/1	0.97	0.39	145,145,145,145	0
22	MG	A	1633	1/1	0.97	0.34	113,113,113,113	0
22	MG	A	1602	1/1	0.97	0.17	145,145,145,145	0
22	MG	A	1806	1/1	0.97	0.13	242,242,242,242	0
22	MG	A	1740	1/1	0.97	0.08	129,129,129,129	0
22	MG	A	1865	1/1	0.97	0.25	180,180,180,180	0
22	MG	A	1842	1/1	0.97	0.17	161,161,161,161	0
22	MG	A	1760	1/1	0.97	0.32	147,147,147,147	0
22	MG	A	1868	1/1	0.97	0.29	144,144,144,144	0
22	MG	A	1743	1/1	0.97	0.19	112,112,112,112	0
22	MG	A	1764	1/1	0.97	0.06	220,220,220,220	0
22	MG	A	1724	1/1	0.97	0.06	133,133,133,133	0
22	MG	A	1786	1/1	0.97	0.05	179,179,179,179	0
22	MG	A	1707	1/1	0.97	0.05	83,83,83,83	0
22	MG	A	1635	1/1	0.97	0.04	101,101,101,101	0
22	MG	A	1616	1/1	0.97	0.10	195,195,195,195	0
22	MG	J	202	1/1	0.97	0.11	344,344,344,344	0
22	MG	A	1631	1/1	0.97	0.14	93,93,93,93	0
22	MG	A	1693	1/1	0.97	0.20	150,150,150,150	0
22	MG	A	1657	1/1	0.97	0.11	136,136,136,136	0
22	MG	A	1680	1/1	0.97	0.10	128,128,128,128	0
22	MG	A	1610	1/1	0.97	0.12	119,119,119,119	0
22	MG	A	1661	1/1	0.97	0.29	141,141,141,141	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	MG	A	1719	1/1	0.97	0.17	108,108,108,108	0
22	MG	A	1797	1/1	0.97	0.14	176,176,176,176	0
22	MG	A	1828	1/1	0.98	0.23	351,351,351,351	0
22	MG	A	1801	1/1	0.98	0.10	135,135,135,135	0
22	MG	A	1831	1/1	0.98	0.34	244,244,244,244	0
22	MG	A	1732	1/1	0.98	0.06	81,81,81,81	0
22	MG	A	1614	1/1	0.98	0.05	144,144,144,144	0
22	MG	A	1804	1/1	0.98	0.23	366,366,366,366	0
22	MG	A	1835	1/1	0.98	0.06	349,349,349,349	0
22	MG	A	1805	1/1	0.98	0.08	162,162,162,162	0
22	MG	A	1620	1/1	0.98	0.07	116,116,116,116	0
22	MG	A	1838	1/1	0.98	0.13	187,187,187,187	0
22	MG	A	1807	1/1	0.98	0.23	254,254,254,254	0
22	MG	A	1679	1/1	0.98	0.06	150,150,150,150	0
22	MG	A	1639	1/1	0.98	0.19	163,163,163,163	0
22	MG	B	302	1/1	0.98	0.07	147,147,147,147	0
22	MG	C	301	1/1	0.98	0.11	165,165,165,165	0
22	MG	A	1660	1/1	0.98	0.08	116,116,116,116	0
22	MG	D	302	1/1	0.98	0.11	122,122,122,122	0
22	MG	A	1694	1/1	0.98	0.12	194,194,194,194	0
22	MG	A	1695	1/1	0.98	0.17	134,134,134,134	0
22	MG	A	1712	1/1	0.98	0.10	151,151,151,151	0
22	MG	A	1742	1/1	0.98	0.11	129,129,129,129	0
22	MG	A	1817	1/1	0.98	0.12	144,144,144,144	0
22	MG	A	1627	1/1	0.98	0.06	110,110,110,110	0
22	MG	A	1668	1/1	0.98	0.14	271,271,271,271	0
22	MG	A	1613	1/1	0.98	0.16	160,160,160,160	0
22	MG	A	1761	1/1	0.98	0.10	157,157,157,157	0
22	MG	A	1762	1/1	0.98	0.06	184,184,184,184	0
22	MG	A	1824	1/1	0.98	0.11	407,407,407,407	0
22	MG	A	1687	1/1	0.98	0.04	162,162,162,162	0
22	MG	A	1703	1/1	0.98	0.14	142,142,142,142	0
22	MG	A	1827	1/1	0.98	0.11	304,304,304,304	0
22	MG	A	1647	1/1	0.99	0.10	138,138,138,138	0
22	MG	A	1701	1/1	0.99	0.03	146,146,146,146	0
22	MG	A	1768	1/1	0.99	0.09	112,112,112,112	0
22	MG	A	1654	1/1	0.99	0.04	121,121,121,121	0
22	MG	A	1648	1/1	0.99	0.09	176,176,176,176	0
22	MG	A	1690	1/1	0.99	0.07	387,387,387,387	0
22	MG	A	1643	1/1	0.99	0.30	146,146,146,146	0
22	MG	A	1681	1/1	0.99	0.09	152,152,152,152	0
22	MG	A	1811	1/1	0.99	0.21	255,255,255,255	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	MG	A	1606	1/1	0.99	0.05	113,113,113,113	0
22	MG	A	1708	1/1	0.99	0.12	127,127,127,127	0
22	MG	A	1741	1/1	0.99	0.07	118,118,118,118	0
22	MG	A	1815	1/1	0.99	0.16	286,286,286,286	0
22	MG	A	1683	1/1	0.99	0.20	175,175,175,175	0
22	MG	A	1658	1/1	0.99	0.07	111,111,111,111	0
22	MG	A	1612	1/1	0.99	0.04	174,174,174,174	0
22	MG	A	1697	1/1	0.99	0.13	335,335,335,335	0
22	MG	A	1698	1/1	0.99	0.09	218,218,218,218	0
22	MG	A	1615	1/1	0.99	0.09	87,87,87,87	0
22	MG	A	1715	1/1	0.99	0.08	88,88,88,88	0
22	MG	A	1823	1/1	0.99	0.10	276,276,276,276	0
23	ZN	D	301	1/1	0.99	0.20	117,117,117,117	0
23	ZN	N	101	1/1	0.99	0.03	233,233,233,233	0
22	MG	A	1800	1/1	1.00	0.03	62,62,62,62	0
22	MG	A	1829	1/1	1.00	0.17	202,202,202,202	0

6.5 Other polymers

There are no such residues in this entry.