



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:52 PM UTC

PDB ID : 4DUZ / pdb_00004duz
Title : Crystal structure of the *Thermus thermophilus* 30S ribosomal subunit with a 16S rRNA mutation, U13C, bound with streptomycin
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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

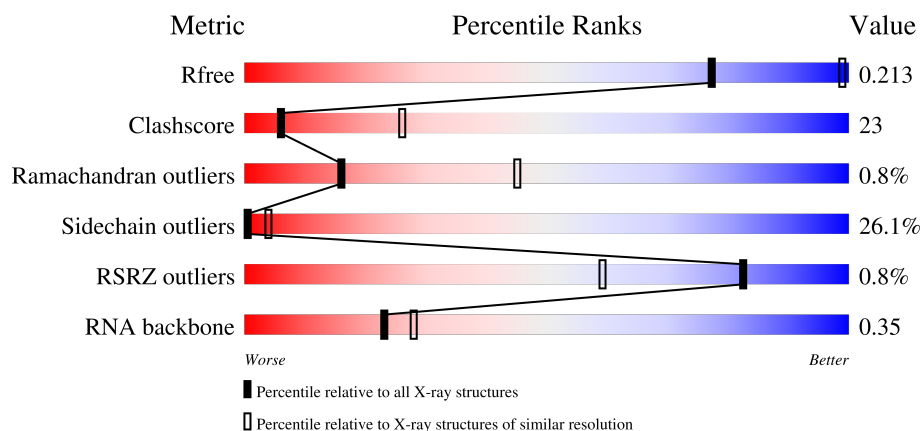
1 Overall quality at a glance

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	33% 46% 20% ..
2	B	256	28% 46% 14% 9%
3	C	239	30% 40% 15% 14%

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Mol	Chain	Length	Quality of chain
4	D	209	
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
23	MG	A	1661	-	-	-	X
23	MG	A	1794	-	-	-	X

2 Entry composition

There are 25 unique types of molecules in this entry. The entry contains 52289 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	0	0
			32507	14477	6012	10506	1512			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	C	U	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			

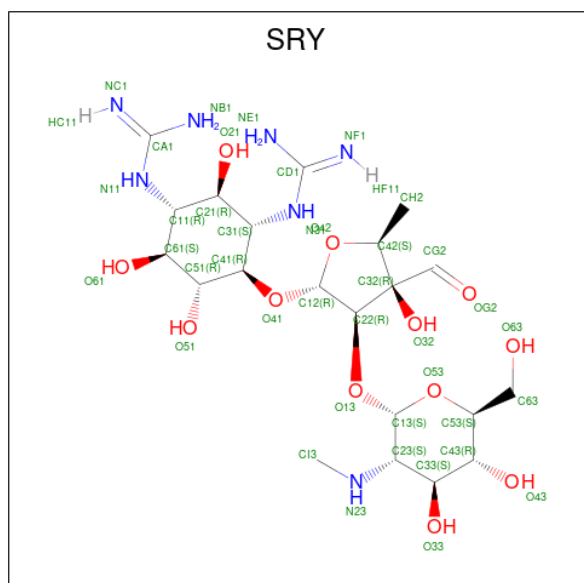
- Molecule 20 is a protein called ribosomal protein S20.

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



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

- Molecule 23 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	A	249	Total 249	Mg 249	0	0
23	B	2	Total 2	Mg 2	0	0
23	D	1	Total 1	Mg 1	0	0
23	E	1	Total 1	Mg 1	0	0
23	H	4	Total 4	Mg 4	0	0
23	J	1	Total 1	Mg 1	0	0
23	M	2	Total 2	Mg 2	0	0
23	P	2	Total 2	Mg 2	0	0
23	Q	2	Total 2	Mg 2	0	0
23	S	1	Total 1	Mg 1	0	0
23	T	2	Total 2	Mg 2	0	0

- Molecule 24 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 25 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	A	369	Total 369	O 369	0	0
25	D	1	Total 1	O 1	0	0
25	E	6	Total 6	O 6	0	0
25	G	1	Total 1	O 1	0	0

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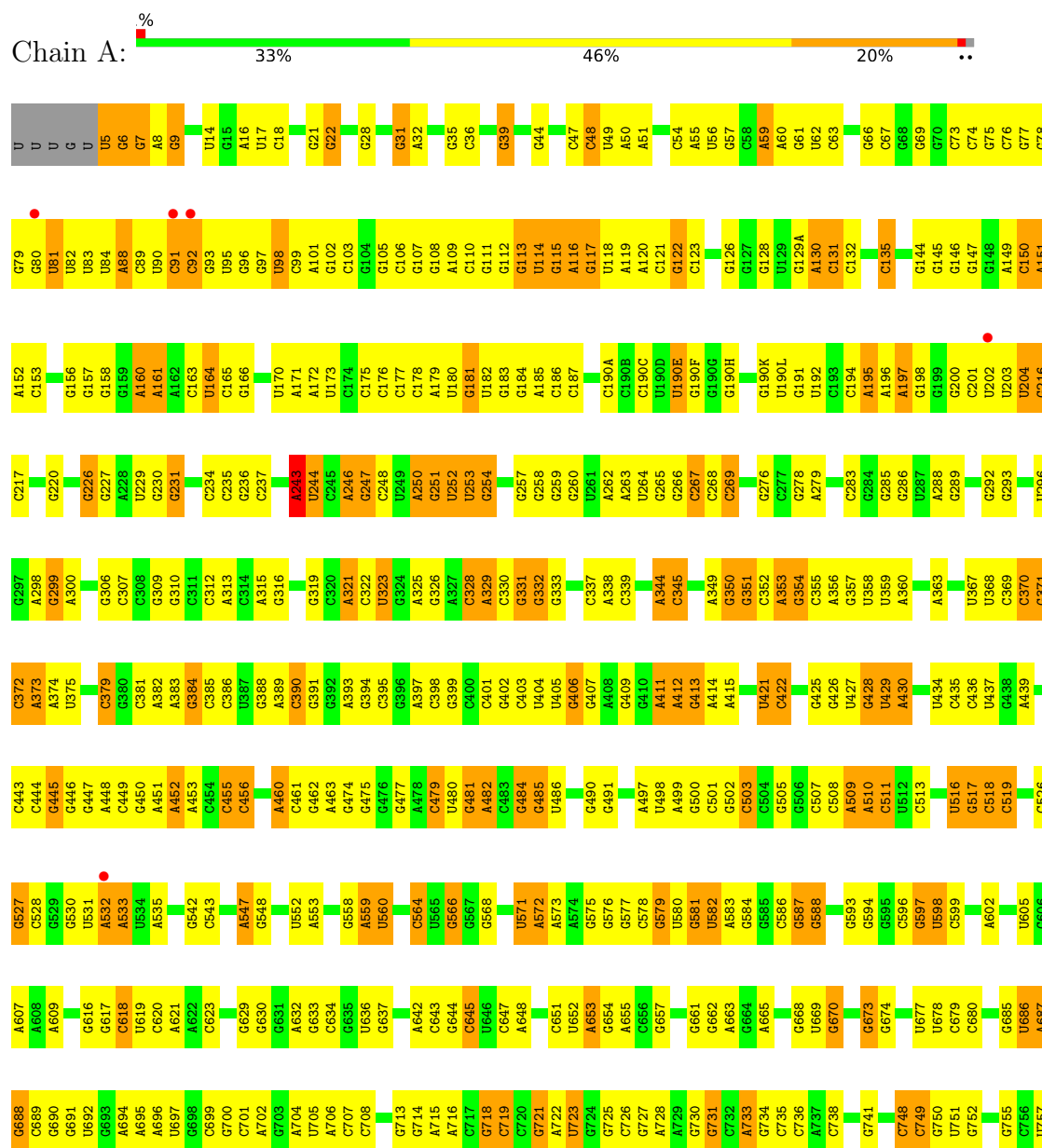
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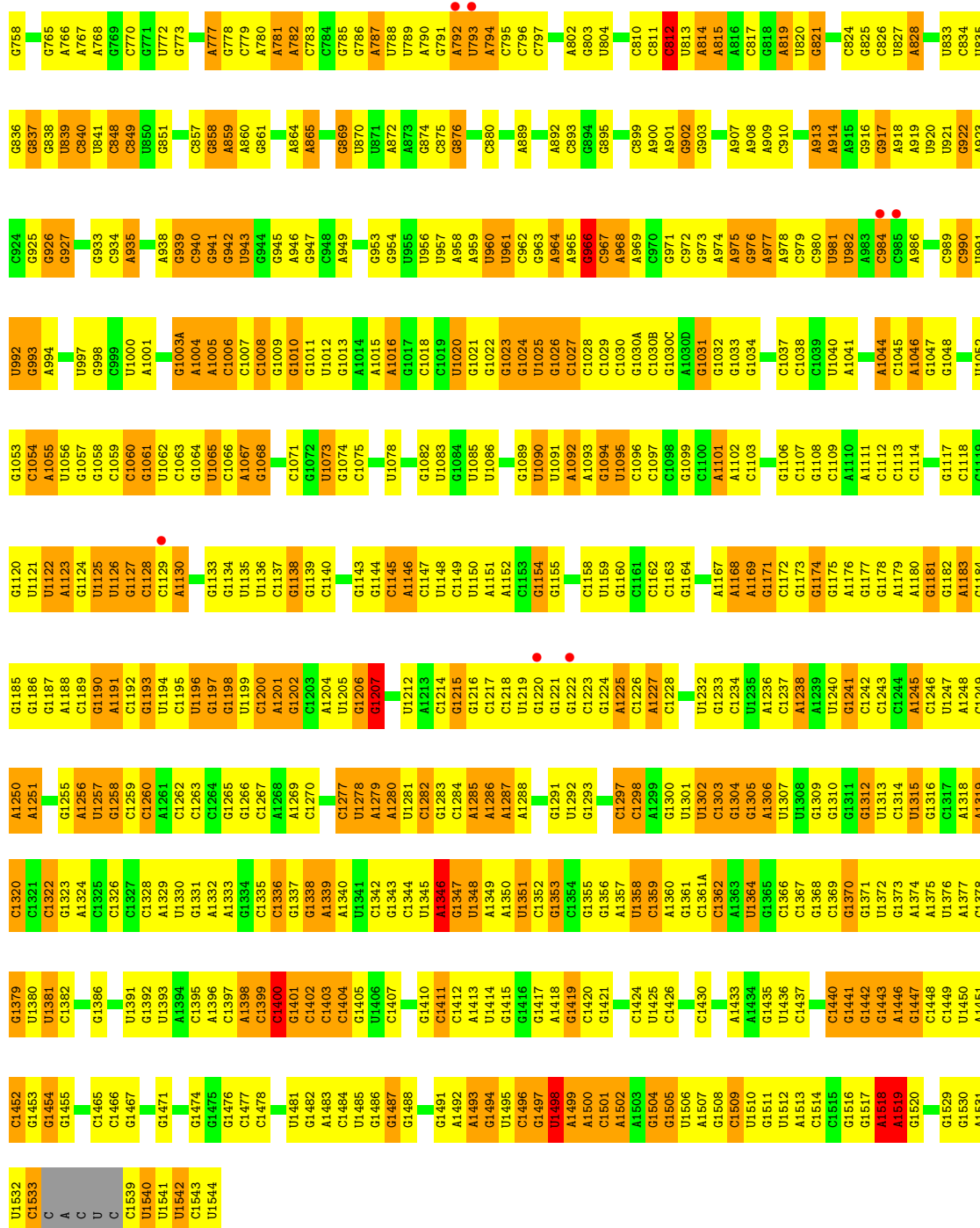
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	L	1	Total	O	0	0
			1	1		
25	P	1	Total	O	0	0
			1	1		
25	Q	4	Total	O	0	0
			4	4		
25	T	2	Total	O	0	0
			2	2		

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.

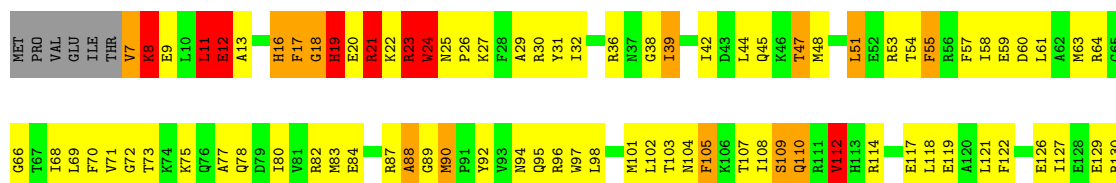
• Molecule 1: 16S rRNA

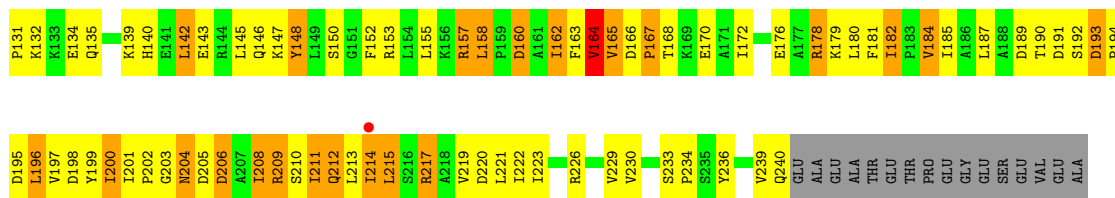




• Molecule 2: ribosomal protein S2

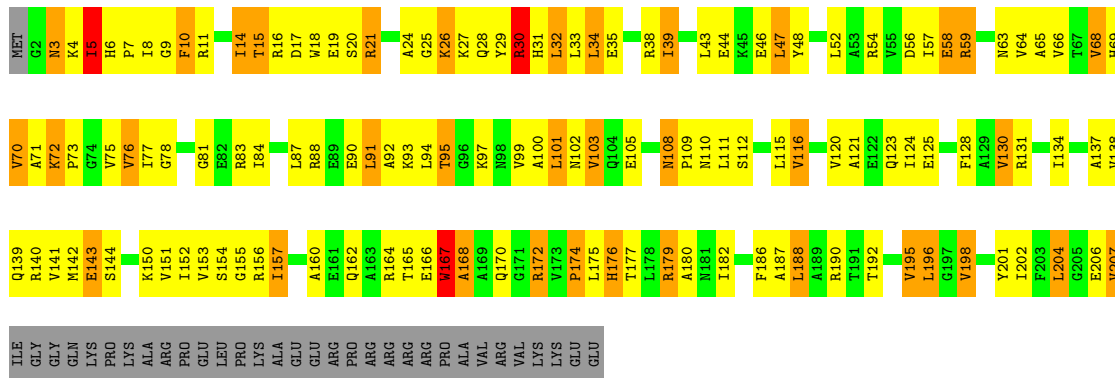
Chain B: 28% 46% 14% 9%





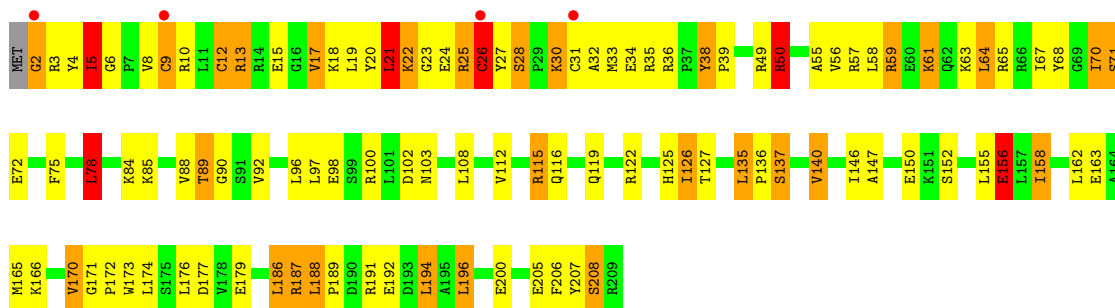
• Molecule 3: ribosomal protein S3

Chain C: 30% 40% 15% 14%



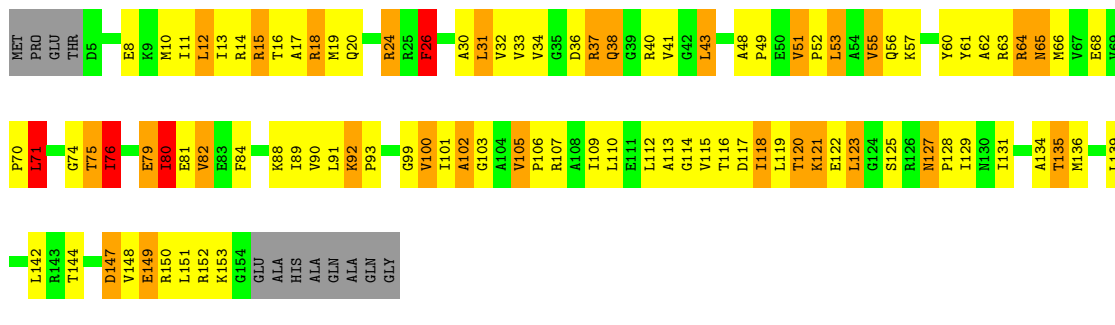
• Molecule 4: ribosomal protein S4

Chain D: 2% 48% 34% 14%

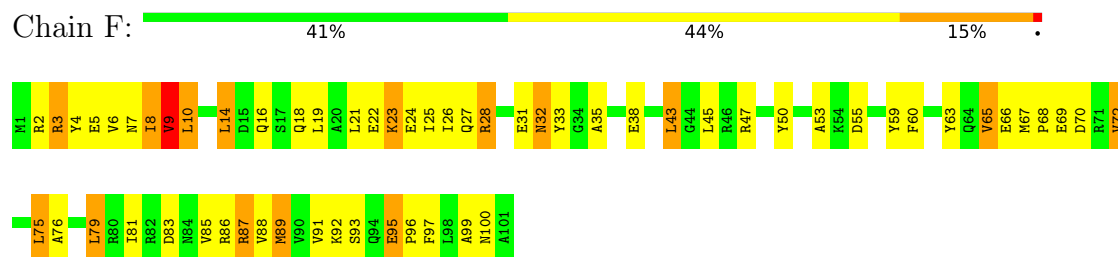


• Molecule 5: ribosomal protein S5

Chain E: 33% 40% 17% 7%



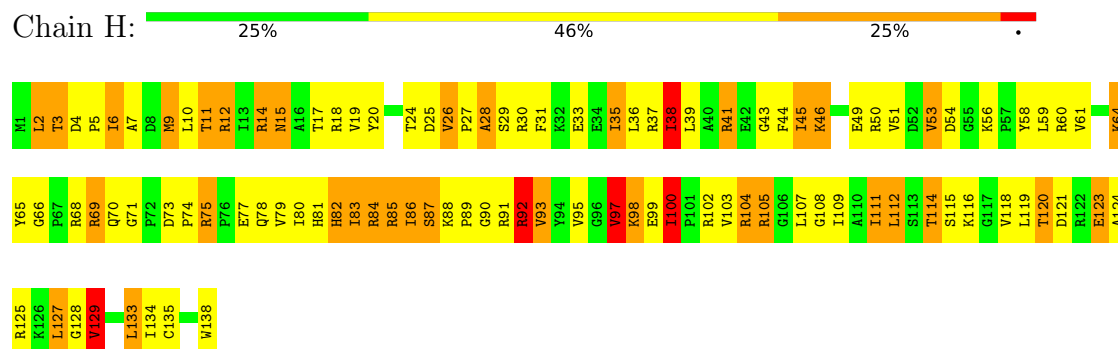
• Molecule 6: ribosomal protein S6



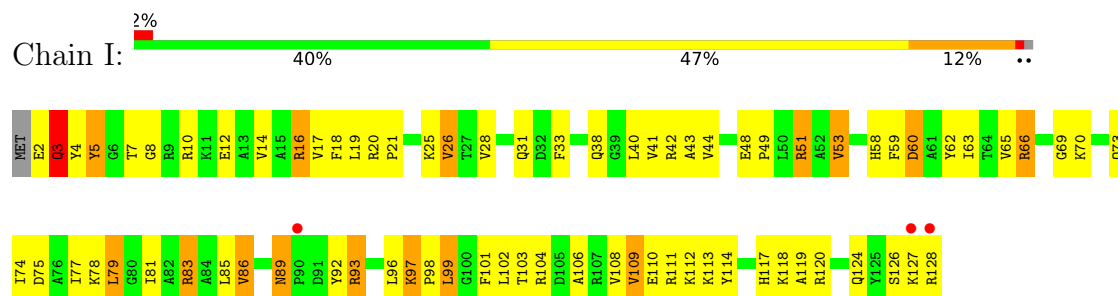
• Molecule 7: ribosomal protein S7



• Molecule 8: ribosomal protein S8

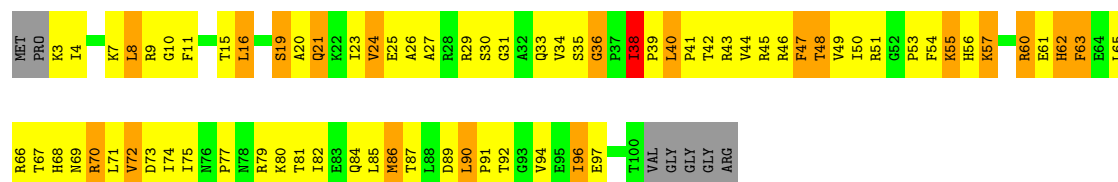


• Molecule 9: ribosomal protein S9

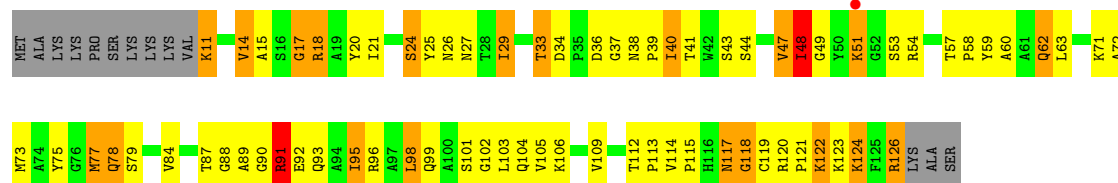


• Molecule 10: ribosomal protein S10

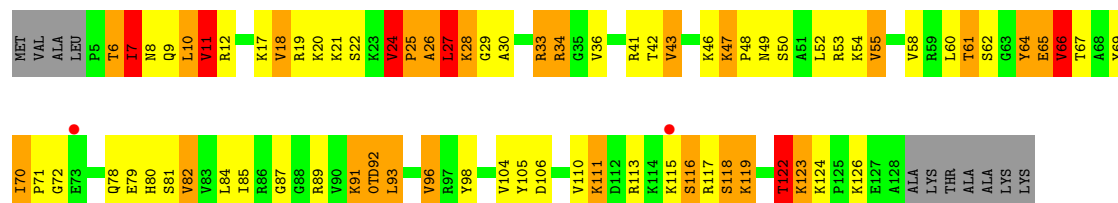




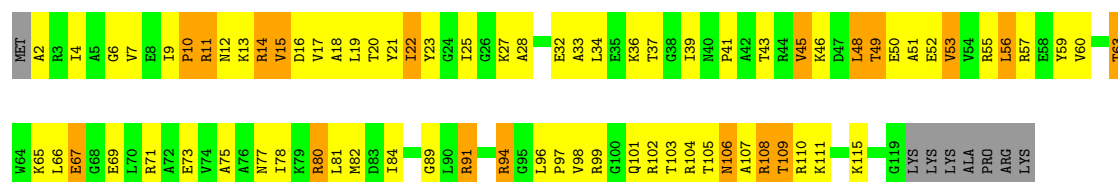
- Molecule 11: ribosomal protein S11



- Molecule 12: ribosomal protein S12



- Molecule 13: ribosomal protein S13

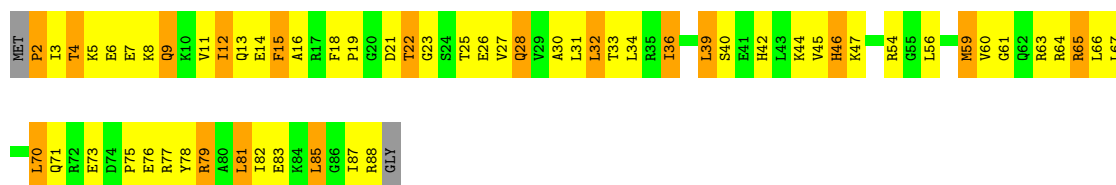


- Molecule 14: ribosomal protein S14



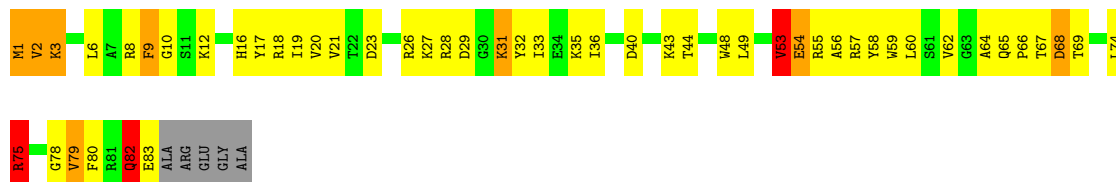
- Molecule 15: ribosomal protein S15





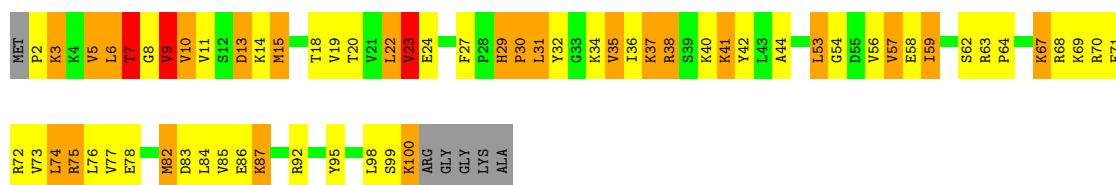
• Molecule 16: ribosomal protein S16

Chain P: 36% 45% 9% 6%



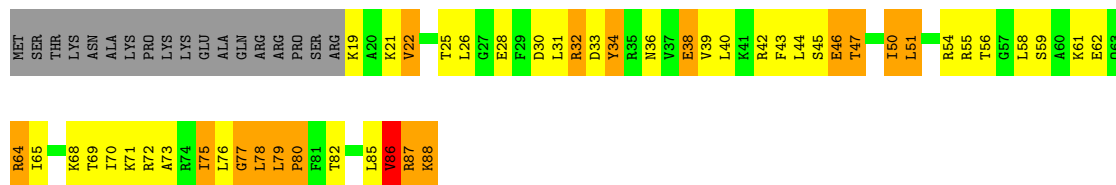
• Molecule 17: ribosomal protein S17

Chain Q: 33% 36% 22% 6%



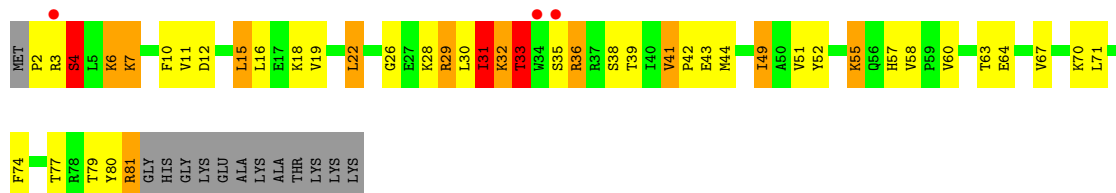
• Molecule 18: ribosomal protein S18

Chain R: 24% 36% 18% 20%

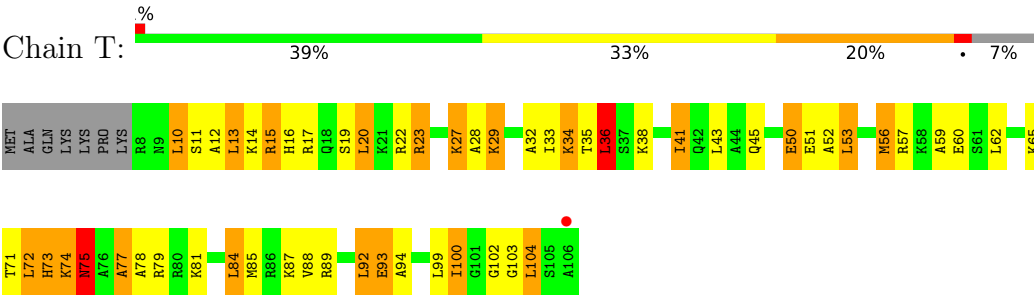


• Molecule 19: ribosomal protein S19

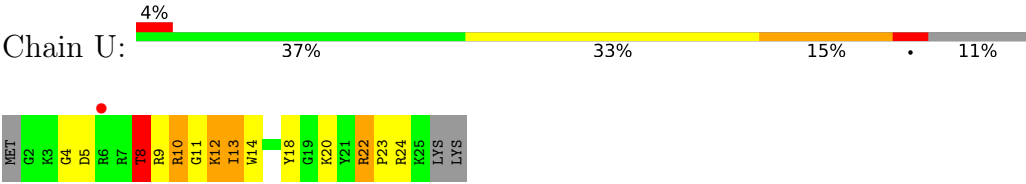
Chain S: 3% 38% 33% 12% 14%



• 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	402.52Å 402.52Å 173.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.56 – 3.65 34.56 – 3.65	Depositor EDS
% Data completeness (in resolution range)	95.6 (34.56-3.65) 95.3 (34.56-3.65)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 3.66Å)	Xtriage
Refinement program	PHENIX dev_978	Depositor
R, R_{free}	0.156 , 0.216 0.155 , 0.213	Depositor DCC
R_{free} test set	7502 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	141.1	Xtriage
Anisotropy	0.199	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 135.0	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	52289	wwPDB-VP
Average B, all atoms (Å ²)	172.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.07% 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: 2MG, 0TD, 7MG, MA6, SRY, PSU, 5MC, UR3, M2G, 4OC, ZN, MG

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	0.70	3/36040 (0.0%)	0.67	4/56243 (0.0%)
2	B	1.01	3/1935 (0.2%)	1.47	41/2609 (1.6%)
3	C	0.83	0/1636	1.25	15/2205 (0.7%)
4	D	0.95	1/1733 (0.1%)	1.45	22/2318 (0.9%)
5	E	1.40	6/1162 (0.5%)	1.58	20/1564 (1.3%)
6	F	0.94	2/856 (0.2%)	1.25	8/1154 (0.7%)
7	G	0.89	0/1276	1.33	11/1709 (0.6%)
8	H	1.41	6/1136 (0.5%)	1.71	20/1527 (1.3%)
9	I	0.82	0/1029	1.20	7/1379 (0.5%)
10	J	0.84	1/805 (0.1%)	1.31	10/1082 (0.9%)
11	K	0.99	1/879 (0.1%)	1.55	13/1187 (1.1%)
12	L	1.12	1/977 (0.1%)	1.75	25/1306 (1.9%)
13	M	0.92	1/947 (0.1%)	1.36	11/1270 (0.9%)
14	N	0.82	0/501	1.29	5/664 (0.8%)
15	O	1.06	2/740 (0.3%)	1.38	5/987 (0.5%)
16	P	1.15	1/716 (0.1%)	1.44	6/963 (0.6%)
17	Q	1.37	7/836 (0.8%)	1.65	9/1117 (0.8%)
18	R	1.01	0/579	1.38	7/768 (0.9%)
19	S	0.85	0/661	1.35	7/890 (0.8%)
20	T	1.03	0/765	1.49	11/1007 (1.1%)
21	U	0.70	0/212	1.35	3/277 (1.1%)
All	All	0.83	35/55421 (0.1%)	0.98	260/82226 (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	3
3	C	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
4	D	0	2
8	H	0	2
10	J	0	2
12	L	0	3
15	O	0	1
17	Q	0	1
18	R	0	1
20	T	0	1
All	All	0	19

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	51	VAL	CA-CB	11.21	1.60	1.54
4	D	5	ILE	CA-CB	8.66	1.66	1.54
5	E	33	VAL	CA-CB	-8.47	1.43	1.54
17	Q	9	VAL	CA-CB	-7.95	1.45	1.54
8	H	61	VAL	CA-CB	-7.64	1.44	1.54
5	E	80	ILE	CA-CB	-7.58	1.44	1.54
17	Q	35	VAL	CA-CB	-7.27	1.45	1.53
17	Q	23	VAL	CA-CB	-7.07	1.45	1.53
5	E	115	VAL	CA-CB	-6.82	1.46	1.54
15	O	82	ILE	CA-CB	-6.67	1.46	1.54
8	H	111	ILE	CA-CB	-6.38	1.46	1.54
8	H	89	PRO	CA-C	-6.35	1.45	1.52
12	L	7	ILE	CA-CB	-6.32	1.45	1.54
6	F	9	VAL	CA-CB	-6.24	1.47	1.54
11	K	48	ILE	CA-CB	-6.20	1.46	1.54
16	P	36	ILE	CA-CB	-6.13	1.47	1.54
13	M	7	VAL	CA-CB	6.01	1.62	1.54
5	E	129	ILE	CA-CB	-5.98	1.46	1.54
17	Q	11	VAL	CA-CB	-5.91	1.47	1.54
10	J	4	ILE	CA-CB	5.87	1.60	1.53
1	A	1403	C	C1'-N1	-5.79	1.39	1.48
17	Q	7	THR	CA-CB	-5.75	1.44	1.53
6	F	76	ALA	CA-C	5.73	1.60	1.52
8	H	28	ALA	CA-CB	-5.70	1.43	1.53
8	H	97	VAL	CA-CB	-5.67	1.46	1.54
2	B	112	VAL	CA-CB	5.54	1.61	1.54
1	A	1498	UR3	O3'-P	5.45	1.61	1.56
8	H	6	ILE	CA-CB	-5.44	1.46	1.54
1	A	1346	A	C3'-O3'	5.42	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	O	60	VAL	CA-CB	-5.41	1.47	1.54
2	B	184	VAL	CA-CB	-5.14	1.48	1.54
17	Q	99	SER	CA-C	5.12	1.59	1.52
5	E	32	VAL	CA-CB	-5.10	1.47	1.54
2	B	21	ARG	CA-C	5.07	1.59	1.52
17	Q	5	VAL	CA-C	-5.03	1.46	1.52

All (260) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	L	26	ALA	N-CA-C	-13.87	94.10	111.02
12	L	24	VAL	CA-C-N	-11.71	105.20	119.84
12	L	24	VAL	C-N-CA	-11.71	105.20	119.84
4	D	3	ARG	N-CA-C	11.34	123.64	111.28
8	H	100	ILE	CA-C-N	11.30	132.01	119.92
8	H	100	ILE	C-N-CA	11.30	132.01	119.92
4	D	26	CYS	N-CA-C	-10.86	100.23	113.15
19	S	6	LYS	N-CA-C	10.86	124.07	108.00
17	Q	29	HIS	CA-C-N	10.83	131.13	119.87
17	Q	29	HIS	C-N-CA	10.83	131.13	119.87
4	D	171	GLY	CA-C-N	10.82	130.42	119.82
4	D	171	GLY	C-N-CA	10.82	130.42	119.82
7	G	111	ARG	CA-C-N	10.46	131.24	119.32
7	G	111	ARG	C-N-CA	10.46	131.24	119.32
12	L	30	ALA	CA-C-N	10.27	129.93	119.56
12	L	30	ALA	C-N-CA	10.27	129.93	119.56
2	B	16	HIS	N-CA-C	10.06	126.80	113.72
12	L	43	VAL	N-CA-C	10.05	121.62	108.35
11	K	17	GLY	N-CA-C	9.79	123.70	110.69
2	B	193	ASP	CA-C-N	9.66	129.02	118.97
2	B	193	ASP	C-N-CA	9.66	129.02	118.97
15	O	36	ILE	CB-CA-C	-9.18	100.13	111.88
20	T	73	HIS	CB-CA-C	-9.10	104.96	115.79
20	T	94	ALA	N-CA-C	-9.05	93.24	108.26
19	S	6	LYS	CB-CA-C	-8.95	103.81	116.34
5	E	48	ALA	N-CA-C	8.85	116.09	108.13
12	L	18	VAL	N-CA-C	8.85	121.35	107.28
2	B	90	MET	N-CA-C	8.85	119.77	109.60
12	L	85	ILE	CB-CA-C	-8.82	100.76	111.08
4	D	30	LYS	N-CA-C	8.28	124.39	113.30
4	D	13	ARG	N-CA-C	8.20	120.21	111.28
4	D	38	TYR	CA-C-N	8.13	128.76	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	38	TYR	C-N-CA	8.13	128.76	120.38
11	K	14	VAL	N-CA-C	8.07	118.65	110.82
8	H	81	HIS	N-CA-C	-8.03	103.28	113.23
19	S	67	VAL	N-CA-C	8.00	118.05	110.53
7	G	127	ALA	N-CA-C	-8.00	101.85	111.69
2	B	208	ILE	N-CA-C	7.87	119.59	110.62
3	C	167	TRP	N-CA-C	7.59	118.70	108.23
17	Q	9	VAL	CB-CA-C	-7.58	99.54	110.83
13	M	15	VAL	N-CA-C	7.55	119.58	111.58
2	B	23	ARG	N-CA-C	-7.51	94.79	110.80
17	Q	14	LYS	N-CA-C	7.50	120.41	111.33
12	L	7	ILE	N-CA-C	-7.44	102.89	111.00
11	K	91	ARG	N-CA-C	-7.40	103.21	111.28
13	M	45	VAL	N-CA-C	7.36	117.48	110.42
10	J	36	GLY	CA-C-N	7.31	128.97	119.84
10	J	36	GLY	C-N-CA	7.31	128.97	119.84
12	L	66	VAL	N-CA-C	7.29	120.99	108.90
2	B	19	HIS	N-CA-C	7.26	120.23	108.76
18	R	79	LEU	CA-C-N	7.26	127.67	119.83
18	R	79	LEU	C-N-CA	7.26	127.67	119.83
4	D	56	VAL	CB-CA-C	-7.20	102.29	112.22
15	O	85	LEU	N-CA-C	7.18	121.27	112.23
11	K	87	THR	CB-CA-C	-7.13	97.68	109.80
5	E	127	ASN	CA-C-N	7.10	126.35	118.97
5	E	127	ASN	C-N-CA	7.10	126.35	118.97
8	H	80	ILE	N-CA-CB	-7.10	103.08	111.60
7	G	148	ASN	N-CA-C	7.06	120.77	112.72
14	N	18	VAL	N-CA-C	7.04	118.68	111.00
5	E	64	ARG	N-CA-C	-7.02	98.86	110.17
8	H	69	ARG	N-CA-C	6.98	120.50	109.81
2	B	12	GLU	N-CA-C	6.97	125.65	110.80
4	D	21	LEU	N-CA-C	-6.95	104.42	113.17
4	D	196	LEU	CA-C-N	6.94	128.51	119.84
4	D	196	LEU	C-N-CA	6.94	128.51	119.84
5	E	92	LYS	N-CA-C	-6.87	100.58	110.40
9	I	26	VAL	N-CA-C	6.83	117.47	107.37
5	E	109	ILE	N-CA-C	6.75	116.84	110.30
3	C	108	ASN	CA-C-N	6.74	128.27	119.84
3	C	108	ASN	C-N-CA	6.74	128.27	119.84
16	P	75	ARG	N-CA-C	-6.72	105.08	113.28
2	B	158	LEU	N-CA-C	6.72	117.33	109.60
2	B	21	ARG	N-CA-C	6.69	125.05	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	76	ILE	CA-C-N	6.67	126.30	119.56
5	E	76	ILE	C-N-CA	6.67	126.30	119.56
17	Q	99	SER	N-CA-C	6.64	124.95	110.80
3	C	47	LEU	N-CA-C	6.63	121.08	112.92
2	B	211	ILE	CB-CA-C	-6.63	103.40	111.88
8	H	38	ILE	CB-CA-C	-6.61	103.36	112.02
13	M	66	LEU	N-CA-C	6.58	118.53	109.18
7	G	8	GLU	N-CA-C	6.58	119.92	110.24
12	L	118	SER	N-CA-C	-6.58	104.03	111.07
2	B	239	VAL	N-CA-C	6.57	117.25	110.36
3	C	72	LYS	CA-C-N	6.56	126.25	119.56
3	C	72	LYS	C-N-CA	6.56	126.25	119.56
10	J	33	GLN	N-CA-C	6.54	118.96	111.11
12	L	17	LYS	CA-C-N	-6.49	114.43	123.13
12	L	17	LYS	C-N-CA	-6.49	114.43	123.13
13	M	49	THR	N-CA-C	-6.49	101.52	110.35
3	C	28	GLN	N-CA-C	6.49	121.34	113.17
2	B	18	GLY	N-CA-C	6.47	120.55	112.79
8	H	75	ARG	CA-C-N	6.46	126.83	119.92
8	H	75	ARG	C-N-CA	6.46	126.83	119.92
19	S	10	PHE	N-CA-C	6.39	119.36	109.07
5	E	71	LEU	N-CA-C	6.38	118.97	109.59
2	B	182	ILE	CA-C-N	6.38	126.88	119.99
2	B	182	ILE	C-N-CA	6.38	126.88	119.99
2	B	20	GLU	N-CA-C	6.38	124.38	110.80
20	T	92	LEU	CA-C-N	-6.35	113.38	122.77
20	T	92	LEU	C-N-CA	-6.35	113.38	122.77
12	L	66	VAL	CB-CA-C	-6.31	99.63	110.30
12	L	122	THR	N-CA-C	6.31	119.78	109.06
11	K	109	VAL	CA-C-N	-6.29	114.05	122.42
11	K	109	VAL	C-N-CA	-6.29	114.05	122.42
8	H	87	SER	N-CA-C	-6.29	100.26	110.20
8	H	115	SER	N-CA-C	-6.28	105.48	113.01
18	R	34	TYR	N-CA-C	-6.26	105.12	112.89
2	B	182	ILE	CB-CA-C	-6.25	105.12	110.94
8	H	2	LEU	N-CA-C	-6.24	102.12	110.55
11	K	117	ASN	N-CA-C	6.24	124.09	110.80
2	B	88	ALA	N-CA-C	-6.24	100.19	109.86
8	H	66	GLY	CA-C-N	6.24	126.42	120.31
8	H	66	GLY	C-N-CA	6.24	126.42	120.31
5	E	32	VAL	CB-CA-C	-6.20	102.05	110.42
7	G	91	VAL	N-CA-C	6.20	118.97	108.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	83	ASP	N-CA-C	-6.19	104.22	110.97
3	C	39	ILE	CB-CA-C	-6.18	104.08	111.81
14	N	39	LEU	N-CA-C	6.17	119.55	109.24
2	B	112	VAL	N-CA-CB	6.17	118.18	110.47
12	L	22	SER	N-CA-C	6.14	118.96	109.07
11	K	118	GLY	N-CA-C	6.13	127.71	113.18
20	T	16	HIS	CB-CA-C	-6.13	101.17	110.92
21	U	22	ARG	CA-C-N	-6.12	114.33	120.21
21	U	22	ARG	C-N-CA	-6.12	114.33	120.21
16	P	19	ILE	CB-CA-C	-6.10	102.24	111.33
19	S	4	SER	N-CA-C	6.10	119.48	108.69
16	P	9	PHE	N-CA-C	6.10	120.74	112.88
4	D	188	LEU	CA-C-N	6.09	125.85	119.76
4	D	188	LEU	C-N-CA	6.09	125.85	119.76
2	B	165	VAL	CA-C-N	-6.05	114.52	122.74
2	B	165	VAL	C-N-CA	-6.05	114.52	122.74
5	E	20	GLN	N-CA-C	-6.04	100.31	109.85
4	D	12	CYS	N-CA-C	-6.04	103.66	111.02
11	K	102	GLY	N-CA-C	-5.99	106.67	115.72
6	F	76	ALA	N-CA-C	5.97	118.58	111.71
4	D	50	ARG	CA-C-N	5.96	125.87	119.85
4	D	50	ARG	C-N-CA	5.96	125.87	119.85
16	P	79	VAL	N-CA-C	-5.93	103.35	111.89
7	G	155	ARG	N-CA-C	5.91	123.40	110.80
2	B	105	PHE	N-CA-C	-5.89	105.19	112.90
10	J	73	ASP	N-CA-C	-5.85	101.39	110.10
4	D	126	ILE	N-CA-C	5.83	116.34	108.17
5	E	129	ILE	CB-CA-C	-5.82	101.74	111.29
2	B	164	VAL	N-CA-C	5.81	116.85	108.48
15	O	11	VAL	CB-CA-C	-5.80	104.47	112.24
6	F	9	VAL	CB-CA-C	-5.79	102.20	110.83
14	N	32	SER	N-CA-C	5.79	117.87	108.26
4	D	78	LEU	CA-CB-CG	-5.76	96.14	116.30
11	K	51	LYS	N-CA-C	5.76	120.02	112.13
14	N	53	LEU	CA-C-N	5.75	126.08	119.92
14	N	53	LEU	C-N-CA	5.75	126.08	119.92
13	M	67	GLU	N-CA-C	5.75	116.51	108.00
5	E	120	THR	CA-C-N	-5.75	113.42	122.73
5	E	120	THR	C-N-CA	-5.75	113.42	122.73
17	Q	31	LEU	CA-CB-CG	-5.73	96.26	116.30
20	T	75	ASN	N-CA-C	-5.71	106.35	113.38
2	B	130	ARG	CA-C-N	5.69	125.69	119.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	130	ARG	C-N-CA	5.69	125.69	119.89
3	C	5	ILE	CB-CA-C	-5.68	101.97	111.29
5	E	103	GLY	N-CA-C	-5.68	104.64	112.25
15	O	46	HIS	CB-CA-C	-5.68	103.50	111.80
18	R	77	GLY	N-CA-C	5.65	122.86	115.40
7	G	77	SER	N-CA-C	5.65	117.64	108.26
1	A	243	A	P-O3'-C3'	5.64	128.67	120.20
3	C	30	ARG	N-CA-C	5.63	117.41	111.28
12	L	67	THR	CB-CA-C	-5.58	100.75	109.84
4	D	8	VAL	CB-CA-C	5.57	116.01	111.05
20	T	34	LYS	N-CA-C	-5.57	105.11	111.07
1	A	1346	A	P-O3'-C3'	5.56	128.54	120.20
18	R	55	ARG	N-CA-C	5.55	120.20	113.38
2	B	196	LEU	N-CA-C	5.55	119.15	112.38
1	A	812	C	C2'-C3'-O3'	5.53	117.79	109.50
10	J	55	LYS	N-CA-C	5.52	116.17	108.00
2	B	233	SER	CA-C-N	5.52	124.87	118.85
2	B	233	SER	C-N-CA	5.52	124.87	118.85
5	E	102	ALA	N-CA-C	5.51	117.45	109.07
20	T	74	LYS	N-CA-C	5.50	117.85	108.67
8	H	53	VAL	CB-CA-C	-5.47	103.65	111.31
12	L	124	LYS	CA-C-N	5.47	125.94	120.14
12	L	124	LYS	C-N-CA	5.47	125.94	120.14
8	H	12	ARG	NE-CZ-NH1	-5.45	116.05	121.50
3	C	174	PRO	N-CA-C	5.44	120.09	112.26
15	O	15	PHE	N-CA-C	5.44	120.02	113.17
11	K	109	VAL	N-CA-C	5.43	115.88	107.78
20	T	36	LEU	N-CA-C	5.43	118.03	111.40
3	C	155	GLY	N-CA-C	5.43	119.53	112.25
17	Q	82	MET	N-CA-C	-5.42	106.67	113.28
7	G	17	VAL	N-CA-C	5.41	116.06	110.82
17	Q	83	ASP	N-CA-C	-5.41	105.39	111.28
8	H	92	ARG	CG-CD-NE	5.39	123.87	112.00
5	E	147	ASP	CB-CA-C	-5.38	101.70	110.85
10	J	38	ILE	N-CA-C	5.36	114.37	108.05
13	M	25	ILE	N-CA-C	5.34	115.68	107.77
21	U	8	THR	N-CA-C	5.33	117.63	109.95
10	J	60	ARG	N-CA-C	5.33	122.16	110.80
2	B	148	TYR	N-CA-C	5.33	118.94	112.23
12	L	119	LYS	N-CA-C	-5.31	102.61	110.48
16	P	82	GLN	N-CA-C	5.31	119.87	113.17
12	L	72	GLY	N-CA-C	5.31	118.75	112.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	93	VAL	CB-CA-C	-5.31	103.23	110.77
3	C	26	LYS	N-CA-C	-5.30	99.51	110.80
9	I	106	ALA	N-CA-C	5.30	119.38	113.02
13	M	28	ALA	N-CA-C	5.30	117.48	111.02
2	B	24	TRP	N-CA-C	5.29	122.06	110.80
8	H	129	VAL	N-CA-C	5.28	117.66	108.90
20	T	100	ILE	CB-CA-C	-5.27	105.11	112.02
3	C	174	PRO	CA-C-O	-5.26	115.78	121.77
2	B	8	LYS	N-CA-C	5.22	116.14	107.73
7	G	9	VAL	CB-CA-C	-5.22	103.54	111.69
6	F	72	VAL	N-CA-C	5.22	115.84	110.36
5	E	26	PHE	N-CA-C	5.22	117.34	109.41
10	J	40	LEU	CA-C-N	5.21	126.36	119.84
10	J	40	LEU	C-N-CA	5.21	126.36	119.84
13	M	67	GLU	CB-CA-C	-5.21	109.04	116.34
13	M	10	PRO	CA-C-O	-5.20	115.23	121.48
3	C	168	ALA	N-CA-C	5.20	121.87	110.80
18	R	80	PRO	N-CA-C	5.19	119.03	111.03
2	B	150	SER	N-CA-C	5.18	117.60	111.33
4	D	10	ARG	N-CA-C	5.18	116.74	111.14
12	L	115	LYS	CA-C-N	-5.17	115.12	123.23
12	L	115	LYS	C-N-CA	-5.17	115.12	123.23
4	D	50	ARG	N-CA-C	-5.17	102.38	109.71
5	E	100	VAL	CB-CA-C	-5.16	102.83	111.29
20	T	77	ALA	N-CA-C	-5.15	105.58	111.14
2	B	90	MET	CA-C-N	5.15	125.43	119.92
2	B	90	MET	C-N-CA	5.15	125.43	119.92
17	Q	67	LYS	N-CA-C	-5.14	102.99	110.24
19	S	33	THR	N-CA-C	5.13	116.78	108.26
6	F	65	VAL	CB-CA-C	-5.13	103.42	110.91
12	L	11	VAL	N-CA-C	5.12	116.46	110.62
19	S	26	GLY	N-CA-C	-5.11	105.24	112.81
8	H	7	ALA	N-CA-C	-5.11	105.61	111.07
11	K	26	ASN	N-CA-C	5.11	118.66	112.23
2	B	167	PRO	N-CA-C	-5.11	107.20	113.84
2	B	204	ASN	N-CA-C	5.11	117.03	107.99
12	L	27	LEU	CB-CA-C	-5.10	109.15	115.89
6	F	85	VAL	N-CA-C	5.10	116.03	108.23
10	J	31	GLY	N-CA-C	5.09	119.87	112.55
11	K	77	MET	N-CA-C	5.08	116.84	110.24
9	I	3	GLN	N-CA-C	5.07	116.68	108.26
13	M	109	THR	CA-C-N	5.06	127.47	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	109	THR	C-N-CA	5.06	127.47	120.29
1	A	117	G	C8-N9-Cl'	-5.05	111.83	127.00
6	F	8	ILE	N-CA-C	5.05	115.13	107.75
16	P	20	VAL	N-CA-C	5.05	115.65	108.42
2	B	70	PHE	CA-C-N	-5.04	116.54	123.14
2	B	70	PHE	C-N-CA	-5.04	116.54	123.14
2	B	200	ILE	CB-CA-C	-5.04	103.16	110.81
9	I	58	HIS	N-CA-C	-5.04	106.97	113.01
7	G	24	THR	N-CA-C	-5.03	105.25	111.33
2	B	89	GLY	N-CA-C	-5.03	106.32	113.86
5	E	61	TYR	N-CA-C	-5.02	105.99	111.82
9	I	5	TYR	N-CA-C	5.02	117.94	109.95
9	I	60	ASP	N-CA-C	-5.02	103.97	110.19
18	R	86	VAL	N-CA-C	5.02	116.52	108.89
2	B	197	VAL	N-CA-C	5.01	116.51	108.89
9	I	4	TYR	N-CA-C	5.01	117.60	109.24
8	H	17	THR	N-CA-C	5.00	117.39	111.33
6	F	88	VAL	N-CA-C	-5.00	101.11	108.11

There are no chirality outliers.

All (19) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	11	LEU	Peptide
2	B	77	ALA	Peptide
2	B	8	LYS	Peptide
3	C	166	GLU	Peptide
3	C	179	ARG	Peptide
3	C	24	ALA	Peptide
4	D	2	GLY	Peptide
4	D	28	SER	Peptide
8	H	27	PRO	Peptide
8	H	90	GLY	Peptide
10	J	86	MET	Peptide
10	J	90	LEU	Peptide
12	L	24	VAL	Peptide
12	L	27	LEU	Peptide
12	L	91	LYS	Peptide
15	O	2	PRO	Peptide
17	Q	13	ASP	Peptide
18	R	86	VAL	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	32507	0	16434	993	0
2	B	1900	0	1951	114	0
3	C	1612	0	1677	106	0
4	D	1703	0	1763	93	0
5	E	1146	0	1207	65	0
6	F	843	0	857	50	0
7	G	1257	0	1296	63	0
8	H	1116	0	1177	88	0
9	I	1010	0	1037	71	0
10	J	792	0	835	54	0
11	K	864	0	881	52	0
12	L	972	0	1058	54	0
13	M	937	0	995	51	0
14	N	492	0	529	46	0
15	O	729	0	768	51	0
16	P	700	0	720	42	0
17	Q	823	0	893	63	0
18	R	574	0	644	38	0
19	S	647	0	673	35	0
20	T	763	0	861	44	0
21	U	208	0	221	18	0
22	A	40	0	37	6	0
23	A	249	0	0	0	0
23	B	2	0	0	0	0
23	D	1	0	0	0	0
23	E	1	0	0	0	0
23	H	4	0	0	0	0
23	J	1	0	0	0	0
23	M	2	0	0	0	0
23	P	2	0	0	0	0
23	Q	2	0	0	0	0
23	S	1	0	0	0	0
23	T	2	0	0	0	0
24	D	1	0	0	0	0
24	N	1	0	0	0	0
25	A	369	0	0	20	0
25	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	E	6	0	0	0	0
25	G	1	0	0	0	0
25	L	1	0	0	0	0
25	P	1	0	0	0	0
25	Q	4	0	0	0	0
25	T	2	0	0	1	0
All	All	52289	0	36514	1978	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 23.

All (1978) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1433:A:N7	1:A:1467:G:N2	2.15	0.95
12:L:24:VAL:HG12	12:L:26:ALA:H	1.33	0.93
17:Q:29:HIS:CD2	17:Q:32:TYR:H	1.88	0.92
1:A:1240:U:OP1	7:G:119:ARG:NH2	2.02	0.92
19:S:11:VAL:HG22	19:S:39:THR:HB	1.49	0.92
10:J:15:THR:HG22	10:J:94:VAL:HG13	1.54	0.90
1:A:1249:C:O2'	9:I:73:GLN:NE2	2.05	0.90
1:A:427:U:OP1	4:D:13:ARG:NH2	2.05	0.89
10:J:38:ILE:HD11	10:J:71:LEU:HB2	1.54	0.89
1:A:279:A:OP2	17:Q:95:TYR:OH	1.90	0.89
1:A:1061:G:H1	1:A:1195:C:H42	1.20	0.88
1:A:1316:G:N2	1:A:1319:A:OP2	2.07	0.87
3:C:150:LYS:HB3	3:C:201:TYR:HB2	1.57	0.85
1:A:1195:C:H3'	1:A:1196:U:H5''	1.55	0.85
1:A:310:G:OP2	16:P:27:LYS:NZ	2.09	0.85
7:G:155:ARG:HA	7:G:155:ARG:HH11	1.42	0.84
8:H:82:HIS:HE1	8:H:84:ARG:HB2	1.42	0.84
1:A:1055:A:O2'	3:C:156:ARG:NH1	2.10	0.84
1:A:384:G:H2'	1:A:385:C:C6	2.13	0.83
1:A:1338:G:H2'	1:A:1339:A:C8	2.14	0.83
8:H:69:ARG:NH2	8:H:75:ARG:O	2.12	0.82
2:B:109:SER:HA	2:B:112:VAL:HG23	1.61	0.82
12:L:27:LEU:C	12:L:29:GLY:H	1.87	0.82
13:M:10:PRO:HB2	13:M:18:ALA:HB1	1.60	0.82
1:A:986:A:O2'	19:S:52:TYR:OH	1.98	0.82
17:Q:29:HIS:HD2	17:Q:32:TYR:H	1.26	0.82
8:H:9:MET:HG3	8:H:26:VAL:HG21	1.60	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:57:THR:HG23	11:K:60:ALA:H	1.44	0.81
1:A:1112:C:H1'	3:C:179:ARG:HH22	1.45	0.81
1:A:869:G:N7	25:A:2219:HOH:O	2.12	0.81
1:A:1055:A:N7	1:A:1200:C:N4	2.29	0.81
3:C:153:VAL:HG12	3:C:154:SER:H	1.46	0.80
12:L:25:PRO:HB3	12:L:27:LEU:HD22	1.62	0.80
1:A:1047:G:H5''	14:N:4:LYS:HD3	1.63	0.80
1:A:407:G:OP1	4:D:115:ARG:NH1	2.15	0.80
1:A:517:G:N1	1:A:533:A:OP2	2.13	0.80
13:M:91:ARG:HB3	13:M:98:VAL:HG22	1.63	0.80
1:A:1009:G:H1	1:A:1020:U:H3	1.28	0.79
1:A:1257:U:H4'	1:A:1258:G:O5'	1.78	0.79
3:C:14:ILE:HB	3:C:15:THR:HG23	1.64	0.79
4:D:13:ARG:HD2	4:D:38:TYR:O	1.82	0.79
1:A:1101:A:H4'	1:A:1102:A:O5'	1.82	0.79
9:I:126:SER:OG	9:I:127:LYS:N	2.06	0.79
1:A:1125:U:OP2	1:A:1145:C:N4	2.16	0.79
1:A:1347:G:H3'	9:I:108:VAL:O	1.82	0.78
1:A:1130:A:H4'	9:I:20:ARG:HH22	1.48	0.78
11:K:40:ILE:HG22	11:K:41:THR:HG23	1.65	0.78
15:O:25:THR:HG21	15:O:70:LEU:HD23	1.65	0.78
1:A:190(A):C:H42	1:A:190(H):G:H1	1.32	0.77
1:A:1309:G:OP2	13:M:99:ARG:NH2	2.17	0.77
5:E:11:ILE:HB	5:E:31:LEU:HB3	1.67	0.77
1:A:1412:C:H2'	1:A:1413:A:C8	2.19	0.77
1:A:91:C:C5	1:A:92:C:H5	2.03	0.77
1:A:337:C:H2'	1:A:338:A:H8	1.49	0.77
1:A:967:5MC:H4'	9:I:128:ARG:HG3	1.66	0.76
1:A:1368:G:H5''	9:I:112:LYS:HB3	1.68	0.76
15:O:33:THR:HG23	15:O:63:ARG:NH1	2.00	0.76
6:F:33:TYR:CD1	6:F:75:LEU:HA	2.20	0.76
3:C:92:ALA:HB2	3:C:99:VAL:HG12	1.67	0.76
7:G:18:TYR:HD2	7:G:59:LEU:HD13	1.50	0.75
3:C:27:LYS:O	3:C:30:ARG:NH2	2.19	0.75
1:A:964:A:O2'	10:J:55:LYS:NZ	2.16	0.75
1:A:92:C:O2'	1:A:93:G:H5'	1.85	0.75
8:H:2:LEU:HD23	8:H:3:THR:N	2.02	0.75
3:C:17:ASP:O	3:C:54:ARG:NH2	2.19	0.75
4:D:64:LEU:HA	4:D:67:ILE:HD12	1.68	0.75
1:A:1435:G:H2'	1:A:1436:U:C6	2.22	0.75
1:A:1369:C:H2'	1:A:1370:G:C8	2.22	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1128:C:O2'	1:A:1130:A:OP2	2.04	0.74
1:A:1113:C:H42	1:A:1187:G:H1	1.34	0.74
8:H:114:THR:HB	8:H:116:LYS:H	1.50	0.74
1:A:1073:U:OP2	5:E:57:LYS:NZ	2.15	0.74
10:J:47:PHE:HB3	14:N:34:TYR:HE2	1.52	0.74
1:A:474:G:H2'	1:A:475:G:H8	1.52	0.73
1:A:1368:G:O2'	10:J:46:ARG:NH2	2.22	0.73
4:D:15:GLU:OE2	4:D:59:ARG:NH2	2.20	0.73
9:I:108:VAL:HG12	9:I:109:VAL:H	1.52	0.73
1:A:1285:A:H4'	1:A:1286:A:O5'	1.88	0.73
7:G:27:ILE:HD12	7:G:40:ALA:HA	1.71	0.73
1:A:1504:G:OP1	1:A:1507:A:H4'	1.88	0.73
15:O:6:GLU:HA	15:O:9:GLN:HB2	1.69	0.73
1:A:793:U:O2'	1:A:794:A:O5'	2.07	0.73
2:B:158:LEU:H	2:B:158:LEU:HD12	1.54	0.73
7:G:15:ASP:HB3	7:G:19:GLY:H	1.54	0.73
3:C:58:GLU:H	3:C:65:ALA:HB3	1.54	0.72
10:J:9:ARG:HH21	10:J:97:GLU:HG3	1.53	0.72
13:M:22:ILE:HG22	13:M:23:TYR:H	1.53	0.72
1:A:1342:C:H2'	1:A:1343:G:H8	1.54	0.72
13:M:75:ALA:HA	13:M:78:ILE:HD12	1.71	0.72
11:K:121:PRO:HG2	11:K:126:ARG:HG2	1.72	0.72
3:C:88:ARG:HA	3:C:91:LEU:HD23	1.71	0.72
12:L:87:GLY:HA2	12:L:98:TYR:HA	1.71	0.72
1:A:1086:U:H3	1:A:1099:G:H22	1.35	0.72
3:C:48:TYR:HA	3:C:52:LEU:HD23	1.70	0.72
3:C:188:LEU:HD21	3:C:195:VAL:HG13	1.71	0.72
6:F:33:TYR:HD1	6:F:75:LEU:HA	1.52	0.72
2:B:132:LYS:NZ	2:B:135:GLN:OE1	2.20	0.72
2:B:213:LEU:HD23	2:B:214:ILE:HD13	1.72	0.71
1:A:926:G:N2	1:A:1542:U:OP1	2.23	0.71
2:B:205:ASP:OD1	2:B:206:ASP:N	2.24	0.71
11:K:43:SER:HB2	11:K:47:VAL:HG11	1.71	0.71
16:P:57:ARG:HG3	16:P:79:VAL:HG12	1.72	0.71
1:A:91:C:C6	1:A:92:C:H5	2.08	0.71
1:A:1059:C:N4	1:A:1198:G:O6	2.14	0.71
1:A:1347:G:O2'	1:A:1348:U:O5'	2.08	0.71
1:A:547:A:OP2	4:D:2:GLY:N	2.24	0.71
10:J:63:PHE:HB3	14:N:57:ARG:O	1.91	0.71
1:A:827:U:H5'	1:A:828:A:OP2	1.92	0.70
1:A:750:G:H1'	15:O:23:GLY:H	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:73:ALA:HB3	18:R:79:LEU:HD12	1.73	0.70
1:A:1057:G:H5''	3:C:154:SER:HB2	1.73	0.70
8:H:26:VAL:HG13	8:H:59:LEU:HB2	1.73	0.70
1:A:1234:C:H1'	1:A:1364:U:O2	1.91	0.70
14:N:18:VAL:HG22	14:N:19:ARG:HD2	1.74	0.70
4:D:22:LYS:HB2	4:D:26:CYS:SG	2.31	0.70
20:T:56:MET:HE2	20:T:85:MET:HA	1.73	0.70
8:H:4:ASP:OD2	8:H:85:ARG:NH1	2.24	0.70
15:O:26:GLU:HG3	15:O:81:LEU:HG	1.74	0.70
1:A:1175:G:H2'	1:A:1176:A:C8	2.26	0.70
1:A:716:A:H1'	11:K:118:GLY:HA2	1.73	0.69
1:A:992:U:O2'	1:A:993:G:OP2	2.10	0.69
1:A:1200:C:O2	1:A:1205:U:N3	2.25	0.69
1:A:337:C:H2'	1:A:338:A:C8	2.28	0.69
1:A:1111:A:H61	3:C:177:THR:HG22	1.57	0.69
15:O:70:LEU:HB3	15:O:78:TYR:HB2	1.74	0.69
3:C:5:ILE:HD11	3:C:10:PHE:HD2	1.55	0.69
6:F:69:GLU:OE1	6:F:69:GLU:N	2.24	0.69
1:A:1347:G:H1'	1:A:1348:U:H5	1.57	0.69
21:U:5:ASP:HB3	21:U:8:THR:OG1	1.92	0.69
1:A:1158:C:N3	1:A:1181:G:N2	2.41	0.69
15:O:12:ILE:HG12	15:O:31:LEU:HD11	1.75	0.69
1:A:93:G:C2	1:A:95:U:C2	2.81	0.69
1:A:718:G:H5''	1:A:718:G:C8	2.28	0.69
1:A:1090:U:H2'	1:A:1091:U:H6	1.57	0.69
1:A:1397:C:O2'	1:A:1398:A:OP1	2.07	0.69
1:A:1400:5MC:H3'	1:A:1401:G:H5'	1.75	0.69
3:C:156:ARG:HB3	3:C:196:LEU:HD22	1.73	0.69
8:H:38:ILE:HD13	8:H:41:ARG:NH2	2.08	0.69
1:A:80:G:H22	1:A:89:C:H42	1.40	0.69
1:A:485:G:O2'	1:A:486:U:OP2	2.10	0.69
9:I:48:GLU:OE1	9:I:51:ARG:NH1	2.23	0.69
1:A:93:G:H2'	1:A:95:U:C6	2.28	0.69
9:I:21:PRO:HA	9:I:59:PHE:HA	1.75	0.69
7:G:22:LEU:HD23	7:G:62:PHE:HE2	1.58	0.68
11:K:90:GLY:HA2	11:K:93:GLN:HB2	1.76	0.68
11:K:101:SER:OG	11:K:103:LEU:N	2.26	0.68
13:M:59:TYR:O	13:M:63:THR:OG1	2.10	0.68
14:N:16:PHE:HB2	14:N:19:ARG:HD3	1.75	0.68
17:Q:29:HIS:HD2	17:Q:32:TYR:N	1.91	0.68
18:R:59:SER:H	18:R:62:GLU:HB2	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:G:C2'	1:A:113:G:H5'	2.24	0.68
12:L:53:ARG:NH1	12:L:92:OTD:OD2	2.27	0.68
1:A:250:A:H4'	1:A:251:G:O5'	1.94	0.68
1:A:1130:A:H4'	9:I:20:ARG:NH2	2.09	0.68
1:A:9:G:OP1	5:E:122:GLU:HG3	1.94	0.68
17:Q:31:LEU:HD23	17:Q:32:TYR:CE2	2.29	0.68
1:A:28:G:O2'	1:A:296:U:OP1	2.10	0.68
1:A:838:G:H2'	1:A:839:U:H5''	1.74	0.68
1:A:1349:A:OP2	9:I:118:LYS:HD3	1.94	0.68
1:A:1278:U:H4'	1:A:1279:A:N3	2.10	0.67
1:A:1510:U:H2'	1:A:1511:G:C8	2.30	0.67
22:A:1601:SRV:H12	22:A:1601:SRV:O63	1.95	0.67
1:A:345:C:OP2	1:A:345:C:H6	1.77	0.67
17:Q:62:SER:OG	17:Q:72:ARG:HG2	1.94	0.67
1:A:21:G:H2'	1:A:22:G:C8	2.29	0.67
1:A:90:U:C4	1:A:91:C:N4	2.62	0.67
1:A:90:U:O4	1:A:91:C:N4	2.27	0.67
1:A:679:C:H2'	1:A:680:C:H6	1.60	0.67
5:E:110:LEU:HD13	5:E:118:ILE:HD13	1.77	0.67
7:G:16:LEU:HD23	9:I:42:ARG:HG2	1.75	0.67
1:A:1356:G:H2'	1:A:1357:A:C8	2.30	0.67
17:Q:38:ARG:N	17:Q:38:ARG:HD2	2.09	0.67
3:C:39:ILE:HD12	3:C:57:ILE:HD13	1.77	0.67
11:K:93:GLN:HA	11:K:96:ARG:HD3	1.76	0.67
14:N:24:CYS:HB3	14:N:33:VAL:HG12	1.75	0.67
4:D:31:CYS:C	4:D:33:MET:H	2.03	0.67
1:A:819:A:H5'	1:A:819:A:H8	1.60	0.66
1:A:1442:G:N2	1:A:1447:G:N7	2.37	0.66
1:A:1492:A:H2'	1:A:1493:A:H4'	1.77	0.66
2:B:101:MET:HA	2:B:108:ILE:HG13	1.77	0.66
1:A:992:U:H3	1:A:1044:A:H62	1.44	0.66
1:A:1305:G:H5''	21:U:4:GLY:HA3	1.77	0.66
9:I:8:GLY:HA2	9:I:79:LEU:HD12	1.77	0.66
15:O:12:ILE:HD11	15:O:31:LEU:HD21	1.78	0.66
1:A:914:A:OP1	22:A:1601:SRV:HI33	1.94	0.66
13:M:19:LEU:HD21	13:M:56:LEU:HD11	1.78	0.66
14:N:40:CYS:HB3	14:N:43:CYS:SG	2.35	0.66
1:A:484:G:O2'	1:A:485:G:OP2	2.11	0.66
1:A:1147:C:O2	9:I:16:ARG:NH2	2.26	0.66
1:A:1367:C:H5'	10:J:60:ARG:NH2	2.11	0.66
6:F:67:MET:HB2	6:F:68:PRO:HD2	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:70:LYS:HG2	7:G:96:GLN:HB3	1.78	0.66
1:A:902:G:H2'	1:A:903:G:H8	1.59	0.66
1:A:1181:G:O2'	1:A:1182:G:O4'	2.12	0.66
1:A:1191:A:OP1	3:C:3:ASN:ND2	2.29	0.66
10:J:49:VAL:HG13	14:N:41:ARG:HB2	1.76	0.66
13:M:19:LEU:O	13:M:22:ILE:HG13	1.94	0.66
1:A:1376:U:OP1	7:G:98:SER:OG	2.08	0.66
3:C:110:ASN:HD22	3:C:140:ARG:HB3	1.60	0.66
16:P:67:THR:HG22	16:P:69:THR:H	1.60	0.66
1:A:78:G:N1	1:A:92:C:C4	2.64	0.66
1:A:1118:C:H1'	1:A:1179:A:C4	2.30	0.66
13:M:11:ARG:HA	13:M:45:VAL:HG11	1.77	0.66
10:J:8:LEU:HD13	10:J:20:ALA:HB2	1.76	0.65
1:A:916:G:H2'	1:A:917:G:H8	1.62	0.65
1:A:946:A:H2'	1:A:947:G:C8	2.30	0.65
1:A:1243:C:OP2	21:U:10:ARG:NH2	2.29	0.65
3:C:93:LYS:HG2	3:C:94:LEU:HD22	1.77	0.65
3:C:131:ARG:HA	3:C:134:ILE:HD12	1.78	0.65
7:G:18:TYR:CD2	7:G:59:LEU:HD13	2.30	0.65
11:K:101:SER:HG	11:K:103:LEU:H	1.44	0.65
1:A:1201:A:H4'	1:A:1202:G:H5'	1.78	0.65
1:A:1323:G:OP2	19:S:3:ARG:NH1	2.29	0.65
19:S:16:LEU:HA	19:S:19:VAL:HG12	1.77	0.65
3:C:83:ARG:O	3:C:87:LEU:HB2	1.97	0.65
7:G:26:PHE:HD1	7:G:101:LEU:HD22	1.61	0.65
21:U:9:ARG:HH22	21:U:23:PRO:HD2	1.61	0.65
14:N:21:TYR:HB2	14:N:23:ARG:HG2	1.79	0.65
16:P:75:ARG:HB2	16:P:80:PHE:CD1	2.30	0.65
1:A:617:G:H1	1:A:623:C:H42	1.44	0.65
2:B:132:LYS:HA	2:B:135:GLN:HB3	1.77	0.65
6:F:32:ASN:O	6:F:32:ASN:ND2	2.27	0.65
1:A:1343:G:H2'	1:A:1344:C:C6	2.32	0.65
8:H:82:HIS:CE1	8:H:84:ARG:HB2	2.27	0.65
17:Q:53:LEU:HB3	17:Q:82:MET:HE1	1.78	0.65
1:A:144:G:H1	1:A:178:C:H42	1.43	0.65
1:A:1513:A:N6	25:A:2057:HOH:O	2.30	0.65
1:A:263:A:OP2	20:T:79:ARG:NH1	2.29	0.65
1:A:1255:G:O2'	1:A:1258:G:N3	2.30	0.65
16:P:75:ARG:HB2	16:P:80:PHE:HD1	1.62	0.65
2:B:97:TRP:HZ2	2:B:102:LEU:HD13	1.62	0.64
19:S:18:LYS:O	19:S:22:LEU:HB2	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:2:ARG:O	6:F:66:GLU:HA	1.98	0.64
1:A:1143:G:H2'	1:A:1144:G:H8	1.61	0.64
12:L:113:ARG:HH22	12:L:116:SER:H	1.45	0.64
17:Q:75:ARG:HH11	17:Q:75:ARG:HB2	1.63	0.64
2:B:209:ARG:HH11	2:B:209:ARG:HG3	1.63	0.64
1:A:93:G:N2	1:A:95:U:H1'	2.12	0.64
1:A:393:A:OP2	16:P:12:LYS:NZ	2.29	0.64
1:A:414:A:OP2	1:A:428:G:N2	2.20	0.64
1:A:1496:C:O2'	1:A:1497:G:H5''	1.98	0.64
12:L:27:LEU:C	12:L:29:GLY:N	2.53	0.64
1:A:1391:U:H2'	1:A:1392:G:C8	2.33	0.64
2:B:131:PRO:HG2	2:B:134:GLU:HG3	1.80	0.64
3:C:167:TRP:HE3	3:C:168:ALA:N	1.95	0.64
9:I:97:LYS:HB2	9:I:102:LEU:HD12	1.80	0.64
1:A:243:A:H4'	1:A:244:U:O5'	1.98	0.64
1:A:679:C:H2'	1:A:680:C:C6	2.33	0.63
7:G:90:GLU:HG2	7:G:91:VAL:H	1.63	0.63
1:A:184:G:H2'	1:A:185:A:H8	1.63	0.63
1:A:839:U:H5'	1:A:840:C:H5	1.64	0.63
1:A:1342:C:H2'	1:A:1343:G:C8	2.34	0.63
17:Q:18:THR:HG23	17:Q:69:LYS:HE3	1.79	0.63
17:Q:29:HIS:CG	17:Q:30:PRO:HD2	2.33	0.63
1:A:718:G:H5''	1:A:718:G:H8	1.63	0.63
3:C:58:GLU:HB3	10:J:92:THR:HG21	1.81	0.63
1:A:945:G:O6	1:A:1236:A:N1	2.31	0.63
6:F:50:TYR:CE1	18:R:77:GLY:HA2	2.34	0.63
8:H:103:VAL:HG12	8:H:108:GLY:HA3	1.79	0.63
1:A:434:U:H2'	1:A:435:C:C6	2.34	0.63
1:A:1442:G:N7	1:A:1446:A:N6	2.47	0.63
9:I:25:LYS:HG3	9:I:60:ASP:OD1	1.98	0.63
1:A:837:G:H1	1:A:849:C:H42	1.47	0.63
1:A:1128:C:OP1	9:I:66:ARG:NH1	2.30	0.63
1:A:1417:G:O2'	1:A:1483:A:N6	2.31	0.63
1:A:1359:C:OP2	14:N:35:ARG:NH1	2.31	0.63
2:B:142:LEU:HD13	2:B:146:GLN:HE22	1.63	0.63
18:R:30:ASP:HB3	18:R:33:ASP:HB2	1.80	0.63
4:D:68:TYR:OH	4:D:98:GLU:OE1	2.11	0.63
10:J:36:GLY:HA2	10:J:72:VAL:HG13	1.79	0.63
1:A:633:G:H2'	1:A:634:C:C6	2.34	0.62
1:A:802:A:H2'	1:A:803:G:O4'	1.99	0.62
5:E:60:TYR:CE1	5:E:64:ARG:HD2	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:65:ASN:ND2	5:E:65:ASN:O	2.32	0.62
1:A:795:C:H5''	1:A:796:C:OP2	1.99	0.62
1:A:1358:U:O2'	1:A:1359:C:OP1	2.17	0.62
1:A:481:G:HO2'	1:A:482:A:H8	1.43	0.62
2:B:21:ARG:HA	2:B:39:ILE:HA	1.82	0.62
1:A:921:U:O2'	5:E:19:MET:O	2.17	0.62
1:A:1251:A:H4'	9:I:12:GLU:OE2	1.99	0.62
1:A:1286:A:H2'	1:A:1287:A:H4'	1.79	0.62
1:A:1255:G:O2'	1:A:1258:G:H1'	1.99	0.62
1:A:299:G:H2'	1:A:300:A:C8	2.35	0.62
1:A:474:G:H2'	1:A:475:G:C8	2.35	0.62
1:A:501:C:H2'	1:A:502:G:C8	2.34	0.62
1:A:190(E):U:O2'	17:Q:63:ARG:NH2	2.32	0.62
1:A:235:C:H5'	17:Q:70:ARG:HG2	1.80	0.62
1:A:1004:A:H5'	1:A:1025:U:H3	1.65	0.62
1:A:1068:G:OP2	1:A:1068:G:H8	1.82	0.62
1:A:1255:G:H2'	1:A:1279:A:H61	1.64	0.62
1:A:1420:C:H2'	1:A:1421:G:H8	1.65	0.62
2:B:12:GLU:HG2	2:B:213:LEU:HD22	1.80	0.62
15:O:33:THR:HA	15:O:63:ARG:HH11	1.64	0.62
19:S:80:TYR:CE1	19:S:81:ARG:HB3	2.34	0.62
1:A:184:G:H2'	1:A:185:A:C8	2.35	0.62
1:A:825:G:H21	8:H:11:THR:HG21	1.65	0.62
3:C:75:VAL:O	3:C:83:ARG:HD3	2.00	0.62
9:I:26:VAL:HB	9:I:33:PHE:HB2	1.82	0.62
1:A:738:C:OP1	6:F:92:LYS:HD3	1.99	0.61
2:B:73:THR:HG21	2:B:96:ARG:HD2	1.81	0.61
15:O:33:THR:HA	15:O:63:ARG:NH1	2.15	0.61
1:A:14:U:O2	1:A:16:A:C8	2.53	0.61
14:N:16:PHE:HD1	14:N:19:ARG:HH11	1.48	0.61
1:A:1143:G:H2'	1:A:1144:G:C8	2.35	0.61
2:B:16:HIS:HB3	2:B:210:SER:HB2	1.83	0.61
2:B:30:ARG:HG3	2:B:31:TYR:CD2	2.35	0.61
4:D:64:LEU:O	4:D:64:LEU:HD22	2.00	0.61
1:A:633:G:H2'	1:A:634:C:H6	1.65	0.61
1:A:815:A:N6	1:A:1509:C:H1'	2.15	0.61
1:A:1179:A:H2'	1:A:1180:A:O4'	2.01	0.61
1:A:1400:5MC:H3'	1:A:1401:G:C5'	2.31	0.61
6:F:70:ASP:OD1	6:F:70:ASP:N	2.33	0.61
13:M:34:LEU:HD13	13:M:41:PRO:HA	1.82	0.61
16:P:6:LEU:HD23	16:P:17:TYR:CD2	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:G:H2'	1:A:95:U:H6	1.62	0.61
6:F:10:LEU:HD12	6:F:59:TYR:HB3	1.81	0.61
8:H:119:LEU:HD12	8:H:124:ALA:HB2	1.83	0.61
1:A:1241:G:H2'	1:A:1242:C:H6	1.65	0.61
7:G:27:ILE:HA	7:G:30:ILE:HD12	1.80	0.61
1:A:79:G:C6	1:A:80:G:C6	2.88	0.61
5:E:17:ALA:HA	5:E:26:PHE:HB3	1.80	0.61
16:P:68:ASP:OD1	16:P:68:ASP:N	2.28	0.61
19:S:36:ARG:HB3	19:S:51:VAL:HG11	1.83	0.61
1:A:685:G:O2'	1:A:686:U:H5''	2.01	0.61
2:B:96:ARG:HE	2:B:97:TRP:H	1.49	0.61
15:O:33:THR:HG23	15:O:63:ARG:HH12	1.64	0.61
1:A:1063:C:H2'	1:A:1064:G:C8	2.36	0.61
3:C:14:ILE:O	3:C:16:ARG:N	2.27	0.61
1:A:518:C:H2'	1:A:530:G:C8	2.35	0.60
1:A:1190:G:O3'	3:C:3:ASN:HB2	2.01	0.60
3:C:134:ILE:O	3:C:138:VAL:HG23	2.01	0.60
1:A:527:7MG:H5''	1:A:527:7MG:H81	1.81	0.60
1:A:902:G:H2'	1:A:903:G:C8	2.35	0.60
1:A:1182:G:H4'	1:A:1183:A:H5'	1.83	0.60
7:G:65:ALA:HB1	7:G:127:ALA:HB3	1.83	0.60
4:D:15:GLU:HG2	4:D:63:LYS:HG3	1.82	0.60
4:D:26:CYS:HA	4:D:31:CYS:HB2	1.82	0.60
10:J:16:LEU:HD13	10:J:68:HIS:HB2	1.83	0.60
10:J:27:ALA:HA	10:J:81:THR:HG23	1.83	0.60
11:K:58:PRO:HD3	11:K:89:ALA:HB1	1.83	0.60
2:B:82:ARG:HG2	2:B:92:TYR:CE1	2.36	0.60
12:L:10:LEU:HD12	17:Q:32:TYR:CZ	2.37	0.60
20:T:65:LYS:O	20:T:68:LYS:HB2	2.02	0.60
5:E:74:GLY:HA3	5:E:116:THR:HG22	1.82	0.60
5:E:90:VAL:O	5:E:91:LEU:HD23	2.01	0.60
7:G:108:ALA:O	7:G:119:ARG:HB3	2.01	0.60
8:H:46:LYS:HG3	8:H:64:LYS:HB2	1.84	0.60
1:A:429:U:OP1	4:D:36:ARG:NH1	2.32	0.60
1:A:1059:C:N3	1:A:1198:G:N1	2.32	0.60
1:A:1236:A:H4'	1:A:1304:G:H4'	1.84	0.60
21:U:8:THR:HG22	21:U:9:ARG:H	1.67	0.60
17:Q:5:VAL:C	17:Q:6:LEU:HD23	2.27	0.60
1:A:355:C:H5'	1:A:389:A:OP2	2.00	0.60
4:D:125:HIS:HD1	4:D:152:SER:HG	1.50	0.60
18:R:46:GLU:OE2	18:R:86:VAL:HG23	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:C:O2	16:P:1:MET:HB2	2.01	0.59
1:A:864:A:H2'	1:A:865:A:C8	2.37	0.59
1:A:1005:A:N6	1:A:1024:G:O2'	2.35	0.59
1:A:1145:C:O2'	1:A:1146:A:O5'	2.18	0.59
1:A:112:G:H2'	1:A:113:G:H5'	1.83	0.59
1:A:706:A:O2'	11:K:29:ILE:HD11	2.02	0.59
1:A:757:U:H2'	1:A:758:G:O4'	2.02	0.59
1:A:1126:U:N3	1:A:1149:C:H1'	2.17	0.59
1:A:1441:G:H4'	1:A:1442:G:C5	2.37	0.59
5:E:81:GLU:HG3	5:E:90:VAL:HG22	1.84	0.59
1:A:79:G:H2'	1:A:80:G:C8	2.37	0.59
3:C:6:HIS:HD2	3:C:9:GLY:H	1.49	0.59
12:L:66:VAL:HG11	12:L:98:TYR:CE1	2.38	0.59
12:L:110:VAL:HA	12:L:111:LYS:HE3	1.83	0.59
1:A:673:G:H5'	6:F:87:ARG:HD2	1.83	0.59
5:E:37:ARG:HB3	5:E:37:ARG:HH11	1.66	0.59
5:E:121:LYS:HG2	5:E:123:LEU:CD2	2.32	0.59
13:M:22:ILE:HG22	13:M:23:TYR:N	2.17	0.59
13:M:96:LEU:HB3	13:M:97:PRO:HD2	1.84	0.59
1:A:76:C:H2'	1:A:77:G:C8	2.37	0.59
2:B:142:LEU:HD13	2:B:146:GLN:NE2	2.18	0.59
20:T:12:ALA:HA	25:T:1302:HOH:O	2.02	0.59
1:A:1410:G:H2'	1:A:1411:C:H6	1.67	0.59
1:A:1391:U:H2'	1:A:1392:G:H8	1.66	0.59
3:C:180:ALA:HB1	3:C:182:ILE:HG13	1.83	0.59
1:A:113:G:H1'	1:A:354:G:H5'	1.85	0.59
1:A:835:U:OP1	18:R:64:ARG:NH2	2.34	0.59
12:L:28:LYS:HE3	12:L:33:ARG:HH12	1.67	0.59
20:T:50:GLU:HA	20:T:100:ILE:HG13	1.85	0.59
9:I:43:ALA:HA	9:I:74:ILE:HD13	1.83	0.59
1:A:160:A:O2'	1:A:161:A:OP1	2.21	0.59
1:A:819:A:H5'	1:A:819:A:C8	2.37	0.59
5:E:71:LEU:HD21	5:E:113:ALA:O	2.03	0.59
8:H:95:VAL:HB	8:H:99:GLU:HB2	1.85	0.59
1:A:92:C:O2	1:A:93:G:C8	2.56	0.58
1:A:758:G:C8	25:A:2216:HOH:O	2.52	0.58
3:C:202:ILE:HG22	3:C:204:LEU:HD23	1.85	0.58
11:K:78:GLN:HA	11:K:103:LEU:HD22	1.84	0.58
13:M:48:LEU:HD12	13:M:53:VAL:HG23	1.85	0.58
1:A:1241:G:H2'	1:A:1242:C:C6	2.38	0.58
4:D:15:GLU:C	4:D:17:VAL:H	2.09	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:U:H2'	1:A:63:C:C6	2.39	0.58
10:J:48:THR:HA	10:J:62:HIS:HB3	1.85	0.58
11:K:73:MET:HG2	11:K:103:LEU:HD21	1.85	0.58
1:A:1009:G:N2	1:A:1010:G:H1'	2.18	0.58
6:F:53:ALA:HB3	6:F:86:ARG:NE	2.19	0.58
14:N:16:PHE:HD1	14:N:19:ARG:NH1	2.01	0.58
1:A:108:G:C6	20:T:15:ARG:HG2	2.38	0.58
1:A:839:U:H5'	1:A:840:C:C5	2.38	0.58
1:A:966:M2G:HM22	1:A:967:5MC:C2	2.39	0.58
1:A:1028:C:H2'	1:A:1029:C:H6	1.69	0.58
1:A:620:C:N1	4:D:135:LEU:HD13	2.19	0.58
1:A:692:U:OP1	11:K:124:LYS:NZ	2.32	0.58
1:A:1516:G:H1'	1:A:1519:MA6:H101	1.86	0.58
8:H:20:TYR:HA	8:H:65:TYR:CZ	2.38	0.58
1:A:80:G:N2	1:A:89:C:H42	2.01	0.58
1:A:90:U:N3	1:A:91:C:N3	2.52	0.58
1:A:1114:C:O2	14:N:60:SER:OG	2.21	0.58
1:A:653:A:O4'	8:H:56:LYS:HE2	2.04	0.58
1:A:938:A:H5'	7:G:76:ARG:HH22	1.69	0.58
1:A:1266:G:N2	1:A:1269:A:OP2	2.35	0.58
1:A:1399:C:H4'	1:A:1400:5MC:H5''	1.85	0.58
1:A:1402:4OC:HM22	1:A:1403:C:H5'	1.85	0.58
1:A:1498:UR3:O2'	1:A:1499:A:OP2	2.14	0.58
3:C:64:VAL:HG11	3:C:99:VAL:HG23	1.85	0.58
18:R:38:GLU:OE1	18:R:38:GLU:HA	2.03	0.58
4:D:127:THR:HB	4:D:147:ALA:HB3	1.86	0.58
4:D:174:LEU:C	4:D:186:LEU:HD21	2.29	0.58
1:A:95:U:H2'	1:A:96:G:H8	1.68	0.58
1:A:975:A:H4'	1:A:976:G:O5'	2.02	0.58
1:A:1123:A:H2	10:J:39:PRO:HG3	1.68	0.58
7:G:28:ASN:HA	7:G:31:MET:HE2	1.86	0.58
8:H:51:VAL:HG11	8:H:60:ARG:HG2	1.84	0.58
12:L:6:THR:OG1	12:L:9:GLN:HG3	2.04	0.58
1:A:677:U:H3	1:A:713:G:H22	1.52	0.57
1:A:1314:C:H41	19:S:6:LYS:HZ2	1.52	0.57
4:D:25:ARG:C	4:D:27:TYR:H	2.09	0.57
7:G:27:ILE:CD1	7:G:40:ALA:HA	2.34	0.57
1:A:279:A:H5'	1:A:279:A:H8	1.68	0.57
1:A:1476:G:H2'	1:A:1477:C:C6	2.39	0.57
10:J:77:PRO:HB2	10:J:82:ILE:HD11	1.84	0.57
1:A:411:A:N7	1:A:413:G:N3	2.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:707:C:H2'	1:A:708:C:C6	2.39	0.57
1:A:780:A:O2'	1:A:781:A:H5''	2.05	0.57
1:A:1163:C:H2'	1:A:1164:G:O4'	2.04	0.57
16:P:53:VAL:O	16:P:56:ALA:N	2.37	0.57
1:A:827:U:H3'	1:A:870:U:O4	2.05	0.57
1:A:1497:G:H2'	1:A:1498:UR3:H5'	1.85	0.57
10:J:11:PHE:CE2	10:J:65:LEU:HD21	2.39	0.57
1:A:909:A:H2'	1:A:910:C:O4'	2.03	0.57
11:K:54:ARG:O	11:K:57:THR:HG22	2.04	0.57
19:S:15:LEU:HD22	19:S:44:MET:HE1	1.84	0.57
1:A:451:A:N6	1:A:481:G:C4	2.72	0.57
1:A:714:G:H2'	1:A:715:A:C8	2.39	0.57
1:A:966:M2G:HM22	1:A:967:5MC:H1'	1.87	0.57
8:H:114:THR:HB	8:H:116:LYS:N	2.19	0.57
16:P:10:GLY:HA3	16:P:16:HIS:H	1.68	0.57
1:A:88:A:H2'	1:A:89:C:C6	2.40	0.57
1:A:243:A:C2	1:A:246:A:C8	2.92	0.57
1:A:750:G:O2'	15:O:21:ASP:OD2	2.23	0.57
1:A:1206:G:H2'	1:A:1207:2MG:C8	2.40	0.57
5:E:80:ILE:HG12	5:E:81:GLU:N	2.16	0.57
10:J:62:HIS:O	14:N:59:ALA:HB3	2.04	0.57
1:A:80:G:H22	1:A:89:C:N4	2.02	0.57
1:A:552:U:H2'	1:A:553:A:C8	2.40	0.57
1:A:571:U:H5''	1:A:572:A:OP2	2.05	0.57
1:A:93:G:H21	1:A:95:U:H1'	1.68	0.57
1:A:481:G:O2'	1:A:482:A:H8	1.88	0.57
1:A:1372:U:H2'	1:A:1373:G:O4'	2.05	0.57
1:A:384:G:H2'	1:A:385:C:H6	1.64	0.57
3:C:112:SER:O	3:C:115:LEU:HB2	2.04	0.57
4:D:187:ARG:NE	4:D:188:LEU:H	2.02	0.57
9:I:79:LEU:O	9:I:83:ARG:HG2	2.05	0.57
11:K:47:VAL:HG12	11:K:48:ILE:HG13	1.87	0.57
13:M:49:THR:HG22	13:M:51:ALA:H	1.70	0.57
15:O:4:THR:HG23	15:O:7:GLU:HB2	1.86	0.57
1:A:321:A:H2'	1:A:322:C:H6	1.70	0.56
1:A:858:G:O6	1:A:869:G:C8	2.58	0.56
1:A:1238:A:H5'	1:A:1336:C:H41	1.70	0.56
1:A:1403:C:O2'	1:A:1404:5MC:H5'	2.05	0.56
5:E:76:ILE:O	5:E:93:PRO:HB3	2.04	0.56
8:H:6:ILE:HB	8:H:85:ARG:NH1	2.20	0.56
4:D:98:GLU:HG2	4:D:189:PRO:HG3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:69:TYR:HE2	12:L:71:PRO:HA	1.68	0.56
12:L:93:LEU:O	12:L:96:VAL:HG23	2.05	0.56
1:A:390:C:O3'	16:P:28:ARG:NH2	2.38	0.56
1:A:687:A:C2	1:A:704:A:C5	2.93	0.56
1:A:838:G:H1	1:A:848:C:H42	1.53	0.56
1:A:1267:C:O2'	21:U:20:LYS:HG3	2.06	0.56
6:F:4:TYR:CE1	6:F:92:LYS:HG2	2.40	0.56
11:K:104:GLN:HG2	11:K:106:LYS:NZ	2.20	0.56
21:U:9:ARG:HH22	21:U:23:PRO:CD	2.17	0.56
1:A:31:G:O2'	1:A:48:C:N4	2.38	0.56
2:B:68:ILE:O	2:B:90:MET:HB3	2.05	0.56
3:C:123:GLN:HE21	3:C:128:PHE:HD2	1.53	0.56
4:D:191:ARG:O	4:D:194:LEU:HD12	2.05	0.56
13:M:12:ASN:H	13:M:45:VAL:HB	1.69	0.56
1:A:1195:C:H3'	1:A:1196:U:C5'	2.32	0.56
1:A:1204:A:H2'	1:A:1205:U:H5'	1.87	0.56
17:Q:95:TYR:HA	17:Q:98:LEU:CD1	2.36	0.56
1:A:60:A:P	1:A:331:G:H22	2.29	0.56
1:A:694:A:N1	1:A:787:A:O2'	2.39	0.56
1:A:1323:G:H2'	1:A:1324:A:C8	2.40	0.56
19:S:12:ASP:CG	19:S:38:SER:HB3	2.30	0.56
5:E:152:ARG:NE	8:H:44:PHE:HE1	2.04	0.56
9:I:17:VAL:HG22	9:I:63:ILE:HD12	1.88	0.56
12:L:7:ILE:O	12:L:11:VAL:HG23	2.06	0.56
15:O:32:LEU:HD12	15:O:63:ARG:HB2	1.88	0.56
1:A:1089:G:C6	1:A:1090:U:N3	2.74	0.56
5:E:116:THR:HG23	5:E:117:ASP:OD2	2.06	0.56
15:O:16:ALA:HB1	15:O:21:ASP:HB3	1.87	0.56
19:S:31:ILE:HG22	19:S:49:ILE:HG12	1.88	0.56
1:A:56:U:H2'	1:A:57:G:H8	1.71	0.56
1:A:126:G:OP1	1:A:605:U:O2'	2.21	0.56
1:A:412:A:H1'	4:D:35:ARG:HH21	1.70	0.56
13:M:14:ARG:HG2	13:M:14:ARG:HH11	1.70	0.56
13:M:49:THR:HB	13:M:52:GLU:H	1.70	0.56
20:T:81:LYS:O	20:T:85:MET:HG3	2.06	0.56
1:A:200:G:H1	1:A:217:C:H42	1.54	0.56
1:A:397:A:O2'	1:A:399:G:OP2	2.20	0.56
4:D:57:ARG:HB3	4:D:206:PHE:HB2	1.88	0.56
9:I:89:ASN:O	9:I:92:TYR:HB2	2.05	0.56
14:N:24:CYS:H	14:N:33:VAL:HG11	1.71	0.56
1:A:758:G:N7	25:A:2216:HOH:O	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1280:A:N7	10:J:40:LEU:HD22	2.21	0.55
2:B:36:ARG:O	2:B:39:ILE:HG12	2.06	0.55
2:B:178:ARG:NH1	8:H:71:GLY:O	2.39	0.55
5:E:15:ARG:HH11	5:E:15:ARG:HG3	1.72	0.55
1:A:501:C:H2'	1:A:502:G:H8	1.69	0.55
1:A:1188:A:O3'	14:N:58:LYS:NZ	2.38	0.55
3:C:167:TRP:HE3	3:C:168:ALA:H	1.51	0.55
4:D:15:GLU:O	4:D:17:VAL:N	2.39	0.55
1:A:463:A:H2'	1:A:474:G:O4'	2.05	0.55
1:A:1004:A:H5'	1:A:1025:U:N3	2.21	0.55
1:A:1352:C:H2'	1:A:1353:G:C8	2.41	0.55
3:C:77:ILE:HG22	3:C:81:GLY:HA2	1.88	0.55
7:G:38:LEU:O	7:G:42:ILE:HG13	2.07	0.55
1:A:629:G:H2'	1:A:630:G:O4'	2.07	0.55
1:A:1113:C:N4	1:A:1187:G:H1	2.02	0.55
1:A:1361(A):C:C2'	1:A:1362:C:H5''	2.36	0.55
5:E:43:LEU:HB3	5:E:136:MET:HE2	1.89	0.55
8:H:86:ILE:HG21	8:H:133:LEU:HD13	1.89	0.55
17:Q:15:MET:HB3	17:Q:18:THR:HB	1.88	0.55
1:A:1496:C:O2'	1:A:1497:G:O4'	2.24	0.55
1:A:858:G:N7	25:A:2220:HOH:O	2.33	0.55
1:A:1228:C:OP1	13:M:108:ARG:NH2	2.39	0.55
1:A:1395:C:C2'	1:A:1396:A:H5'	2.37	0.55
2:B:180:LEU:HB2	2:B:182:ILE:CD1	2.37	0.55
4:D:18:LYS:HB3	4:D:20:TYR:HE2	1.72	0.55
13:M:12:ASN:N	13:M:45:VAL:HB	2.22	0.55
2:B:24:TRP:CZ3	2:B:26:PRO:HA	2.42	0.55
2:B:72:GLY:HA3	2:B:165:VAL:HG22	1.87	0.55
9:I:48:GLU:N	9:I:49:PRO:HD2	2.22	0.55
16:P:2:VAL:O	16:P:64:ALA:HA	2.07	0.55
16:P:53:VAL:O	16:P:55:ARG:N	2.39	0.55
1:A:89:C:H2'	1:A:90:U:O4'	2.07	0.55
1:A:322:C:C2'	1:A:323:U:H5'	2.37	0.55
1:A:933:G:OP2	7:G:3:ARG:HB2	2.06	0.55
1:A:1054:C:H3'	1:A:1054:C:H6	1.71	0.55
1:A:1117:G:H5''	9:I:104:ARG:NH2	2.22	0.55
1:A:1191:A:H2'	1:A:1192:C:H6	1.72	0.55
1:A:1284:C:OP2	1:A:1285:A:O2'	2.22	0.55
2:B:45:GLN:O	2:B:48:MET:HB2	2.06	0.55
5:E:79:GLU:HB3	5:E:92:LYS:HA	1.88	0.55
2:B:71:VAL:O	2:B:164:VAL:HA	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:119:GLU:OE1	2:B:153:ARG:NH2	2.40	0.55
13:M:11:ARG:HG3	13:M:12:ASN:N	2.22	0.55
16:P:9:PHE:HD2	16:P:18:ARG:HG3	1.72	0.55
1:A:838:G:C2'	1:A:839:U:H5''	2.37	0.55
4:D:9:CYS:O	4:D:12:CYS:HB2	2.07	0.55
17:Q:7:THR:HA	17:Q:57:VAL:O	2.07	0.55
18:R:44:LEU:HD21	18:R:70:ILE:HD13	1.89	0.55
20:T:11:SER:HA	20:T:13:LEU:HD11	1.89	0.55
1:A:350:G:H5''	1:A:350:G:H8	1.72	0.54
1:A:1217:C:OP1	14:N:5:ALA:HB1	2.06	0.54
1:A:1282:C:H2'	1:A:1283:G:O4'	2.06	0.54
10:J:25:GLU:HB3	10:J:29:ARG:HH21	1.72	0.54
1:A:580:U:H2'	1:A:581:G:O4'	2.07	0.54
1:A:1430:C:C2	1:A:1471:G:N2	2.76	0.54
2:B:97:TRP:HH2	2:B:176:GLU:CD	2.14	0.54
11:K:62:GLN:HG3	11:K:63:LEU:N	2.21	0.54
15:O:39:LEU:HB3	15:O:56:LEU:HD13	1.88	0.54
17:Q:8:GLY:O	17:Q:56:VAL:HA	2.07	0.54
1:A:1095:U:OP1	1:A:1108:G:N2	2.33	0.54
1:A:1305:G:N2	1:A:1331:G:H1'	2.22	0.54
1:A:1414:U:H2'	1:A:1415:G:H8	1.73	0.54
4:D:102:ASP:OD1	4:D:103:ASN:N	2.37	0.54
7:G:79:ARG:HB2	7:G:84:ASN:CG	2.32	0.54
1:A:620:C:H2'	1:A:621:A:O4'	2.07	0.54
1:A:1171:G:H2'	1:A:1172:C:H6	1.73	0.54
1:A:1443:G:H5'	1:A:1446:A:H5'	1.88	0.54
3:C:156:ARG:NH1	3:C:160:ALA:O	2.41	0.54
5:E:75:THR:HB	5:E:117:ASP:O	2.08	0.54
10:J:53:PRO:HA	14:N:41:ARG:HH22	1.72	0.54
11:K:92:GLU:O	11:K:95:ILE:HG13	2.08	0.54
1:A:781:A:C5	1:A:802:A:C2	2.96	0.54
1:A:1298:C:O2'	7:G:114:ARG:NH1	2.41	0.54
2:B:17:PHE:HD1	2:B:18:GLY:N	2.04	0.54
12:L:54:LYS:HB3	12:L:70:ILE:HD12	1.90	0.54
17:Q:9:VAL:HG12	17:Q:54:GLY:HA2	1.89	0.54
1:A:35:G:H2'	1:A:36:C:H6	1.72	0.54
3:C:6:HIS:CD2	3:C:9:GLY:H	2.25	0.54
3:C:120:VAL:O	3:C:124:ILE:HG12	2.07	0.54
4:D:35:ARG:O	4:D:36:ARG:HG3	2.07	0.54
5:E:34:VAL:HG12	5:E:62:ALA:HB1	1.89	0.54
1:A:735:C:H1'	18:R:75:ILE:HD12	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:984:C:H42	1:A:1221:G:H1	1.55	0.54
1:A:1302:U:H5''	25:A:2227:HOH:O	2.07	0.54
9:I:89:ASN:O	9:I:92:TYR:N	2.37	0.54
15:O:22:THR:O	15:O:27:VAL:HG11	2.07	0.54
1:A:447:G:N1	1:A:485:G:O2'	2.40	0.54
1:A:526:C:O3'	22:A:1601:SRY:HI31	2.07	0.54
1:A:815:A:H62	1:A:1509:C:H1'	1.72	0.54
1:A:858:G:N7	25:A:2218:HOH:O	2.40	0.54
1:A:1347:G:H1'	1:A:1348:U:C5	2.41	0.54
1:A:1361(A):C:O2'	1:A:1362:C:H6	1.91	0.54
1:A:1518:MA6:H102	1:A:1519:MA6:H103	1.90	0.54
13:M:16:ASP:OD1	13:M:16:ASP:N	2.40	0.54
1:A:369:C:OP2	1:A:388:G:N2	2.39	0.54
1:A:503:C:OP2	12:L:116:SER:HB3	2.07	0.54
1:A:1061:G:H1	1:A:1195:C:N4	1.98	0.54
1:A:1065:U:H5	1:A:1190:G:C4	2.25	0.54
2:B:184:VAL:HG23	2:B:198:ASP:H	1.73	0.54
1:A:1367:C:OP2	9:I:112:LYS:NZ	2.41	0.54
2:B:21:ARG:HG2	2:B:23:ARG:HH11	1.73	0.54
4:D:9:CYS:SG	4:D:31:CYS:O	2.65	0.54
1:A:1424:C:H2'	1:A:1425:U:H6	1.73	0.53
2:B:105:PHE:HE2	2:B:157:ARG:HA	1.73	0.53
3:C:110:ASN:ND2	3:C:140:ARG:HB3	2.22	0.53
13:M:14:ARG:HG2	13:M:14:ARG:NH1	2.23	0.53
16:P:75:ARG:HH11	16:P:75:ARG:HG3	1.72	0.53
1:A:532:A:O2'	1:A:533:A:OP1	2.22	0.53
1:A:558:G:H5''	1:A:559:A:H3'	1.89	0.53
2:B:88:ALA:HB2	2:B:219:VAL:HG13	1.90	0.53
7:G:26:PHE:CD1	7:G:101:LEU:HD22	2.43	0.53
8:H:11:THR:O	8:H:12:ARG:C	2.50	0.53
10:J:82:ILE:HA	10:J:85:LEU:HD12	1.90	0.53
18:R:36:ASN:O	18:R:40:LEU:HG	2.08	0.53
1:A:90:U:C4	1:A:91:C:C4	2.96	0.53
1:A:620:C:C2	4:D:135:LEU:HD13	2.43	0.53
1:A:973:G:O2'	14:N:29:ARG:NH2	2.40	0.53
1:A:1511:G:H2'	1:A:1512:U:O4'	2.09	0.53
1:A:1518:MA6:H2'	1:A:1519:MA6:C8	2.38	0.53
21:U:13:ILE:HA	21:U:22:ARG:NH1	2.23	0.53
1:A:254:G:OP1	17:Q:67:LYS:O	2.25	0.53
1:A:321:A:C2	1:A:333:G:C2	2.96	0.53
1:A:381:C:H2'	1:A:382:A:O4'	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394:G:H2'	1:A:395:C:C6	2.44	0.53
1:A:564:C:C5	17:Q:31:LEU:HD21	2.43	0.53
1:A:1504:G:C3'	1:A:1505:G:H5'	2.37	0.53
9:I:103:THR:HG22	9:I:104:ARG:O	2.08	0.53
17:Q:40:LYS:HD3	17:Q:42:TYR:CZ	2.43	0.53
1:A:462:G:H21	16:P:82:GLN:HE21	1.57	0.53
1:A:954:G:H21	1:A:1227:A:H62	1.55	0.53
1:A:1008:C:H42	1:A:1021:G:H1	1.56	0.53
1:A:1502:A:H2'	1:A:1504:G:C8	2.42	0.53
3:C:87:LEU:HD22	3:C:101:LEU:HD11	1.89	0.53
10:J:8:LEU:HD23	10:J:96:ILE:HG23	1.88	0.53
15:O:22:THR:OG1	15:O:23:GLY:N	2.40	0.53
1:A:49:U:O2'	1:A:50:A:H2'	2.08	0.53
1:A:1392:G:H2'	1:A:1393:U:H6	1.74	0.53
1:A:1404:5MC:H2'	1:A:1405:G:O4'	2.09	0.53
1:A:1539:C:H2'	1:A:1540:PSU:H6	1.73	0.53
2:B:23:ARG:O	2:B:24:TRP:HD1	1.91	0.53
4:D:31:CYS:O	4:D:31:CYS:SG	2.66	0.53
6:F:95:GLU:HG3	6:F:96:PRO:HD2	1.90	0.53
7:G:54:THR:HG22	7:G:56:GLN:H	1.74	0.53
8:H:53:VAL:HB	8:H:58:TYR:CD1	2.44	0.53
11:K:41:THR:HG21	11:K:71:LYS:HB3	1.90	0.53
13:M:107:ALA:HB3	13:M:111:LYS:HE3	1.89	0.53
17:Q:27:PHE:CZ	17:Q:36:ILE:HD11	2.43	0.53
18:R:39:VAL:HG13	18:R:40:LEU:HD23	1.91	0.53
1:A:117:G:O5'	1:A:117:G:H8	1.92	0.53
1:A:405:U:O4	4:D:2:GLY:HA3	2.08	0.53
1:A:1007:C:H2'	1:A:1008:C:C5	2.43	0.53
1:A:1403:C:H2'	1:A:1404:5MC:C6	2.44	0.53
1:A:1532:U:H2'	1:A:1533:C:H3'	1.91	0.53
2:B:223:ILE:HG21	2:B:230:VAL:HB	1.90	0.53
8:H:15:ASN:N	8:H:15:ASN:OD1	2.41	0.53
1:A:596:C:C2'	1:A:597:G:H5'	2.38	0.53
1:A:976:G:OP2	1:A:1358:U:H1'	2.08	0.53
1:A:1448:C:H2'	1:A:1449:C:H6	1.74	0.53
2:B:82:ARG:HG2	2:B:92:TYR:HE1	1.73	0.53
4:D:173:TRP:HB2	4:D:187:ARG:O	2.09	0.53
10:J:7:LYS:HA	10:J:71:LEU:HD13	1.91	0.53
1:A:383:A:C6	1:A:384:G:H1'	2.44	0.53
1:A:685:G:C2'	1:A:686:U:H5''	2.38	0.52
1:A:1198:G:H2'	1:A:1199:U:C6	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1347:G:HO2'	1:A:1348:U:P	2.33	0.52
2:B:180:LEU:HB2	2:B:182:ILE:HD12	1.90	0.52
7:G:73:MET:SD	7:G:90:GLU:HA	2.49	0.52
9:I:118:LYS:O	9:I:120:ARG:N	2.39	0.52
1:A:560:U:H5'	1:A:566:G:N2	2.24	0.52
1:A:673:G:H2'	1:A:674:G:C8	2.44	0.52
10:J:51:ARG:CZ	10:J:61:GLU:HB2	2.38	0.52
10:J:69:ASN:C	10:J:70:ARG:HG2	2.34	0.52
13:M:99:ARG:HB2	13:M:101:GLN:HE22	1.73	0.52
15:O:87:ILE:HG22	15:O:88:ARG:N	2.23	0.52
2:B:21:ARG:HG3	2:B:22:LYS:H	1.73	0.52
3:C:73:PRO:HG3	3:C:105:GLU:CD	2.33	0.52
5:E:84:PHE:HB2	5:E:134:ALA:HB2	1.91	0.52
20:T:71:THR:O	20:T:72:LEU:HD23	2.09	0.52
1:A:838:G:N2	1:A:849:C:C2	2.77	0.52
1:A:1305:G:H3'	21:U:4:GLY:O	2.10	0.52
2:B:19:HIS:CE1	2:B:204:ASN:ND2	2.77	0.52
6:F:53:ALA:HB3	6:F:86:ARG:HE	1.73	0.52
8:H:97:VAL:HG12	8:H:98:LYS:HD3	1.92	0.52
13:M:23:TYR:CZ	13:M:71:ARG:HD3	2.44	0.52
14:N:21:TYR:N	14:N:21:TYR:CD1	2.77	0.52
16:P:6:LEU:HD23	16:P:17:TYR:CG	2.45	0.52
1:A:1517:G:H5''	25:A:2084:HOH:O	2.08	0.52
17:Q:6:LEU:O	17:Q:58:GLU:HA	2.09	0.52
1:A:1006:C:H41	1:A:1024:G:H21	1.56	0.52
1:A:1121:U:H2'	1:A:1122:U:C6	2.45	0.52
7:G:62:PHE:CE2	7:G:66:VAL:HG21	2.44	0.52
1:A:170:U:O2'	1:A:171:A:H5'	2.08	0.52
1:A:1144:G:N2	1:A:1146:A:H62	2.07	0.52
1:A:1177:G:N2	1:A:1181:G:O6	2.43	0.52
1:A:1305:G:C8	1:A:1305:G:OP2	2.63	0.52
1:A:1359:C:H1'	1:A:1361(A):C:H41	1.74	0.52
2:B:90:MET:HE2	2:B:226:ARG:HH22	1.73	0.52
9:I:2:GLU:HG3	9:I:3:GLN:OE1	2.09	0.52
13:M:52:GLU:HG2	13:M:55:ARG:HH21	1.75	0.52
16:P:75:ARG:HG2	16:P:75:ARG:O	2.09	0.52
1:A:191:G:N2	20:T:103:GLY:O	2.42	0.52
1:A:1171:G:H2'	1:A:1172:C:C6	2.45	0.52
2:B:189:ASP:HB3	2:B:203:GLY:O	2.10	0.52
5:E:24:ARG:HB2	5:E:26:PHE:HE2	1.75	0.52
10:J:91:PRO:O	10:J:94:VAL:HG22	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:66:VAL:HG11	12:L:98:TYR:HE1	1.75	0.52
1:A:79:G:C2	1:A:80:G:C4	2.98	0.52
1:A:248:C:O2'	1:A:283:C:H4'	2.09	0.52
1:A:1347:G:O2'	1:A:1348:U:P	2.68	0.52
1:A:1505:G:C8	1:A:1505:G:H3'	2.44	0.52
2:B:12:GLU:OE1	2:B:12:GLU:HA	2.09	0.52
5:E:81:GLU:CD	5:E:88:LYS:HE3	2.35	0.52
7:G:60:LYS:HD2	7:G:63:LYS:HE2	1.90	0.52
8:H:11:THR:OG1	8:H:14:ARG:NH1	2.32	0.52
8:H:64:LYS:HG2	8:H:79:VAL:HG21	1.91	0.52
16:P:21:VAL:HG21	16:P:59:TRP:CD1	2.44	0.52
1:A:1012:U:H2'	1:A:1013:G:C8	2.45	0.52
3:C:30:ARG:H	3:C:30:ARG:HD3	1.75	0.52
1:A:83:U:C2'	1:A:84:U:H5'	2.40	0.51
1:A:385:C:H2'	1:A:386:C:C6	2.44	0.51
1:A:436:C:H2'	1:A:437:U:H6	1.75	0.51
1:A:581:G:O3'	15:O:64:ARG:NH2	2.43	0.51
1:A:1145:C:HO2'	1:A:1146:A:P	2.32	0.51
12:L:62:SER:OG	12:L:64:TYR:HB2	2.09	0.51
1:A:8:A:N7	4:D:208:SER:OG	2.44	0.51
1:A:316:G:H1	1:A:337:C:H42	1.59	0.51
1:A:445:G:H8	1:A:445:G:O5'	1.91	0.51
1:A:833:U:H2'	1:A:834:C:C6	2.45	0.51
1:A:1248:A:N3	9:I:70:LYS:HE3	2.25	0.51
6:F:97:PHE:H	18:R:32:ARG:HH12	1.59	0.51
11:K:58:PRO:HA	11:K:90:GLY:HA3	1.91	0.51
16:P:26:ARG:HD2	16:P:31:LYS:O	2.10	0.51
1:A:251:G:H4'	1:A:252:U:OP1	2.07	0.51
1:A:1347:G:N2	1:A:1373:G:H2'	2.25	0.51
6:F:7:ASN:HB2	6:F:89:MET:O	2.09	0.51
8:H:100:ILE:HG23	8:H:112:LEU:HD21	1.93	0.51
15:O:26:GLU:OE1	15:O:77:ARG:HD2	2.10	0.51
17:Q:74:LEU:HD22	17:Q:75:ARG:HG2	1.91	0.51
1:A:1222:G:OP1	19:S:77:THR:HG21	2.11	0.51
1:A:1395:C:O2'	1:A:1396:A:H5'	2.10	0.51
2:B:139:LYS:O	2:B:143:GLU:HG3	2.09	0.51
8:H:86:ILE:HG21	8:H:133:LEU:HB3	1.92	0.51
13:M:2:ALA:O	13:M:10:PRO:HD2	2.10	0.51
19:S:4:SER:O	19:S:6:LYS:NZ	2.44	0.51
20:T:10:LEU:HD13	20:T:11:SER:N	2.24	0.51
1:A:425:G:H2'	1:A:426:G:H5'	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:690:G:H2'	1:A:691:G:O4'	2.09	0.51
1:A:704:A:C2	1:A:705:U:H1'	2.45	0.51
8:H:9:MET:CG	8:H:26:VAL:HG21	2.37	0.51
20:T:17:ARG:O	20:T:20:LEU:HB2	2.10	0.51
1:A:118:U:H3'	1:A:288:A:H61	1.76	0.51
1:A:278:G:C6	17:Q:95:TYR:HD2	2.27	0.51
1:A:838:G:H1	1:A:848:C:N4	2.08	0.51
2:B:157:ARG:H	2:B:157:ARG:HD2	1.75	0.51
5:E:36:ASP:C	5:E:38:GLN:H	2.18	0.51
9:I:42:ARG:NH2	9:I:75:ASP:OD1	2.43	0.51
12:L:126:LYS:N	12:L:126:LYS:HD2	2.26	0.51
1:A:428:G:H4'	1:A:429:U:O5'	2.11	0.51
1:A:510:A:H5''	1:A:511:C:P	2.51	0.51
1:A:938:A:H5'	7:G:76:ARG:HH12	1.75	0.51
1:A:1424:C:H2'	1:A:1425:U:C6	2.45	0.51
6:F:100:ASN:O	6:F:100:ASN:ND2	2.43	0.51
10:J:42:THR:HG23	10:J:67:THR:O	2.10	0.51
18:R:76:LEU:HB3	18:R:78:LEU:HD21	1.93	0.51
1:A:106:C:O2	1:A:379:C:H4'	2.11	0.51
1:A:647:C:H2'	1:A:648:A:H8	1.76	0.51
1:A:935:A:N6	7:G:3:ARG:HG3	2.25	0.51
1:A:1329:A:H2'	1:A:1330:U:H6	1.76	0.51
2:B:189:ASP:O	2:B:192:SER:OG	2.29	0.51
2:B:217:ARG:O	2:B:220:ASP:HB2	2.10	0.51
8:H:84:ARG:O	8:H:135:CYS:HB2	2.11	0.51
11:K:104:GLN:HB3	11:K:106:LYS:HE2	1.92	0.51
18:R:46:GLU:OE2	18:R:85:LEU:HD12	2.10	0.51
1:A:344:A:H5'	1:A:345:C:C5	2.45	0.51
1:A:836:G:OP1	18:R:61:LYS:NZ	2.37	0.51
1:A:857:C:H3'	25:A:2218:HOH:O	2.09	0.51
3:C:91:LEU:HG	3:C:99:VAL:HG11	1.92	0.51
3:C:172:ARG:NH2	3:C:174:PRO:HG3	2.26	0.51
1:A:62:U:O2'	1:A:379:C:O2	2.29	0.51
1:A:216:G:C2	1:A:217:C:C4	2.99	0.51
1:A:976:G:H4'	1:A:977:A:OP1	2.11	0.51
1:A:1095:U:P	1:A:1108:G:H22	2.34	0.51
1:A:1186:G:H2'	1:A:1187:G:O4'	2.10	0.51
1:A:1243:C:H5''	21:U:8:THR:CG2	2.41	0.51
1:A:1360:A:OP2	14:N:35:ARG:NH2	2.44	0.51
1:A:60:A:H4'	1:A:61:G:O5'	2.10	0.50
1:A:731:G:OP1	1:A:766:A:H1'	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:15:PHE:CD2	15:O:30:ALA:HB2	2.46	0.50
17:Q:37:LYS:C	17:Q:38:ARG:HD2	2.36	0.50
1:A:60:A:O5'	1:A:331:G:N2	2.44	0.50
1:A:235:C:N4	25:A:1970:HOH:O	2.44	0.50
1:A:1366:C:H2'	1:A:1367:C:H6	1.76	0.50
1:A:1450:U:H2'	1:A:1452:C:N4	2.26	0.50
4:D:15:GLU:CD	4:D:59:ARG:HH21	2.18	0.50
7:G:91:VAL:HG12	7:G:92:SER:N	2.27	0.50
1:A:321:A:H2'	1:A:322:C:C6	2.46	0.50
1:A:1255:G:H2'	1:A:1279:A:N6	2.24	0.50
1:A:1447:G:H2'	1:A:1447:G:N3	2.25	0.50
2:B:240:GLN:OE1	2:B:240:GLN:N	2.45	0.50
3:C:66:VAL:HG12	3:C:68:VAL:HG23	1.93	0.50
7:G:69:VAL:HG21	7:G:104:LEU:HD21	1.92	0.50
18:R:22:VAL:HG23	18:R:56:THR:HA	1.92	0.50
1:A:92:C:H2'	1:A:93:G:H8	1.76	0.50
1:A:390:C:H2'	1:A:391:G:C8	2.46	0.50
1:A:826:C:H2'	1:A:827:U:H6	1.76	0.50
1:A:957:U:O2'	1:A:959:A:N7	2.38	0.50
3:C:70:VAL:HG13	3:C:72:LYS:H	1.76	0.50
4:D:21:LEU:HD21	4:D:67:ILE:O	2.11	0.50
1:A:91:C:C6	1:A:92:C:C5	2.96	0.50
1:A:157:G:H2'	1:A:158:G:H8	1.75	0.50
1:A:481:G:O2'	1:A:482:A:C8	2.58	0.50
1:A:782:A:H2'	1:A:783:C:O4'	2.12	0.50
1:A:1303:C:H2'	1:A:1304:G:H5'	1.93	0.50
1:A:1332:A:H2'	1:A:1333:A:C8	2.47	0.50
1:A:1543:C:O5'	1:A:1543:C:H6	1.95	0.50
2:B:122:PHE:CE2	2:B:139:LYS:HD3	2.46	0.50
6:F:4:TYR:HB2	6:F:65:VAL:CG2	2.41	0.50
6:F:91:VAL:HG12	6:F:92:LYS:O	2.12	0.50
10:J:29:ARG:NH1	10:J:84:GLN:OE1	2.35	0.50
8:H:50:ARG:HA	8:H:59:LEU:HD23	1.92	0.50
10:J:65:LEU:HD23	10:J:66:ARG:N	2.27	0.50
12:L:111:LYS:HE3	12:L:111:LYS:H	1.75	0.50
19:S:22:LEU:HD21	19:S:28:LYS:HB2	1.92	0.50
20:T:29:LYS:O	20:T:32:ALA:HB3	2.12	0.50
1:A:778:G:H2'	1:A:779:C:O4'	2.11	0.50
1:A:1500:A:H5''	1:A:1501:C:OP2	2.12	0.50
5:E:51:VAL:N	5:E:52:PRO:HD2	2.27	0.50
1:A:455:C:C2'	1:A:456:C:H5'	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:721:G:C6	1:A:733:A:C2	3.00	0.50
1:A:781:A:C4	1:A:802:A:C2	3.00	0.50
1:A:1494:G:C2	1:A:1495:U:C4	3.00	0.50
12:L:82:VAL:O	12:L:106:ASP:HB2	2.11	0.50
1:A:5:U:H4'	1:A:6:G:O5'	2.11	0.50
1:A:1016:A:O2'	1:A:1217:C:O2	2.29	0.50
4:D:152:SER:O	4:D:155:LEU:HB2	2.12	0.50
8:H:2:LEU:HD23	8:H:3:THR:H	1.75	0.50
8:H:124:ALA:O	8:H:128:GLY:N	2.45	0.50
1:A:1040:U:H2'	1:A:1041:A:H8	1.76	0.49
1:A:1486:G:H2'	1:A:1487:G:O4'	2.12	0.49
1:A:77:G:N1	1:A:93:G:C5	2.80	0.49
1:A:353:A:H5'	1:A:353:A:H8	1.77	0.49
15:O:2:PRO:O	15:O:3:ILE:HG13	2.11	0.49
1:A:78:G:C6	1:A:92:C:N4	2.80	0.49
1:A:95:U:O2'	1:A:96:G:H5'	2.12	0.49
1:A:578:C:O2'	1:A:728:A:N3	2.43	0.49
1:A:583:A:H2'	1:A:584:G:O4'	2.12	0.49
1:A:677:U:H2'	1:A:678:U:H6	1.76	0.49
1:A:978:A:O2'	1:A:1322:C:N3	2.44	0.49
1:A:1046:A:H3'	1:A:1047:G:H8	1.78	0.49
1:A:1370:G:C2	1:A:1371:G:N7	2.80	0.49
1:A:1442:G:C5	1:A:1446:A:N6	2.80	0.49
6:F:23:LYS:O	6:F:27:GLN:HG2	2.12	0.49
8:H:120:THR:HG23	8:H:123:GLU:OE1	2.12	0.49
1:A:149:A:H2'	1:A:150:C:C6	2.47	0.49
1:A:156:G:H1	1:A:165:C:H42	1.59	0.49
1:A:1392:G:H21	1:A:1502:A:H8	1.59	0.49
4:D:102:ASP:HB3	4:D:136:PRO:HB3	1.94	0.49
5:E:149:GLU:O	5:E:153:LYS:HB2	2.12	0.49
1:A:75:G:N1	1:A:96:G:C6	2.80	0.49
1:A:98:U:H2'	1:A:99:C:C6	2.48	0.49
1:A:865:A:O5'	1:A:865:A:H8	1.96	0.49
1:A:908:A:C2	1:A:909:A:C4	3.00	0.49
1:A:1126:U:H3	1:A:1149:C:H1'	1.77	0.49
2:B:18:GLY:HA3	2:B:42:ILE:H	1.76	0.49
3:C:10:PHE:C	3:C:10:PHE:CD1	2.91	0.49
3:C:18:TRP:CD1	14:N:54:PRO:HA	2.47	0.49
1:A:35:G:H2'	1:A:36:C:C6	2.48	0.49
1:A:409:G:OP1	4:D:24:GLU:O	2.31	0.49
1:A:705:U:H5''	1:A:706:A:OP2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:790:A:H3'	1:A:791:G:C8	2.48	0.49
3:C:43:LEU:HD23	3:C:47:LEU:HD13	1.94	0.49
9:I:18:PHE:CD1	9:I:62:TYR:HD2	2.31	0.49
1:A:325:A:H2'	1:A:326:G:O4'	2.13	0.49
1:A:997:U:H2'	1:A:998:G:O4'	2.13	0.49
2:B:97:TRP:CH2	2:B:176:GLU:CD	2.90	0.49
5:E:99:GLY:O	5:E:101:ILE:HG12	2.12	0.49
8:H:20:TYR:HA	8:H:65:TYR:CE2	2.48	0.49
8:H:121:ASP:HB2	8:H:125:ARG:NH2	2.28	0.49
12:L:78:GLN:HG2	12:L:81:SER:HB3	1.95	0.49
16:P:10:GLY:CA	16:P:16:HIS:H	2.26	0.49
21:U:18:TYR:CD2	21:U:24:ARG:HA	2.48	0.49
1:A:1513:A:H2'	1:A:1514:C:C6	2.47	0.49
3:C:152:ILE:HG22	3:C:153:VAL:O	2.13	0.49
8:H:28:ALA:CB	8:H:59:LEU:HG	2.43	0.49
9:I:108:VAL:HG12	9:I:109:VAL:N	2.23	0.49
12:L:25:PRO:C	12:L:27:LEU:HB2	2.37	0.49
1:A:7:G:H5'	1:A:298:A:H5'	1.94	0.49
1:A:186:C:H2'	1:A:187:C:C6	2.47	0.49
1:A:688:G:H1	1:A:699:C:H42	1.60	0.49
1:A:825:G:H2'	1:A:826:C:O4'	2.13	0.49
1:A:986:A:H4'	19:S:55:LYS:HZ3	1.77	0.49
1:A:1030:C:H2'	1:A:1030(A):G:C8	2.48	0.49
1:A:1347:G:O6	9:I:10:ARG:NH2	2.37	0.49
8:H:45:ILE:O	8:H:45:ILE:HG12	2.08	0.49
9:I:99:LEU:HB3	9:I:101:PHE:CD1	2.47	0.49
10:J:24:VAL:HG22	10:J:72:VAL:HG11	1.95	0.49
11:K:27:ASN:ND2	11:K:29:ILE:HG22	2.28	0.49
11:K:115:PRO:C	11:K:117:ASN:H	2.21	0.49
14:N:12:ARG:HG2	14:N:14:PRO:HD3	1.94	0.49
1:A:673:G:H5'	6:F:87:ARG:CD	2.42	0.49
1:A:1005:A:H8	1:A:1006:C:C6	2.31	0.49
2:B:59:GLU:HB2	2:B:221:LEU:HD21	1.94	0.49
3:C:35:GLU:O	3:C:39:ILE:HG13	2.13	0.49
3:C:164:ARG:HG2	3:C:165:THR:N	2.27	0.49
7:G:65:ALA:HB2	7:G:128:ALA:HB2	1.95	0.49
8:H:41:ARG:NH1	8:H:123:GLU:OE2	2.42	0.49
11:K:84:VAL:HG11	11:K:91:ARG:HD3	1.95	0.49
1:A:149:A:H2'	1:A:150:C:H6	1.78	0.48
1:A:1173:G:C6	1:A:1174:G:C5	3.01	0.48
1:A:1250:A:H2	1:A:1353:G:H21	1.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1351:U:H4'	7:G:33:ASP:OD2	2.13	0.48
6:F:9:VAL:HG13	6:F:60:PHE:CD2	2.48	0.48
7:G:91:VAL:HG11	7:G:96:GLN:HG3	1.95	0.48
10:J:82:ILE:H	10:J:82:ILE:HD12	1.77	0.48
12:L:34:ARG:HB2	12:L:105:TYR:CE1	2.47	0.48
15:O:5:LYS:O	15:O:8:LYS:N	2.44	0.48
18:R:73:ALA:CB	18:R:79:LEU:HD12	2.42	0.48
1:A:338:A:C2	1:A:339:C:C2	3.01	0.48
1:A:411:A:H62	1:A:413:G:N2	2.11	0.48
1:A:654:G:H2'	1:A:655:A:C8	2.48	0.48
1:A:1074:G:O4'	2:B:104:ASN:HB2	2.12	0.48
1:A:1399:C:C6	1:A:1502:A:N6	2.81	0.48
1:A:1412:C:H2'	1:A:1413:A:H8	1.75	0.48
5:E:90:VAL:C	5:E:91:LEU:HD23	2.38	0.48
1:A:122:G:C2	1:A:123:C:C2	3.01	0.48
1:A:1023:G:H3'	1:A:1024:G:C5'	2.43	0.48
1:A:1291:G:H2'	1:A:1292:U:C6	2.48	0.48
3:C:20:SER:O	14:N:54:PRO:HB3	2.14	0.48
6:F:32:ASN:HD22	6:F:32:ASN:C	2.17	0.48
9:I:111:ARG:HH22	10:J:62:HIS:HE1	1.60	0.48
12:L:113:ARG:HH12	12:L:116:SER:N	2.12	0.48
14:N:20:ALA:C	14:N:21:TYR:HD1	2.21	0.48
1:A:91:C:C5	1:A:92:C:C5	2.93	0.48
1:A:954:G:N2	1:A:1227:A:H62	2.11	0.48
1:A:1054:C:OP1	1:A:1197:G:OP1	2.31	0.48
1:A:1249:C:HO2'	9:I:73:GLN:NE2	2.08	0.48
2:B:17:PHE:CD1	2:B:18:GLY:N	2.81	0.48
2:B:212:GLN:HE21	2:B:212:GLN:C	2.21	0.48
3:C:153:VAL:HG12	3:C:154:SER:N	2.23	0.48
8:H:86:ILE:HG22	8:H:87:SER:N	2.28	0.48
12:L:27:LEU:CA	12:L:29:GLY:H	2.27	0.48
13:M:67:GLU:OE1	13:M:71:ARG:NH2	2.47	0.48
1:A:688:G:H2'	1:A:689:C:H6	1.78	0.48
1:A:765:G:C6	1:A:812:C:C2	3.01	0.48
1:A:1502:A:H2'	1:A:1504:G:N7	2.28	0.48
2:B:160:ASP:OD2	2:B:160:ASP:N	2.46	0.48
20:T:67:ALA:HB2	20:T:77:ALA:HB2	1.95	0.48
1:A:259:G:H2'	1:A:260:G:O4'	2.13	0.48
1:A:344:A:H5'	1:A:345:C:H5	1.78	0.48
1:A:373:A:H1'	1:A:481:G:N3	2.27	0.48
1:A:953:G:H2'	1:A:954:G:O4'	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1265:G:C6	1:A:1266:G:C6	3.01	0.48
1:A:1413:A:C2	1:A:1488:G:C2	3.01	0.48
3:C:44:GLU:HG3	3:C:52:LEU:HD22	1.96	0.48
4:D:170:VAL:HG13	4:D:174:LEU:HB2	1.95	0.48
6:F:35:ALA:HA	6:F:67:MET:HB3	1.95	0.48
8:H:104:ARG:HG2	8:H:104:ARG:HH11	1.78	0.48
13:M:34:LEU:CD1	13:M:41:PRO:HA	2.42	0.48
14:N:15:LYS:HE2	14:N:16:PHE:CZ	2.49	0.48
17:Q:29:HIS:CD2	17:Q:31:LEU:H	2.31	0.48
17:Q:63:ARG:HG2	17:Q:64:PRO:N	2.29	0.48
1:A:78:G:C2	1:A:92:C:C2	3.02	0.48
1:A:1426:C:H42	1:A:1474:G:H1	1.61	0.48
2:B:172:ILE:H	2:B:172:ILE:HD12	1.78	0.48
3:C:71:ALA:HB1	3:C:109:PRO:HB3	1.96	0.48
5:E:11:ILE:HG22	5:E:12:LEU:HD13	1.95	0.48
18:R:45:SER:HB3	18:R:47:THR:O	2.14	0.48
1:A:1255:G:C8	1:A:1279:A:N6	2.78	0.48
1:A:1265:G:H2'	1:A:1266:G:O4'	2.14	0.48
2:B:38:GLY:O	2:B:39:ILE:HD13	2.14	0.48
2:B:47:THR:OG1	2:B:202:PRO:O	2.32	0.48
6:F:6:VAL:HB	6:F:63:TYR:HB2	1.96	0.48
13:M:16:ASP:HB3	13:M:34:LEU:HD12	1.95	0.48
13:M:37:THR:HB	13:M:39:ILE:HG13	1.95	0.48
20:T:84:LEU:O	20:T:88:VAL:HG23	2.14	0.48
1:A:267:C:H2'	1:A:268:C:C6	2.49	0.48
1:A:429:U:H1'	1:A:430:A:H5''	1.96	0.48
1:A:880:C:OP1	12:L:12:ARG:NH1	2.46	0.48
2:B:44:LEU:HD23	2:B:44:LEU:HA	1.67	0.48
4:D:61:LYS:HE2	4:D:72:GLU:OE2	2.13	0.48
4:D:88:VAL:O	4:D:92:VAL:HG23	2.13	0.48
7:G:22:LEU:O	7:G:25:ALA:HB3	2.14	0.48
13:M:17:VAL:O	13:M:20:THR:HB	2.13	0.48
13:M:52:GLU:HG2	13:M:55:ARG:NH2	2.29	0.48
14:N:16:PHE:CD1	14:N:19:ARG:NH1	2.82	0.48
1:A:919:A:O2'	1:A:920:U:H5'	2.14	0.48
1:A:1082:G:O2'	1:A:1083:U:H5'	2.14	0.48
1:A:1346:A:O2'	1:A:1347:G:OP2	2.26	0.48
1:A:93:G:C2	1:A:95:U:N1	2.82	0.47
1:A:267:C:H2'	1:A:268:C:H6	1.79	0.47
1:A:299:G:C6	1:A:300:A:C6	3.02	0.47
1:A:402:G:C6	1:A:403:C:C4	3.02	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:528:C:H41	12:L:49:ASN:CG	2.21	0.47
1:A:1201:A:H4'	1:A:1202:G:C5'	2.44	0.47
1:A:1368:G:OP2	9:I:112:LYS:HD3	2.14	0.47
4:D:4:TYR:HE2	4:D:6:GLY:C	2.22	0.47
4:D:15:GLU:O	4:D:17:VAL:HG13	2.14	0.47
4:D:187:ARG:HD2	4:D:187:ARG:HA	1.65	0.47
14:N:36:PHE:C	14:N:36:PHE:CD1	2.92	0.47
17:Q:44:ALA:HB1	17:Q:72:ARG:HA	1.95	0.47
21:U:5:ASP:O	21:U:11:GLY:HA3	2.14	0.47
1:A:357:G:H1'	1:A:368:U:O2	2.14	0.47
1:A:594:G:H1	1:A:645:C:H42	1.62	0.47
1:A:766:A:C8	1:A:814:A:N6	2.82	0.47
1:A:1314:C:H41	19:S:6:LYS:NZ	2.11	0.47
3:C:139:GLN:O	3:C:143:GLU:HB2	2.14	0.47
5:E:127:ASN:HA	5:E:128:PRO:HD3	1.75	0.47
15:O:18:PHE:HD1	15:O:19:PRO:O	1.97	0.47
21:U:10:ARG:HA	21:U:13:ILE:HB	1.96	0.47
1:A:236:G:H2'	1:A:237:C:O4'	2.13	0.47
1:A:581:G:C8	25:A:2214:HOH:O	2.66	0.47
1:A:767:A:H2'	1:A:768:A:O4'	2.14	0.47
1:A:858:G:C8	25:A:2218:HOH:O	2.56	0.47
1:A:939:G:H5''	7:G:102:ARG:NH1	2.30	0.47
9:I:118:LYS:C	9:I:120:ARG:H	2.21	0.47
10:J:50:ILE:HG22	10:J:60:ARG:HD3	1.96	0.47
12:L:47:LYS:HE2	12:L:47:LYS:HB2	1.56	0.47
1:A:96:G:H2'	1:A:97:G:C8	2.49	0.47
1:A:103:C:O2'	1:A:172:A:N1	2.31	0.47
1:A:632:A:H2'	1:A:633:G:H5'	1.96	0.47
1:A:925:G:C2	1:A:927:G:C8	3.02	0.47
1:A:976:G:N7	1:A:1358:U:N3	2.61	0.47
1:A:1007:C:H2'	1:A:1008:C:H5	1.77	0.47
1:A:1009:G:N2	1:A:1020:U:O2	2.48	0.47
1:A:1028:C:N4	1:A:1034:G:H21	2.13	0.47
1:A:1361(A):C:O2'	1:A:1362:C:O4'	2.32	0.47
3:C:94:LEU:HD13	3:C:94:LEU:HA	1.67	0.47
4:D:4:TYR:C	4:D:5:ILE:HG13	2.38	0.47
5:E:40:ARG:HB3	5:E:66:MET:HE2	1.96	0.47
9:I:112:LYS:HG2	9:I:113:LYS:N	2.30	0.47
18:R:43:PHE:O	18:R:51:LEU:HB2	2.15	0.47
21:U:13:ILE:HG22	21:U:14:TRP:N	2.29	0.47
1:A:88:A:H2'	1:A:89:C:H6	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:C:OP1	20:T:17:ARG:NH1	2.47	0.47
1:A:407:G:O2'	4:D:116:GLN:HG3	2.13	0.47
1:A:781:A:H2'	1:A:782:A:H5'	1.96	0.47
1:A:788:U:H2'	1:A:789:U:O4'	2.14	0.47
1:A:1368:G:C5'	9:I:112:LYS:HB3	2.42	0.47
2:B:126:GLU:HA	2:B:129:GLU:HG3	1.96	0.47
5:E:31:LEU:HD23	5:E:31:LEU:HA	1.55	0.47
5:E:52:PRO:O	5:E:55:VAL:HG12	2.14	0.47
5:E:152:ARG:CZ	8:H:44:PHE:HE1	2.28	0.47
12:L:55:VAL:HG12	12:L:69:TYR:HA	1.95	0.47
1:A:106:C:C2'	1:A:107:G:H5'	2.45	0.47
1:A:123:C:OP1	1:A:312:C:H5'	2.14	0.47
1:A:130:A:H1'	1:A:263:A:O2'	2.15	0.47
1:A:778:G:H8	1:A:778:G:O5'	1.96	0.47
1:A:941:G:C6	1:A:942:G:C8	3.03	0.47
1:A:1144:G:H22	1:A:1146:A:H62	1.62	0.47
4:D:23:GLY:HA3	4:D:112:VAL:HG12	1.96	0.47
4:D:140:VAL:HG11	4:D:146:ILE:HD11	1.96	0.47
4:D:174:LEU:O	4:D:186:LEU:HD11	2.14	0.47
17:Q:87:LYS:HA	17:Q:87:LYS:HE3	1.97	0.47
20:T:36:LEU:HA	20:T:36:LEU:HD23	1.49	0.47
21:U:12:LYS:HB3	21:U:22:ARG:HD2	1.96	0.47
1:A:62:U:H2'	1:A:63:C:H6	1.78	0.47
1:A:766:A:OP2	25:A:2188:HOH:O	2.21	0.47
1:A:1003(A):G:H3'	1:A:1004:A:H5''	1.97	0.47
1:A:1022:G:H2'	1:A:1023:G:H5''	1.97	0.47
1:A:1074:G:C6	1:A:1075:C:C4	3.02	0.47
1:A:1106:G:H5''	3:C:172:ARG:HB3	1.96	0.47
1:A:1117:G:N2	1:A:1180:A:O2'	2.47	0.47
2:B:98:LEU:HB2	2:B:101:MET:HG3	1.96	0.47
3:C:10:PHE:C	3:C:10:PHE:HD1	2.23	0.47
3:C:59:ARG:HE	3:C:59:ARG:HB2	1.60	0.47
3:C:167:TRP:CE3	3:C:168:ALA:N	2.75	0.47
4:D:32:ALA:O	4:D:36:ARG:N	2.48	0.47
4:D:100:ARG:NH1	4:D:137:SER:HA	2.30	0.47
5:E:84:PHE:CB	5:E:134:ALA:HB2	2.45	0.47
8:H:36:LEU:HD23	8:H:36:LEU:HA	1.72	0.47
10:J:47:PHE:HB3	14:N:34:TYR:CE2	2.42	0.47
11:K:98:LEU:HD12	11:K:98:LEU:HA	1.54	0.47
15:O:33:THR:O	15:O:36:ILE:HB	2.15	0.47
18:R:79:LEU:HD23	18:R:80:PRO:HD2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:G:O2'	1:A:607:A:N1	2.48	0.47
1:A:707:C:H5''	11:K:20:TYR:CD2	2.50	0.47
1:A:723:U:O2	1:A:723:U:H2'	2.14	0.47
1:A:824:C:H42	1:A:876:G:H1	1.63	0.47
1:A:953:G:C5'	1:A:965:A:H61	2.27	0.47
1:A:1240:U:C2	7:G:32:ARG:HD2	2.50	0.47
1:A:1357:A:H5''	1:A:1358:U:OP2	2.15	0.47
3:C:54:ARG:H	3:C:69:HIS:HB2	1.79	0.47
4:D:30:LYS:C	4:D:32:ALA:H	2.21	0.47
5:E:139:LEU:HD23	5:E:139:LEU:HA	1.61	0.47
16:P:67:THR:HG22	16:P:69:THR:N	2.27	0.47
18:R:46:GLU:OE2	18:R:86:VAL:N	2.30	0.47
20:T:52:ALA:O	20:T:56:MET:HB2	2.15	0.47
20:T:56:MET:HG3	20:T:88:VAL:HG21	1.97	0.47
1:A:941:G:C2	1:A:1343:G:C2	3.03	0.47
1:A:1262:C:H2'	1:A:1263:C:C6	2.50	0.47
2:B:55:PHE:HA	2:B:58:ILE:HG12	1.95	0.47
4:D:61:LYS:HD3	4:D:206:PHE:CE2	2.49	0.47
4:D:173:TRP:C	4:D:186:LEU:HG	2.39	0.47
9:I:96:LEU:HB3	9:I:102:LEU:HG	1.97	0.47
13:M:4:ILE:HG23	13:M:57:ARG:HA	1.97	0.47
16:P:75:ARG:C	16:P:78:GLY:H	2.23	0.47
1:A:160:A:HO2'	1:A:161:A:P	2.37	0.47
1:A:328:C:O2	1:A:328:C:H2'	2.15	0.47
1:A:699:C:C2'	1:A:700:G:H5'	2.45	0.47
1:A:1314:C:H2'	1:A:1315:U:C6	2.50	0.47
1:A:1358:U:H5''	14:N:35:ARG:HG3	1.96	0.47
1:A:1361:G:H8	1:A:1361:G:O5'	1.98	0.47
6:F:24:GLU:HG3	6:F:28:ARG:HD2	1.97	0.47
7:G:26:PHE:HA	7:G:101:LEU:HD13	1.96	0.47
9:I:63:ILE:HG21	9:I:77:ILE:HG12	1.96	0.47
11:K:34:ASP:O	11:K:37:GLY:N	2.31	0.47
12:L:93:LEU:HD12	12:L:96:VAL:HG21	1.95	0.47
17:Q:84:LEU:HD23	17:Q:84:LEU:HA	1.49	0.47
1:A:44:G:N2	1:A:399:G:C4	2.83	0.46
1:A:1053:G:HO2'	1:A:1199:U:H5	1.62	0.46
1:A:1109:C:OP2	3:C:176:HIS:ND1	2.47	0.46
1:A:1361(A):C:H2'	1:A:1362:C:H5''	1.97	0.46
1:A:1450:U:H2'	1:A:1452:C:H41	1.78	0.46
22:A:1601:SRY:OG2	12:L:91:LYS:NZ	2.47	0.46
2:B:103:THR:N	2:B:176:GLU:OE1	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:28:ALA:HB2	8:H:59:LEU:HG	1.98	0.46
8:H:73:ASP:HA	8:H:74:PRO:HD2	1.68	0.46
8:H:97:VAL:HG23	8:H:129:VAL:C	2.40	0.46
1:A:192:U:H4'	20:T:57:ARG:HD2	1.97	0.46
1:A:204:U:H4'	1:A:216:G:OP1	2.14	0.46
1:A:509:A:H5''	4:D:55:ALA:HB2	1.97	0.46
1:A:839:U:C5'	1:A:840:C:H5	2.28	0.46
1:A:942:G:N3	1:A:943:U:C6	2.83	0.46
1:A:1381:U:C5	1:A:1382:C:C5	3.03	0.46
2:B:30:ARG:HG3	2:B:31:TYR:CE2	2.49	0.46
12:L:117:ARG:HB3	12:L:122:THR:O	2.15	0.46
17:Q:75:ARG:HB2	17:Q:75:ARG:NH1	2.30	0.46
19:S:12:ASP:OD2	19:S:35:SER:OG	2.32	0.46
1:A:150:C:H2'	1:A:151:A:O5'	2.16	0.46
1:A:657:G:H4'	15:O:28:GLN:HG3	1.96	0.46
3:C:91:LEU:O	3:C:95:THR:HG23	2.16	0.46
4:D:61:LYS:HD2	4:D:207:TYR:OH	2.16	0.46
5:E:8:GLU:OE1	5:E:63:ARG:NH2	2.49	0.46
6:F:33:TYR:CD1	6:F:75:LEU:HD23	2.50	0.46
9:I:99:LEU:HD13	9:I:101:PHE:HE1	1.80	0.46
11:K:18:ARG:HB3	11:K:33:THR:HG23	1.96	0.46
14:N:21:TYR:N	14:N:21:TYR:HD1	2.12	0.46
16:P:58:TYR:CD1	16:P:58:TYR:C	2.93	0.46
1:A:101:A:H2'	1:A:102:G:H8	1.81	0.46
1:A:130:A:C8	17:Q:63:ARG:HG3	2.50	0.46
1:A:353:A:H5'	1:A:353:A:C8	2.50	0.46
1:A:369:C:C2'	1:A:370:C:H5'	2.45	0.46
1:A:374:A:H2'	1:A:375:U:C6	2.51	0.46
1:A:411:A:C5	1:A:413:G:N3	2.84	0.46
1:A:436:C:C2	1:A:437:U:C5	3.04	0.46
1:A:1126:U:H2'	1:A:1127:G:H5'	1.97	0.46
3:C:34:LEU:HD22	3:C:38:ARG:HE	1.80	0.46
4:D:173:TRP:O	4:D:186:LEU:HG	2.15	0.46
8:H:69:ARG:N	8:H:74:PRO:O	2.46	0.46
9:I:20:ARG:O	9:I:60:ASP:N	2.49	0.46
15:O:39:LEU:HD13	15:O:56:LEU:HB2	1.97	0.46
19:S:31:ILE:HA	19:S:31:ILE:HD13	1.78	0.46
1:A:695:A:C2	1:A:787:A:H1'	2.51	0.46
1:A:837:G:H1	1:A:849:C:N4	2.13	0.46
1:A:1064:G:N2	1:A:1190:G:H2'	2.31	0.46
1:A:1347:G:H22	1:A:1374:A:P	2.39	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1374:A:C4	1:A:1375:A:C8	3.03	0.46
8:H:97:VAL:O	8:H:100:ILE:HG13	2.16	0.46
13:M:77:ASN:O	13:M:80:ARG:HB3	2.16	0.46
17:Q:74:LEU:HB3	17:Q:75:ARG:HG2	1.97	0.46
1:A:748:C:H4'	1:A:749:C:O5'	2.16	0.46
1:A:1237:C:N4	1:A:1336:C:O2	2.48	0.46
1:A:1305:G:O2'	1:A:1306:A:P	2.73	0.46
4:D:100:ARG:HH12	4:D:137:SER:HB3	1.81	0.46
1:A:131:C:O2	1:A:262:A:H2	1.97	0.46
1:A:195:A:H5'	1:A:196:A:OP2	2.15	0.46
1:A:235:C:C5'	17:Q:70:ARG:HG2	2.45	0.46
1:A:547:A:H4'	1:A:548:G:O5'	2.15	0.46
2:B:87:ARG:HH21	2:B:219:VAL:HG12	1.79	0.46
2:B:90:MET:HE2	2:B:226:ARG:NH2	2.30	0.46
5:E:117:ASP:OD2	5:E:117:ASP:N	2.48	0.46
8:H:38:ILE:HD13	8:H:41:ARG:HH21	1.78	0.46
9:I:5:TYR:HH	9:I:7:THR:HG1	1.60	0.46
12:L:92:0TD:OD1	12:L:92:0TD:N	2.44	0.46
16:P:60:LEU:HA	16:P:60:LEU:HD23	1.56	0.46
20:T:84:LEU:HD22	20:T:88:VAL:CG2	2.46	0.46
1:A:460:A:C6	1:A:462:G:C6	3.04	0.46
1:A:620:C:H2'	1:A:621:A:C8	2.51	0.46
1:A:1117:G:H4'	9:I:104:ARG:NH1	2.30	0.46
1:A:1191:A:C4	1:A:1192:C:C5	3.04	0.46
1:A:1287:A:H2	1:A:1353:G:N3	2.13	0.46
1:A:1410:G:C4	1:A:1411:C:C5	3.04	0.46
2:B:147:LYS:HZ2	2:B:148:TYR:HE2	1.61	0.46
4:D:25:ARG:C	4:D:27:TYR:N	2.73	0.46
4:D:205:GLU:O	4:D:208:SER:HB3	2.16	0.46
8:H:86:ILE:HD12	8:H:86:ILE:HG23	1.66	0.46
15:O:32:LEU:HD22	15:O:32:LEU:HA	1.76	0.46
15:O:36:ILE:HG12	15:O:59:MET:HG2	1.98	0.46
1:A:179:A:H2'	1:A:180:U:H6	1.81	0.46
1:A:394:G:H2'	1:A:395:C:H6	1.79	0.46
1:A:413:G:C8	1:A:413:G:H3'	2.51	0.46
1:A:977:A:O2'	1:A:978:A:H5''	2.16	0.46
1:A:1064:G:OP1	1:A:1386:G:H4'	2.16	0.46
1:A:1175:G:H2'	1:A:1176:A:H8	1.78	0.46
1:A:1189:C:H4'	3:C:10:PHE:CE2	2.50	0.46
1:A:1337:G:H5''	1:A:1338:G:OP1	2.16	0.46
3:C:25:GLY:HA2	3:C:29:TYR:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:155:LEU:HD23	4:D:156:GLU:N	2.30	0.46
5:E:118:ILE:O	5:E:119:LEU:HD23	2.15	0.46
6:F:8:ILE:HD13	6:F:26:ILE:HD13	1.96	0.46
8:H:120:THR:HG23	8:H:123:GLU:CD	2.41	0.46
10:J:38:ILE:HD11	10:J:71:LEU:N	2.30	0.46
16:P:8:ARG:HG2	16:P:10:GLY:H	1.80	0.46
1:A:106:C:H2'	1:A:107:G:O4'	2.15	0.46
1:A:181:G:C6	1:A:194:C:N3	2.84	0.46
1:A:197:A:N3	1:A:198:G:H1'	2.30	0.46
1:A:316:G:OP2	1:A:351:G:O2'	2.34	0.46
1:A:668:G:H1'	15:O:46:HIS:HD2	1.81	0.46
1:A:1090:U:H2'	1:A:1091:U:C6	2.45	0.46
2:B:201:ILE:HG21	2:B:214:ILE:HG21	1.98	0.46
7:G:138:LYS:HE2	7:G:139:GLU:HG3	1.98	0.46
9:I:17:VAL:HG11	9:I:81:ILE:HA	1.98	0.46
9:I:49:PRO:O	9:I:53:VAL:HB	2.16	0.46
16:P:74:LEU:HD22	16:P:79:VAL:HG21	1.98	0.46
20:T:20:LEU:O	20:T:23:ARG:HB3	2.16	0.46
1:A:190(K):G:H2'	1:A:190(L):U:C6	2.52	0.45
1:A:699:C:H2'	1:A:700:G:H5'	1.97	0.45
1:A:750:G:N3	15:O:23:GLY:HA3	2.30	0.45
1:A:972:C:H4'	10:J:57:LYS:CD	2.46	0.45
1:A:1151:A:H5''	10:J:41:PRO:HA	1.98	0.45
1:A:1193:G:H2'	1:A:1194:U:H6	1.81	0.45
1:A:1338:G:C6	1:A:1339:A:C6	3.04	0.45
2:B:155:LEU:HD23	2:B:155:LEU:HA	1.74	0.45
4:D:78:LEU:HD21	4:D:96:LEU:HB3	1.98	0.45
9:I:66:ARG:HE	9:I:66:ARG:HB2	1.43	0.45
17:Q:31:LEU:HD12	17:Q:31:LEU:HA	1.55	0.45
19:S:28:LYS:HD3	19:S:31:ILE:HG12	1.98	0.45
20:T:43:LEU:H	20:T:43:LEU:HG	1.40	0.45
1:A:200:G:H2'	1:A:201:C:O4'	2.17	0.45
1:A:331:G:H5'	25:A:1996:HOH:O	2.16	0.45
1:A:372:C:H4'	1:A:373:A:O5'	2.16	0.45
1:A:411:A:N6	1:A:413:G:C2	2.84	0.45
1:A:518:C:H1'	12:L:50:SER:HB3	1.98	0.45
1:A:696:A:N1	1:A:797:C:O2'	2.46	0.45
1:A:735:C:H5'	18:R:71:LYS:HD3	1.98	0.45
1:A:738:C:P	6:F:92:LYS:HD3	2.56	0.45
1:A:1107:C:C4	1:A:1108:G:C8	3.04	0.45
1:A:1279:A:OP2	10:J:9:ARG:NH1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1392:G:O2'	1:A:1393:U:H5'	2.17	0.45
3:C:17:ASP:OD1	3:C:21:ARG:NH1	2.49	0.45
4:D:30:LYS:O	4:D:32:ALA:N	2.49	0.45
8:H:25:ASP:OD1	8:H:60:ARG:HD3	2.15	0.45
8:H:87:SER:HA	8:H:93:VAL:HG23	1.98	0.45
8:H:97:VAL:HG23	8:H:129:VAL:O	2.16	0.45
12:L:58:VAL:O	12:L:65:GLU:HA	2.16	0.45
14:N:14:PRO:O	14:N:15:LYS:HB3	2.16	0.45
16:P:53:VAL:O	16:P:54:GLU:C	2.59	0.45
19:S:49:ILE:O	19:S:60:VAL:HG12	2.16	0.45
19:S:74:PHE:CD1	19:S:74:PHE:N	2.85	0.45
1:A:98:U:H2'	1:A:99:C:H6	1.80	0.45
1:A:234:C:H2'	1:A:235:C:C6	2.52	0.45
1:A:237:C:OP2	17:Q:40:LYS:NZ	2.40	0.45
1:A:597:G:H2'	1:A:598:U:H5'	1.99	0.45
1:A:647:C:H2'	1:A:648:A:C8	2.52	0.45
1:A:980:C:H3'	1:A:981:U:H6	1.81	0.45
1:A:1046:A:H5'	1:A:1047:G:OP2	2.17	0.45
1:A:1053:G:O2'	1:A:1199:U:H5	1.99	0.45
1:A:1124:G:H5'	10:J:35:SER:O	2.17	0.45
1:A:1216:G:H5''	14:N:5:ALA:HB2	1.98	0.45
1:A:1221:G:C4	1:A:1222:G:C8	3.04	0.45
1:A:1359:C:P	14:N:35:ARG:HH11	2.40	0.45
1:A:1435:G:H8	1:A:1435:G:O5'	2.00	0.45
4:D:177:ASP:OD2	4:D:179:GLU:HB2	2.16	0.45
5:E:89:ILE:HG21	5:E:135:THR:HA	1.99	0.45
7:G:87:VAL:HA	7:G:88:PRO:HD3	1.71	0.45
9:I:93:ARG:HB3	9:I:93:ARG:HH11	1.81	0.45
1:A:83:U:O2'	1:A:84:U:H5'	2.16	0.45
1:A:958:A:C5	19:S:55:LYS:HB2	2.50	0.45
1:A:978:A:OP1	1:A:1361:G:N2	2.46	0.45
1:A:986:A:H4'	19:S:55:LYS:NZ	2.32	0.45
1:A:1064:G:H1'	1:A:1190:G:H21	1.81	0.45
1:A:1092:A:H5'	7:G:4:ARG:NH1	2.31	0.45
1:A:1348:U:O2'	9:I:120:ARG:HD2	2.16	0.45
1:A:1417:G:N2	1:A:1484:C:C4	2.84	0.45
1:A:1465:C:H2'	1:A:1466:C:O4'	2.16	0.45
2:B:194:PRO:HA	2:B:200:ILE:HD11	1.98	0.45
6:F:5:GLU:OE1	18:R:34:TYR:OH	2.24	0.45
7:G:17:VAL:HG12	7:G:18:TYR:HD1	1.82	0.45
7:G:40:ALA:CB	9:I:41:VAL:HG21	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:25:PRO:HB3	12:L:27:LEU:CD2	2.42	0.45
20:T:20:LEU:HA	20:T:20:LEU:HD13	1.66	0.45
1:A:509:A:OP2	25:A:2198:HOH:O	2.21	0.45
1:A:654:G:H2'	1:A:655:A:H8	1.81	0.45
1:A:1102:A:H2'	1:A:1103:C:H6	1.82	0.45
1:A:1292:U:H2'	1:A:1293:G:H8	1.81	0.45
2:B:24:TRP:HA	2:B:191:ASP:HA	1.99	0.45
3:C:101:LEU:HD23	3:C:102:ASN:H	1.82	0.45
3:C:116:VAL:HG21	3:C:202:ILE:HD11	1.97	0.45
3:C:179:ARG:HD2	3:C:206:GLU:HG3	1.98	0.45
7:G:138:LYS:HG2	7:G:139:GLU:N	2.31	0.45
11:K:11:LYS:HB2	11:K:11:LYS:NZ	2.31	0.45
20:T:75:ASN:O	20:T:78:ALA:N	2.49	0.45
1:A:425:G:C2'	1:A:426:G:H5'	2.47	0.45
1:A:922:G:C6	1:A:923:A:C6	3.05	0.45
1:A:1094:G:OP2	1:A:1095:U:C5	2.69	0.45
1:A:1226:C:H4'	1:A:1227:A:OP1	2.16	0.45
1:A:1504:G:H4'	1:A:1505:G:H5'	1.97	0.45
1:A:1507:A:C2	1:A:1508:G:C4	3.05	0.45
6:F:33:TYR:HD1	6:F:75:LEU:HD23	1.81	0.45
13:M:106:ASN:N	13:M:106:ASN:OD1	2.49	0.45
17:Q:77:VAL:HG12	17:Q:78:GLU:N	2.30	0.45
1:A:105:G:H2'	1:A:106:C:C6	2.51	0.45
1:A:128:G:O3'	17:Q:3:LYS:NZ	2.49	0.45
1:A:578:C:H2'	1:A:579:G:O4'	2.16	0.45
1:A:734:G:H21	18:R:75:ILE:HD13	1.82	0.45
1:A:1320:C:OP1	19:S:70:LYS:HE2	2.17	0.45
5:E:82:VAL:O	5:E:82:VAL:HG12	2.15	0.45
7:G:120:ILE:O	7:G:124:LEU:HB2	2.17	0.45
8:H:104:ARG:HG3	8:H:138:TRP:CD2	2.51	0.45
12:L:123:LYS:H	12:L:123:LYS:HG2	1.45	0.45
13:M:94:ARG:HB3	13:M:96:LEU:CD1	2.46	0.45
15:O:79:ARG:O	15:O:83:GLU:HG2	2.17	0.45
1:A:110:C:H2'	1:A:111:G:O4'	2.16	0.45
1:A:586:C:OP1	17:Q:34:LYS:NZ	2.50	0.45
1:A:1189:C:P	10:J:51:ARG:HH22	2.40	0.45
1:A:1410:G:C4	1:A:1491:G:N2	2.85	0.45
2:B:215:LEU:HD23	2:B:215:LEU:HA	1.58	0.45
4:D:126:ILE:HD13	4:D:126:ILE:HA	1.70	0.45
7:G:15:ASP:OD2	7:G:16:LEU:N	2.49	0.45
12:L:11:VAL:HG23	12:L:11:VAL:H	1.40	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:28:LYS:HG2	19:S:29:ARG:H	1.82	0.45
1:A:78:G:H5'	1:A:79:G:OP2	2.16	0.45
1:A:90:U:C4	1:A:91:C:N3	2.85	0.45
1:A:113:G:H2'	1:A:114:U:C6	2.52	0.45
1:A:113:G:C2	1:A:315:A:N1	2.85	0.45
1:A:946:A:H2'	1:A:947:G:H8	1.79	0.45
1:A:1008:C:O4'	1:A:1023:G:N2	2.50	0.45
1:A:1047:G:H2'	1:A:1048:G:H5'	1.99	0.45
1:A:1054:C:H3'	1:A:1054:C:C6	2.52	0.45
1:A:1060:C:OP1	14:N:45:ARG:NH2	2.50	0.45
1:A:1400:5MC:H4'	1:A:1544:U:C5	2.52	0.45
1:A:1476:G:H2'	1:A:1477:C:H6	1.81	0.45
2:B:47:THR:O	2:B:51:LEU:HB2	2.17	0.45
2:B:189:ASP:OD1	2:B:205:ASP:HB3	2.16	0.45
3:C:7:PRO:HB3	3:C:11:ARG:HH21	1.81	0.45
3:C:26:LYS:HD3	3:C:26:LYS:HA	1.81	0.45
5:E:13:ILE:HG22	5:E:30:ALA:HA	1.99	0.45
6:F:99:ALA:HB2	18:R:31:LEU:HG	1.99	0.45
7:G:70:LYS:NZ	7:G:97:GLN:HA	2.32	0.45
8:H:4:ASP:CG	8:H:85:ARG:NH1	2.75	0.45
13:M:78:ILE:HA	13:M:81:LEU:HD23	1.97	0.45
1:A:81:U:H3'	1:A:81:U:H6	1.82	0.45
1:A:247:G:OP2	17:Q:100:LYS:HD2	2.16	0.45
1:A:452:A:C2	1:A:453:A:C4	3.05	0.45
1:A:942:G:C2	1:A:943:U:C6	3.05	0.45
1:A:1133:G:C2	1:A:1134:G:C8	3.05	0.45
1:A:1418:A:H61	1:A:1482:G:H1'	1.81	0.45
1:A:1494:G:H2'	1:A:1495:U:H6	1.81	0.45
8:H:9:MET:HE1	8:H:35:ILE:HG21	1.99	0.45
9:I:2:GLU:OE2	9:I:3:GLN:NE2	2.50	0.45
14:N:12:ARG:HB3	14:N:13:THR:H	1.50	0.45
15:O:81:LEU:HD23	15:O:81:LEU:HA	1.78	0.45
16:P:21:VAL:HG21	16:P:59:TRP:CG	2.52	0.45
16:P:57:ARG:HG3	16:P:79:VAL:CG1	2.45	0.45
1:A:89:C:N3	1:A:90:U:N3	2.65	0.44
1:A:428:G:C5	1:A:430:A:C6	3.05	0.44
1:A:559:A:H4'	1:A:560:U:O5'	2.17	0.44
1:A:725:G:O2'	1:A:726:C:H5'	2.17	0.44
1:A:960:U:H1'	1:A:1223:C:H5'	1.99	0.44
1:A:1031:G:C8	1:A:1032:G:N7	2.85	0.44
1:A:1349:A:H2'	1:A:1350:A:O4'	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:130:VAL:HG11	3:C:157:ILE:HG23	1.99	0.44
4:D:163:GLU:HG3	4:D:166:LYS:HE3	1.99	0.44
7:G:58:PRO:O	7:G:61:VAL:HB	2.17	0.44
8:H:4:ASP:CG	8:H:85:ARG:HH11	2.23	0.44
1:A:429:U:H4'	1:A:430:A:O5'	2.17	0.44
1:A:674:G:H5'	6:F:50:TYR:CE2	2.52	0.44
1:A:1232:U:H5''	9:I:124:GLN:O	2.17	0.44
7:G:20:ASP:OD1	7:G:21:VAL:N	2.50	0.44
11:K:15:ALA:HA	11:K:77:MET:HA	1.97	0.44
12:L:84:LEU:HB3	12:L:104:VAL:HG11	1.99	0.44
20:T:13:LEU:H	20:T:13:LEU:HG	1.51	0.44
1:A:96:G:H2'	1:A:97:G:H8	1.82	0.44
1:A:108:G:O6	20:T:15:ARG:HG2	2.17	0.44
1:A:371:G:O2'	1:A:372:C:H5'	2.17	0.44
1:A:918:A:H2'	1:A:919:A:C8	2.53	0.44
1:A:1454:G:H2'	1:A:1455:G:H8	1.82	0.44
2:B:184:VAL:HG22	2:B:198:ASP:OD2	2.17	0.44
3:C:90:GLU:OE1	3:C:93:LYS:HD2	2.18	0.44
4:D:65:ARG:HG3	4:D:70:ILE:HG22	1.99	0.44
8:H:111:ILE:HG22	8:H:134:ILE:HB	1.99	0.44
9:I:2:GLU:HG3	9:I:3:GLN:CD	2.42	0.44
14:N:19:ARG:H	14:N:19:ARG:HG2	1.46	0.44
1:A:80:G:N2	1:A:90:U:H3	2.16	0.44
1:A:98:U:C2	1:A:99:C:C5	3.05	0.44
1:A:961:U:H2'	1:A:962:C:O4'	2.18	0.44
1:A:1008:C:N4	1:A:1021:G:H1	2.14	0.44
1:A:1067:A:H4'	1:A:1068:G:O5'	2.17	0.44
1:A:1250:A:O2'	1:A:1370:G:O2'	2.29	0.44
1:A:1355:G:H2'	1:A:1356:G:H8	1.83	0.44
1:A:1497:G:C2'	1:A:1498:UR3:H5'	2.47	0.44
5:E:90:VAL:O	5:E:120:THR:HA	2.17	0.44
6:F:14:LEU:HD13	6:F:18:GLN:HB3	1.99	0.44
19:S:11:VAL:HA	19:S:38:SER:HB2	2.00	0.44
1:A:1494:G:C2	1:A:1495:U:C5	3.06	0.44
3:C:32:LEU:HG	3:C:59:ARG:NH1	2.33	0.44
8:H:100:ILE:CG2	8:H:112:LEU:HD21	2.48	0.44
17:Q:10:VAL:O	17:Q:10:VAL:HG22	2.17	0.44
17:Q:22:LEU:HD22	17:Q:41:LYS:HG3	1.99	0.44
1:A:80:G:H1	1:A:89:C:H42	1.65	0.44
1:A:434:U:C4	1:A:435:C:N4	2.85	0.44
1:A:532:A:H2'	1:A:533:A:C5'	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:914:A:P	22:A:1601:SRY:HI33	2.57	0.44
1:A:1060:C:O2	10:J:56:HIS:NE2	2.51	0.44
1:A:1477:C:H2'	1:A:1478:C:H6	1.82	0.44
2:B:96:ARG:NE	2:B:97:TRP:H	2.13	0.44
2:B:107:THR:HG23	2:B:110:GLN:OE1	2.17	0.44
8:H:9:MET:HE3	8:H:9:MET:HB3	1.73	0.44
10:J:10:GLY:O	10:J:67:THR:HA	2.17	0.44
15:O:14:GLU:HG2	15:O:15:PHE:CE1	2.53	0.44
1:A:230:G:H2'	1:A:231:G:O4'	2.18	0.44
1:A:250:A:O4'	1:A:252:U:C6	2.71	0.44
1:A:413:G:H3'	1:A:413:G:H8	1.82	0.44
1:A:874:G:C2'	1:A:875:C:H5'	2.48	0.44
1:A:972:C:H4'	10:J:57:LYS:HG2	2.00	0.44
1:A:1064:G:H21	1:A:1190:G:H2'	1.82	0.44
1:A:1329:A:H2'	1:A:1330:U:O4'	2.18	0.44
2:B:162:ILE:O	2:B:185:ILE:HD12	2.18	0.44
4:D:22:LYS:HG3	4:D:26:CYS:SG	2.57	0.44
6:F:4:TYR:CZ	6:F:72:VAL:HG21	2.52	0.44
6:F:22:GLU:O	6:F:26:ILE:HG13	2.17	0.44
11:K:88:GLY:O	11:K:89:ALA:C	2.60	0.44
12:L:25:PRO:CA	12:L:27:LEU:HB2	2.48	0.44
13:M:67:GLU:O	13:M:71:ARG:HG2	2.17	0.44
1:A:59:A:H3'	1:A:331:G:N2	2.33	0.44
1:A:89:C:N3	1:A:90:U:C2	2.86	0.44
1:A:103:C:OP2	20:T:14:LYS:HD2	2.18	0.44
1:A:257:G:H1	1:A:269:C:H42	1.66	0.44
1:A:772:U:H2'	1:A:773:G:O4'	2.18	0.44
1:A:869:G:C5	25:A:2219:HOH:O	2.67	0.44
1:A:956:U:C2	1:A:1225:A:C2	3.06	0.44
1:A:978:A:C6	1:A:1318:A:C6	3.06	0.44
1:A:1032:G:H8	1:A:1032:G:O5'	2.00	0.44
1:A:1154:G:C6	1:A:1155:G:C5	3.06	0.44
1:A:1189:C:H4'	3:C:10:PHE:HE2	1.83	0.44
1:A:1245:A:H5''	1:A:1246:C:OP2	2.18	0.44
1:A:1358:U:H3'	1:A:1359:C:C5	2.53	0.44
1:A:1392:G:H2'	1:A:1393:U:C6	2.53	0.44
1:A:1420:C:H2'	1:A:1421:G:C8	2.47	0.44
2:B:61:LEU:HG	2:B:66:GLY:HA3	1.99	0.44
5:E:11:ILE:HD13	5:E:11:ILE:HA	1.74	0.44
5:E:152:ARG:HB3	8:H:43:GLY:HA3	1.99	0.44
6:F:95:GLU:O	18:R:32:ARG:NH1	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:24:SER:OG	11:K:25:TYR:N	2.49	0.44
16:P:1:MET:O	16:P:3:LYS:HG2	2.17	0.44
18:R:25:THR:OG1	18:R:42:ARG:NH1	2.50	0.44
19:S:41:VAL:HB	19:S:42:PRO:HD2	1.99	0.44
1:A:78:G:C6	1:A:92:C:C4	3.06	0.44
1:A:93:G:N2	1:A:95:U:C2	2.86	0.44
1:A:312:C:H2'	1:A:313:A:O4'	2.18	0.44
1:A:619:U:C4	4:D:135:LEU:HD21	2.53	0.44
1:A:643:C:C2'	1:A:644:G:H5'	2.47	0.44
1:A:858:G:O6	25:A:2220:HOH:O	2.21	0.44
1:A:979:C:C5	1:A:980:C:C4	3.06	0.44
1:A:1093:A:N3	1:A:1109:C:O2'	2.43	0.44
2:B:217:ARG:HA	2:B:217:ARG:HD3	1.76	0.44
4:D:207:TYR:HD2	4:D:207:TYR:HA	1.64	0.44
8:H:82:HIS:CD2	8:H:138:TRP:NE1	2.86	0.44
11:K:38:ASN:HA	11:K:39:PRO:HD3	1.58	0.44
12:L:8:ASN:OD1	17:Q:34:LYS:HE2	2.17	0.44
12:L:48:PRO:HG2	12:L:92:0TD:H3	2.00	0.44
15:O:75:PRO:O	15:O:79:ARG:HD3	2.18	0.44
17:Q:53:LEU:HD13	17:Q:53:LEU:HA	1.56	0.44
1:A:192:U:H5'	20:T:102:GLY:O	2.18	0.43
1:A:1492:A:C2'	1:A:1493:A:H4'	2.45	0.43
4:D:84:LYS:HB3	4:D:84:LYS:HE2	1.88	0.43
10:J:38:ILE:HD11	10:J:71:LEU:H	1.83	0.43
1:A:113:G:H2'	1:A:114:U:H6	1.82	0.43
1:A:128:G:OP1	17:Q:2:PRO:HD2	2.18	0.43
1:A:145:G:H1	1:A:177:C:H42	1.65	0.43
1:A:406:G:H21	4:D:119:GLN:HE22	1.64	0.43
1:A:1250:A:C6	1:A:1251:A:C6	3.07	0.43
1:A:1255:G:N2	1:A:1259:C:O2	2.46	0.43
4:D:135:LEU:H	4:D:135:LEU:HG	1.64	0.43
5:E:65:ASN:O	5:E:65:ASN:CG	2.60	0.43
8:H:107:LEU:HD23	8:H:107:LEU:N	2.34	0.43
8:H:119:LEU:HD12	8:H:124:ALA:CB	2.47	0.43
11:K:18:ARG:HB3	11:K:20:TYR:HE1	1.83	0.43
1:A:16:A:C2	1:A:920:U:C2	3.07	0.43
1:A:109:A:C6	1:A:326:G:C6	3.06	0.43
1:A:114:U:O2'	1:A:115:G:H5'	2.18	0.43
1:A:253:U:H2'	1:A:254:G:H8	1.82	0.43
1:A:359:U:H2'	1:A:360:A:C8	2.54	0.43
1:A:509:A:O2'	1:A:510:A:OP1	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:892:A:C2	1:A:907:A:C4	3.07	0.43
1:A:939:G:H2'	1:A:940:C:C6	2.53	0.43
1:A:966:M2G:HM22	1:A:967:5MC:O2	2.18	0.43
1:A:1026:G:C8	1:A:1027:C:C5	3.07	0.43
1:A:1500:A:OP2	1:A:1505:G:OP1	2.36	0.43
3:C:43:LEU:O	3:C:47:LEU:HB2	2.18	0.43
6:F:33:TYR:HD1	6:F:75:LEU:CA	2.28	0.43
6:F:33:TYR:CE1	6:F:75:LEU:HA	2.52	0.43
7:G:22:LEU:HD12	7:G:22:LEU:HA	1.69	0.43
8:H:86:ILE:CG2	8:H:133:LEU:HB3	2.47	0.43
9:I:86:VAL:HG23	9:I:96:LEU:HD22	2.00	0.43
13:M:65:LYS:HE3	13:M:69:GLU:HG2	2.00	0.43
15:O:40:SER:O	15:O:44:LYS:HG2	2.18	0.43
1:A:157:G:H2'	1:A:158:G:C8	2.54	0.43
1:A:599:C:O2'	8:H:129:VAL:HG12	2.17	0.43
1:A:728:A:C8	15:O:54:ARG:NH1	2.86	0.43
1:A:1089:G:C2	1:A:1097:C:C2	3.06	0.43
1:A:1199:U:H4'	10:J:54:PHE:CD1	2.53	0.43
2:B:87:ARG:O	2:B:223:ILE:HD11	2.18	0.43
2:B:166:ASP:OD1	2:B:167:PRO:HD2	2.18	0.43
3:C:153:VAL:HA	3:C:198:VAL:HG12	1.99	0.43
7:G:47:CYS:O	7:G:50:ILE:HB	2.19	0.43
8:H:85:ARG:NE	8:H:87:SER:O	2.51	0.43
11:K:18:ARG:CB	11:K:33:THR:HG23	2.49	0.43
17:Q:22:LEU:HD22	17:Q:22:LEU:HA	1.69	0.43
17:Q:23:VAL:HG21	17:Q:42:TYR:CD1	2.53	0.43
1:A:445:G:H2'	1:A:446:G:C8	2.53	0.43
1:A:455:C:H2'	1:A:456:C:H5'	1.99	0.43
1:A:518:C:H4'	1:A:519:C:O5'	2.18	0.43
1:A:1255:G:H22	1:A:1283:G:H1'	1.83	0.43
1:A:1277:C:O2'	1:A:1279:A:H1'	2.18	0.43
3:C:95:THR:C	3:C:97:LYS:H	2.26	0.43
18:R:46:GLU:HG3	18:R:47:THR:N	2.31	0.43
20:T:29:LYS:HE2	20:T:29:LYS:HB2	1.58	0.43
1:A:115:G:O2'	1:A:116:A:OP2	2.22	0.43
1:A:257:G:H2'	1:A:258:G:O4'	2.19	0.43
1:A:500:G:C6	1:A:501:C:N4	2.87	0.43
1:A:1060:C:C2'	1:A:1061:G:H5'	2.49	0.43
1:A:1330:U:H2'	1:A:1331:G:H5'	2.00	0.43
1:A:1516:G:H8	1:A:1516:G:O5'	2.02	0.43
2:B:101:MET:O	2:B:105:PHE:HA	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:15:GLU:C	4:D:17:VAL:N	2.75	0.43
6:F:27:GLN:O	6:F:31:GLU:HG3	2.19	0.43
6:F:91:VAL:HG13	18:R:72:ARG:NH2	2.34	0.43
12:L:69:TYR:CE2	12:L:71:PRO:HA	2.51	0.43
14:N:36:PHE:C	14:N:36:PHE:HD1	2.27	0.43
15:O:87:ILE:HG22	15:O:88:ARG:HB2	2.01	0.43
17:Q:29:HIS:ND1	17:Q:30:PRO:HD2	2.33	0.43
19:S:22:LEU:HD11	19:S:31:ILE:HG13	2.01	0.43
19:S:31:ILE:HG23	19:S:32:LYS:N	2.33	0.43
1:A:509:A:C8	1:A:509:A:H3'	2.53	0.43
1:A:1148:U:H2'	1:A:1149:C:H6	1.84	0.43
1:A:1150:U:O4	1:A:1151:A:N6	2.50	0.43
1:A:1181:G:C5	1:A:1182:G:C6	3.07	0.43
4:D:13:ARG:NH2	4:D:36:ARG:HH22	2.17	0.43
5:E:37:ARG:O	5:E:114:GLY:HA3	2.19	0.43
7:G:155:ARG:HA	7:G:155:ARG:NH1	2.22	0.43
8:H:36:LEU:O	8:H:37:ARG:C	2.60	0.43
11:K:27:ASN:HD22	11:K:29:ILE:HG22	1.83	0.43
19:S:33:THR:O	19:S:51:VAL:HA	2.18	0.43
1:A:587:G:O2'	1:A:588:G:OP2	2.32	0.43
1:A:593:G:H2'	1:A:594:G:O4'	2.19	0.43
1:A:836:G:C6	1:A:851:G:C6	3.06	0.43
1:A:949:A:C2	1:A:1233:G:N3	2.87	0.43
1:A:1028:C:O2'	1:A:1029:C:H5'	2.18	0.43
3:C:76:VAL:HG11	3:C:103:VAL:HG11	2.00	0.43
3:C:76:VAL:HG12	3:C:77:ILE:HD13	2.01	0.43
4:D:17:VAL:HG21	4:D:63:LYS:HD3	2.01	0.43
5:E:11:ILE:HG22	5:E:12:LEU:N	2.33	0.43
14:N:53:LEU:HD12	14:N:56:VAL:HG21	2.01	0.43
20:T:14:LYS:O	20:T:15:ARG:C	2.61	0.43
1:A:253:U:H2'	1:A:254:G:C8	2.54	0.43
1:A:428:G:H1'	1:A:429:U:OP2	2.19	0.43
1:A:500:G:C6	1:A:501:C:C4	3.07	0.43
1:A:860:A:H2'	1:A:861:G:O4'	2.19	0.43
1:A:940:C:H5''	1:A:941:G:OP2	2.19	0.43
1:A:1060:C:C2	1:A:1198:G:C2	3.07	0.43
1:A:1255:G:N1	1:A:1283:G:C2	2.87	0.43
1:A:1287:A:H2'	1:A:1288:A:C8	2.53	0.43
1:A:1328:C:C2'	1:A:1329:A:H5'	2.49	0.43
2:B:17:PHE:HA	2:B:44:LEU:HD11	2.00	0.43
2:B:44:LEU:HA	2:B:47:THR:HB	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:79:LEU:HD23	6:F:79:LEU:HA	1.66	0.43
8:H:6:ILE:O	8:H:10:LEU:HG	2.19	0.43
11:K:48:ILE:HG22	11:K:49:GLY:H	1.83	0.43
16:P:32:TYR:CE2	16:P:35:LYS:HB2	2.54	0.43
20:T:53:LEU:HD22	20:T:53:LEU:HA	1.81	0.43
21:U:8:THR:HG22	21:U:9:ARG:N	2.33	0.43
1:A:92:C:C2	1:A:93:G:C8	3.06	0.43
1:A:299:G:H8	1:A:299:G:O5'	2.02	0.43
1:A:413:G:O6	4:D:36:ARG:NE	2.52	0.43
1:A:662:G:H2'	1:A:663:A:C8	2.54	0.43
1:A:968:A:C8	1:A:1062:U:H4'	2.53	0.43
1:A:1015:A:H2'	1:A:1016:A:O4'	2.19	0.43
1:A:1015:A:O2'	1:A:1218:C:O2'	2.32	0.43
1:A:1200:C:OP1	1:A:1201:A:H2'	2.19	0.43
1:A:1225:A:H2'	1:A:1225:A:N3	2.33	0.43
3:C:18:TRP:NE1	14:N:54:PRO:HA	2.34	0.43
4:D:38:TYR:HB2	4:D:39:PRO:HD2	2.01	0.43
4:D:68:TYR:CD2	4:D:97:LEU:HD22	2.54	0.43
8:H:10:LEU:HD22	8:H:83:ILE:HD12	1.99	0.43
10:J:26:ALA:HA	10:J:29:ARG:CZ	2.49	0.43
17:Q:6:LEU:HD23	17:Q:6:LEU:N	2.34	0.43
19:S:6:LYS:HB3	19:S:7:LYS:H	1.31	0.43
1:A:39:G:O6	1:A:547:A:H2'	2.18	0.42
1:A:119:A:H2'	25:A:2149:HOH:O	2.17	0.42
1:A:197:A:H1'	1:A:198:G:O4'	2.19	0.42
1:A:265:G:H2'	1:A:267:C:C5	2.54	0.42
1:A:1033:G:H2'	1:A:1034:G:O4'	2.19	0.42
1:A:1368:G:OP1	9:I:111:ARG:NH2	2.47	0.42
2:B:114:ARG:HH21	2:B:118:LEU:HD21	1.84	0.42
5:E:51:VAL:HG12	5:E:52:PRO:HD3	2.01	0.42
6:F:3:ARG:NE	6:F:38:GLU:OE2	2.51	0.42
8:H:65:TYR:HA	8:H:79:VAL:HG23	1.99	0.42
9:I:97:LYS:N	9:I:98:PRO:HD2	2.34	0.42
11:K:44:SER:H	11:K:47:VAL:HB	1.83	0.42
13:M:13:LYS:HB2	13:M:18:ALA:HB2	2.01	0.42
16:P:43:LYS:HE2	16:P:43:LYS:HB2	1.90	0.42
17:Q:20:THR:HG22	17:Q:41:LYS:HG2	2.01	0.42
1:A:74:C:H2'	1:A:75:G:C8	2.54	0.42
1:A:146:G:N2	1:A:147:G:C4	2.87	0.42
1:A:503:C:H6	1:A:503:C:O5'	2.03	0.42
1:A:575:G:O2'	1:A:821:G:H5'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:793:U:HO2'	1:A:794:A:C5'	2.26	0.42
1:A:935:A:H61	7:G:3:ARG:HG3	1.83	0.42
1:A:1057:G:C4	1:A:1058:G:C8	3.07	0.42
1:A:1260:C:O5'	1:A:1284:C:H4'	2.20	0.42
1:A:1357:A:H2'	1:A:1358:U:C6	2.54	0.42
2:B:57:PHE:O	2:B:58:ILE:C	2.61	0.42
2:B:98:LEU:HB2	2:B:101:MET:CG	2.50	0.42
3:C:8:ILE:HG23	3:C:16:ARG:HG2	2.02	0.42
3:C:34:LEU:HD13	3:C:38:ARG:HE	1.84	0.42
3:C:73:PRO:HG3	3:C:105:GLU:OE1	2.19	0.42
6:F:45:LEU:HD23	6:F:45:LEU:HA	1.87	0.42
11:K:95:ILE:O	11:K:99:GLN:HG3	2.19	0.42
11:K:112:THR:HA	11:K:113:PRO:HD2	1.91	0.42
13:M:15:VAL:HG12	13:M:34:LEU:HD11	2.00	0.42
13:M:36:LYS:HD2	13:M:59:TYR:OH	2.18	0.42
15:O:85:LEU:HD23	15:O:85:LEU:HA	1.54	0.42
1:A:107:G:N2	1:A:108:G:H1'	2.35	0.42
1:A:197:A:H4'	1:A:198:G:O5'	2.20	0.42
1:A:993:G:H2'	1:A:993:G:N3	2.35	0.42
1:A:1200:C:O2	1:A:1200:C:H2'	2.20	0.42
2:B:54:THR:OG1	2:B:199:TYR:HB3	2.20	0.42
3:C:137:ALA:O	3:C:141:VAL:HG23	2.19	0.42
8:H:104:ARG:HG2	8:H:104:ARG:NH1	2.35	0.42
8:H:105:ARG:HD3	8:H:105:ARG:HA	1.79	0.42
10:J:19:SER:O	10:J:23:ILE:HG12	2.19	0.42
11:K:48:ILE:HG13	11:K:48:ILE:H	1.42	0.42
12:L:98:TYR:N	12:L:98:TYR:CD1	2.87	0.42
13:M:94:ARG:HB3	13:M:96:LEU:HD12	2.00	0.42
16:P:78:GLY:C	16:P:80:PHE:N	2.75	0.42
20:T:41:ILE:HA	20:T:41:ILE:HD12	1.67	0.42
1:A:81:U:H5'	1:A:82:U:OP1	2.20	0.42
1:A:96:G:C2	1:A:97:G:C4	3.08	0.42
1:A:229:U:H4'	16:P:33:ILE:HD13	2.00	0.42
1:A:285:G:O2'	1:A:286:G:H5'	2.20	0.42
1:A:586:C:C2'	1:A:587:G:H5'	2.49	0.42
1:A:643:C:H2'	1:A:644:G:H5'	2.01	0.42
1:A:678:U:H1'	1:A:777:A:O3'	2.20	0.42
1:A:811:C:H4'	1:A:900:A:N6	2.34	0.42
1:A:975:A:H5'	1:A:975:A:H8	1.83	0.42
1:A:1168:A:H2'	1:A:1169:A:C8	2.54	0.42
2:B:7:VAL:HG11	2:B:221:LEU:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:78:GLN:HB2	2:B:94:ASN:OD1	2.19	0.42
2:B:193:ASP:HA	2:B:194:PRO:HD2	1.72	0.42
5:E:112:LEU:HA	5:E:112:LEU:HD23	1.87	0.42
8:H:83:ILE:O	8:H:83:ILE:HG22	2.18	0.42
12:L:7:ILE:O	12:L:10:LEU:N	2.52	0.42
15:O:42:HIS:HD1	15:O:42:HIS:C	2.28	0.42
1:A:152:A:OP2	1:A:153:C:N4	2.43	0.42
1:A:558:G:C5'	1:A:559:A:H3'	2.48	0.42
1:A:602:A:C2	1:A:637:G:C2	3.08	0.42
1:A:981:U:H5''	1:A:982:U:O5'	2.19	0.42
1:A:1057:G:C5	1:A:1058:G:N7	2.88	0.42
1:A:1095:U:H2'	1:A:1096:C:O4'	2.19	0.42
1:A:1510:U:H2'	1:A:1511:G:H8	1.81	0.42
5:E:88:LYS:HB3	5:E:123:LEU:HB2	2.02	0.42
5:E:147:ASP:O	5:E:150:ARG:HB3	2.19	0.42
11:K:72:ALA:HB1	11:K:77:MET:CG	2.50	0.42
14:N:18:VAL:O	14:N:20:ALA:N	2.53	0.42
20:T:27:LYS:HG3	20:T:28:ALA:N	2.33	0.42
1:A:175:C:H2'	1:A:176:C:H6	1.85	0.42
1:A:229:U:O2'	16:P:23:ASP:HB2	2.19	0.42
1:A:276:G:O3'	17:Q:68:ARG:NH1	2.53	0.42
1:A:402:G:C6	1:A:403:C:C5	3.08	0.42
1:A:687:A:C2	1:A:704:A:C6	3.08	0.42
1:A:826:C:H2'	1:A:827:U:C6	2.54	0.42
1:A:960:U:H4'	1:A:961:U:C5'	2.50	0.42
1:A:1030(A):G:N3	1:A:1030(C):G:OP2	2.53	0.42
1:A:1089:G:C6	1:A:1090:U:C4	3.08	0.42
1:A:1144:G:C2	1:A:1145:C:O2	2.72	0.42
1:A:1215:G:H2'	1:A:1215:G:N3	2.34	0.42
1:A:1226:C:N4	13:M:104:ARG:HG3	2.35	0.42
1:A:1540:PSU:O4	1:A:1540:PSU:H2'	2.19	0.42
2:B:11:LEU:O	2:B:13:ALA:N	2.51	0.42
6:F:43:LEU:HD13	6:F:43:LEU:HA	1.83	0.42
9:I:12:GLU:HG2	9:I:12:GLU:O	2.19	0.42
13:M:6:GLY:O	13:M:67:GLU:HG2	2.20	0.42
15:O:4:THR:OG1	15:O:5:LYS:N	2.52	0.42
17:Q:24:GLU:CD	17:Q:37:LYS:HD2	2.45	0.42
1:A:81:U:H3'	1:A:81:U:C6	2.55	0.42
1:A:226:G:N2	25:A:2108:HOH:O	2.13	0.42
1:A:279:A:H5'	1:A:279:A:C8	2.53	0.42
1:A:371:G:C2'	1:A:372:C:H5'	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:579:G:H2'	1:A:580:U:C6	2.54	0.42
1:A:1089:G:C6	1:A:1090:U:C2	3.08	0.42
2:B:73:THR:HG23	2:B:95:GLN:O	2.20	0.42
6:F:9:VAL:HG13	6:F:60:PHE:CE2	2.54	0.42
7:G:122:HIS:O	7:G:125:MET:HG3	2.19	0.42
11:K:120:ARG:HH11	11:K:120:ARG:HD3	1.65	0.42
12:L:28:LYS:HD2	12:L:33:ARG:NH2	2.35	0.42
13:M:18:ALA:O	13:M:21:TYR:HB2	2.20	0.42
15:O:61:GLY:O	15:O:65:ARG:HD2	2.19	0.42
15:O:70:LEU:HD22	15:O:70:LEU:HA	1.46	0.42
16:P:40:ASP:HB3	16:P:48:TRP:HB2	2.01	0.42
17:Q:20:THR:CG2	17:Q:41:LYS:HG2	2.49	0.42
17:Q:27:PHE:CD1	17:Q:27:PHE:C	2.98	0.42
18:R:51:LEU:HB3	18:R:56:THR:HG23	2.01	0.42
18:R:59:SER:N	18:R:62:GLU:OE1	2.53	0.42
18:R:87:ARG:HB3	18:R:88:LYS:H	1.67	0.42
1:A:89:C:C2	1:A:90:U:C2	3.07	0.42
1:A:507:C:OP2	1:A:508:C:O2'	2.38	0.42
1:A:785:G:H2'	1:A:786:G:H5'	2.02	0.42
1:A:922:G:N1	1:A:923:A:C2	2.88	0.42
1:A:1056:U:H2'	1:A:1057:G:H8	1.84	0.42
1:A:1058:G:C6	1:A:1059:C:C4	3.07	0.42
2:B:126:GLU:HG2	2:B:129:GLU:HB2	2.00	0.42
3:C:78:GLY:HA3	3:C:83:ARG:HB2	2.01	0.42
3:C:99:VAL:HG22	3:C:100:ALA:O	2.19	0.42
14:N:40:CYS:HB3	14:N:43:CYS:H	1.83	0.42
17:Q:15:MET:CB	17:Q:18:THR:HB	2.50	0.42
20:T:34:LYS:O	20:T:38:LYS:HE3	2.19	0.42
1:A:443:C:H2'	1:A:444:C:H6	1.85	0.42
1:A:479:C:H2'	1:A:480:U:O4'	2.20	0.42
1:A:510:A:P	25:A:2199:HOH:O	2.77	0.42
1:A:1303:C:C2'	1:A:1304:G:H5'	2.50	0.42
2:B:145:LEU:HA	2:B:145:LEU:HD23	1.66	0.42
13:M:99:ARG:NH1	19:S:2:PRO:HD3	2.35	0.42
13:M:107:ALA:CB	13:M:111:LYS:HE3	2.49	0.42
15:O:14:GLU:HG2	15:O:15:PHE:HE1	1.85	0.42
1:A:404:U:H2'	1:A:405:U:H6	1.85	0.42
1:A:597:G:H2'	1:A:598:U:C5'	2.49	0.42
1:A:651:C:O2'	1:A:652:U:H5'	2.20	0.42
1:A:1008:C:O5'	1:A:1008:C:H6	2.03	0.42
1:A:1329:A:H2'	1:A:1330:U:C6	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:176:GLU:O	2:B:179:LYS:N	2.52	0.42
3:C:32:LEU:O	3:C:35:GLU:HB3	2.20	0.42
5:E:102:ALA:HB1	5:E:106:PRO:HB2	2.02	0.42
13:M:33:ALA:O	13:M:37:THR:OG1	2.35	0.42
15:O:87:ILE:CG2	15:O:88:ARG:N	2.83	0.42
17:Q:29:HIS:CD2	17:Q:32:TYR:N	2.67	0.42
17:Q:59:ILE:CG2	17:Q:71:PHE:HD1	2.33	0.42
1:A:791:G:N2	1:A:792:A:H62	2.18	0.41
1:A:1089:G:O6	1:A:1090:U:N3	2.52	0.41
1:A:1150:U:H4'	10:J:41:PRO:HG3	2.01	0.41
1:A:1190:G:OP1	3:C:4:LYS:HA	2.19	0.41
1:A:1371:G:H4'	9:I:69:GLY:HA3	2.01	0.41
1:A:1419:G:C6	1:A:1420:C:C4	3.08	0.41
3:C:139:GLN:HG2	3:C:170:GLN:OE1	2.20	0.41
6:F:50:TYR:HE1	18:R:77:GLY:HA2	1.82	0.41
18:R:54:ARG:HE	18:R:54:ARG:HB2	1.48	0.41
1:A:164:U:H2'	1:A:165:C:C6	2.55	0.41
1:A:194:C:O3'	20:T:68:LYS:HE2	2.20	0.41
1:A:393:A:C2	1:A:394:G:C8	3.07	0.41
1:A:642:A:C5	1:A:643:C:C4	3.09	0.41
1:A:1378:C:H2'	1:A:1379:G:O4'	2.20	0.41
2:B:83:MET:SD	2:B:234:PRO:HB2	2.61	0.41
4:D:21:LEU:HD22	4:D:21:LEU:HA	1.93	0.41
4:D:165:MET:HE3	4:D:165:MET:HB3	1.90	0.41
7:G:15:ASP:OD1	7:G:18:TYR:HB2	2.20	0.41
10:J:48:THR:OG1	10:J:62:HIS:CD2	2.73	0.41
1:A:76:C:H2'	1:A:77:G:H8	1.82	0.41
1:A:113:G:C2	1:A:315:A:C2	3.09	0.41
1:A:719:C:O2'	18:R:50:ILE:O	2.36	0.41
1:A:838:G:C3'	1:A:839:U:H5''	2.51	0.41
1:A:859:A:H2'	1:A:860:A:O4'	2.19	0.41
1:A:892:A:C5	1:A:893:C:C4	3.07	0.41
1:A:901:A:N7	1:A:902:G:H1'	2.34	0.41
1:A:921:U:O2'	5:E:18:ARG:HG3	2.20	0.41
1:A:958:A:H1'	19:S:55:LYS:HD3	2.01	0.41
1:A:982:U:O2	1:A:1222:G:N2	2.53	0.41
1:A:1063:C:H2'	1:A:1064:G:H8	1.82	0.41
1:A:1218:C:H2'	1:A:1219:U:C6	2.55	0.41
1:A:1442:G:C6	1:A:1446:A:N7	2.88	0.41
3:C:179:ARG:HD2	3:C:207:VAL:HA	2.01	0.41
4:D:49:ARG:HG3	4:D:50:ARG:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:88:PRO:O	7:G:89:MET:HB3	2.21	0.41
9:I:8:GLY:N	9:I:83:ARG:HD2	2.35	0.41
10:J:38:ILE:HD12	10:J:38:ILE:O	2.20	0.41
15:O:42:HIS:C	15:O:42:HIS:ND1	2.78	0.41
1:A:75:G:C6	1:A:96:G:C6	3.09	0.41
1:A:329:A:C5	1:A:332:G:C6	3.09	0.41
1:A:1031:G:H3'	1:A:1031:G:H8	1.85	0.41
2:B:29:ALA:HA	2:B:32:ILE:HG13	2.01	0.41
2:B:84:GLU:HB3	2:B:219:VAL:HG21	2.01	0.41
4:D:68:TYR:CE2	4:D:97:LEU:HB3	2.54	0.41
4:D:158:ILE:HD13	4:D:158:ILE:HA	1.69	0.41
6:F:14:LEU:HD22	6:F:18:GLN:OE1	2.20	0.41
7:G:16:LEU:HD11	9:I:44:VAL:HB	2.02	0.41
7:G:18:TYR:HD1	7:G:18:TYR:N	2.18	0.41
8:H:92:ARG:HH11	8:H:92:ARG:CG	2.33	0.41
9:I:111:ARG:HD2	14:N:61:TRP:OXT	2.20	0.41
15:O:59:MET:HB2	15:O:59:MET:HE3	1.80	0.41
16:P:1:MET:HE3	16:P:1:MET:HB3	1.88	0.41
1:A:1312:G:N2	1:A:1313:U:H1'	2.36	0.41
22:A:1601:SRY:HI32	22:A:1601:SRY:C22	2.50	0.41
3:C:29:TYR:CE2	3:C:33:LEU:HD11	2.56	0.41
3:C:172:ARG:HH22	3:C:174:PRO:HG3	1.85	0.41
5:E:80:ILE:O	5:E:80:ILE:HG23	2.21	0.41
8:H:119:LEU:HB3	8:H:123:GLU:HB3	2.02	0.41
10:J:43:ARG:HD3	10:J:45:ARG:NH2	2.36	0.41
16:P:74:LEU:O	16:P:79:VAL:HG23	2.20	0.41
19:S:11:VAL:HG12	19:S:15:LEU:HD11	2.02	0.41
1:A:131:C:O2'	1:A:262:A:O2'	2.34	0.41
1:A:132:C:H4'	20:T:74:LYS:HD2	2.03	0.41
1:A:264:U:C2'	1:A:265:G:H5'	2.49	0.41
1:A:451:A:H8	1:A:451:A:OP1	2.04	0.41
1:A:519:C:OP2	12:L:50:SER:OG	2.33	0.41
1:A:526:C:OP1	1:A:913:A:H3'	2.21	0.41
1:A:642:A:C6	1:A:643:C:C4	3.08	0.41
1:A:941:G:C6	1:A:942:G:N7	2.89	0.41
1:A:1040:U:O4	1:A:1041:A:N6	2.53	0.41
1:A:1267:C:O2	21:U:20:LYS:HD2	2.20	0.41
1:A:1345:U:C2	1:A:1377:A:C2	3.09	0.41
1:A:1397:C:HO2'	1:A:1398:A:P	2.37	0.41
2:B:97:TRP:CZ2	2:B:101:MET:HB2	2.55	0.41
2:B:163:PHE:HA	2:B:185:ILE:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:181:PHE:CD2	8:H:70:GLN:HB3	2.56	0.41
7:G:18:TYR:N	7:G:18:TYR:CD1	2.89	0.41
8:H:30:ARG:O	8:H:33:GLU:N	2.54	0.41
8:H:30:ARG:O	8:H:31:PHE:C	2.62	0.41
11:K:17:GLY:HA3	11:K:77:MET:HE1	2.03	0.41
14:N:4:LYS:HE2	14:N:4:LYS:HB3	1.89	0.41
1:A:421:U:H5'	1:A:422:C:H5	1.86	0.41
1:A:427:U:OP2	4:D:36:ARG:NH2	2.53	0.41
1:A:490:G:C6	1:A:491:G:N7	2.88	0.41
1:A:730:G:C5	1:A:731:G:H1'	2.56	0.41
1:A:977:A:C2'	1:A:978:A:H5''	2.50	0.41
1:A:1071:C:H5''	5:E:49:PRO:HG2	2.02	0.41
1:A:1091:U:O2	1:A:1093:A:C8	2.74	0.41
1:A:1481:U:O2'	1:A:1482:G:H5'	2.21	0.41
1:A:1494:G:H2'	1:A:1495:U:C6	2.56	0.41
3:C:138:VAL:HG22	3:C:151:VAL:HG23	2.02	0.41
5:E:106:PRO:O	5:E:107:ARG:C	2.61	0.41
8:H:77:GLU:HG2	8:H:78:GLN:H	1.84	0.41
8:H:118:VAL:C	8:H:119:LEU:HD23	2.45	0.41
17:Q:18:THR:HG22	17:Q:19:VAL:N	2.35	0.41
18:R:58:LEU:HB3	18:R:62:GLU:HB3	2.03	0.41
20:T:89:ARG:NH2	20:T:104:LEU:HB3	2.36	0.41
1:A:77:G:N1	1:A:93:G:C6	2.89	0.41
1:A:78:G:O6	1:A:92:C:N4	2.54	0.41
1:A:403:C:OP1	4:D:137:SER:OG	2.29	0.41
1:A:727:G:H4'	1:A:741:G:H22	1.86	0.41
1:A:1135:U:O2'	1:A:1138:G:O6	2.33	0.41
1:A:1256:A:H4'	1:A:1257:U:O5'	2.19	0.41
2:B:25:ASN:C	2:B:27:LYS:N	2.77	0.41
2:B:211:ILE:O	2:B:215:LEU:HB2	2.20	0.41
3:C:108:ASN:N	3:C:109:PRO:HD3	2.35	0.41
4:D:64:LEU:CD1	4:D:75:PHE:HZ	2.34	0.41
4:D:89:THR:O	4:D:90:GLY:C	2.62	0.41
5:E:52:PRO:HG2	5:E:53:LEU:H	1.86	0.41
5:E:118:ILE:HG12	5:E:119:LEU:N	2.35	0.41
7:G:15:ASP:OD2	7:G:44:TYR:OH	2.39	0.41
8:H:65:TYR:CD1	8:H:65:TYR:N	2.88	0.41
14:N:42:ILE:H	14:N:42:ILE:HG13	1.64	0.41
1:A:116:A:H8	1:A:116:A:O5'	2.04	0.41
1:A:306:G:H2'	1:A:307:C:H6	1.85	0.41
1:A:617:G:N2	1:A:618:C:N3	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:791:G:H2'	1:A:792:A:C8	2.56	0.41
1:A:982:U:O2	1:A:1222:G:N1	2.54	0.41
1:A:1001:A:H61	1:A:1041:A:N6	2.19	0.41
1:A:1247:U:O2	1:A:1291:G:N1	2.54	0.41
1:A:1442:G:C5	1:A:1446:A:C6	3.09	0.41
2:B:80:ILE:HD12	2:B:212:GLN:HG3	2.02	0.41
2:B:152:PHE:CE1	2:B:155:LEU:HD12	2.55	0.41
3:C:142:MET:HE3	3:C:142:MET:HB3	1.75	0.41
3:C:186:PHE:CD2	3:C:187:ALA:N	2.88	0.41
5:E:131:ILE:HD13	5:E:131:ILE:HA	1.95	0.41
8:H:124:ALA:HA	8:H:127:LEU:HB2	2.03	0.41
9:I:99:LEU:HB3	9:I:101:PHE:CE1	2.55	0.41
11:K:29:ILE:C	11:K:29:ILE:HD12	2.45	0.41
11:K:99:GLN:OE1	11:K:105:VAL:HG21	2.21	0.41
11:K:122:LYS:O	11:K:123:LYS:C	2.62	0.41
13:M:82:MET:HA	13:M:89:GLY:HA3	2.03	0.41
15:O:15:PHE:CZ	15:O:85:LEU:HD21	2.56	0.41
16:P:65:GLN:HA	16:P:66:PRO:HD2	1.97	0.41
20:T:10:LEU:HD22	20:T:10:LEU:HA	1.57	0.41
20:T:22:ARG:O	20:T:23:ARG:C	2.64	0.41
20:T:59:ALA:O	20:T:60:GLU:C	2.63	0.41
20:T:74:LYS:HD3	20:T:74:LYS:HA	1.71	0.41
21:U:13:ILE:HA	21:U:22:ARG:HH12	1.86	0.41
1:A:35:G:O2'	12:L:118:SER:O	2.30	0.41
1:A:448:A:C2	1:A:449:C:C4	3.09	0.41
1:A:652:U:O4	1:A:752:G:O2'	2.28	0.41
1:A:990:C:C4	1:A:1216:G:N2	2.89	0.41
1:A:1064:G:H1'	1:A:1190:G:N2	2.37	0.41
1:A:1111:A:N6	3:C:177:THR:HG22	2.31	0.41
1:A:1189:C:H5''	1:A:1190:G:OP2	2.21	0.41
4:D:28:SER:O	4:D:30:LYS:N	2.46	0.41
5:E:142:LEU:HD23	5:E:142:LEU:HA	1.81	0.41
8:H:82:HIS:C	8:H:82:HIS:ND1	2.79	0.41
17:Q:59:ILE:CG2	17:Q:71:PHE:CD1	3.04	0.41
1:A:16:A:C2	1:A:920:U:O2	2.74	0.40
1:A:234:C:H2'	1:A:235:C:H6	1.87	0.40
1:A:370:C:C2'	1:A:371:G:H5'	2.50	0.40
1:A:374:A:C6	1:A:375:U:C4	3.09	0.40
1:A:401:C:H2'	1:A:402:G:C8	2.57	0.40
1:A:707:C:H5''	11:K:20:TYR:HD2	1.84	0.40
1:A:966:M2G:N3	1:A:966:M2G:H2'	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1037:C:H2'	1:A:1038:C:C5	2.57	0.40
1:A:1205:U:H2'	1:A:1206:G:C8	2.56	0.40
1:A:1245:A:N1	1:A:1293:G:C2	2.89	0.40
1:A:1368:G:OP2	9:I:114:TYR:N	2.54	0.40
2:B:222:ILE:HG21	2:B:222:ILE:HD13	1.85	0.40
3:C:121:ALA:O	3:C:125:GLU:HG3	2.21	0.40
7:G:47:CYS:HA	7:G:50:ILE:HG12	2.03	0.40
11:K:59:TYR:O	11:K:62:GLN:N	2.51	0.40
15:O:45:VAL:HG12	15:O:46:HIS:H	1.87	0.40
1:A:17:U:H2'	1:A:18:C:C6	2.56	0.40
1:A:363:A:OP1	12:L:61:THR:OG1	2.30	0.40
1:A:582:U:OP1	15:O:64:ARG:NH2	2.53	0.40
1:A:636:U:H2'	1:A:637:G:C8	2.56	0.40
1:A:976:G:C8	1:A:1358:U:C2	3.09	0.40
1:A:1250:A:H2	1:A:1353:G:N2	2.19	0.40
1:A:1440:C:C2'	1:A:1441:G:H5'	2.51	0.40
1:A:1516:G:H1'	1:A:1519:MA6:C10	2.51	0.40
2:B:114:ARG:O	2:B:117:GLU:HG2	2.21	0.40
3:C:35:GLU:OE1	3:C:97:LYS:NZ	2.54	0.40
3:C:179:ARG:HA	3:C:179:ARG:HD3	1.84	0.40
5:E:105:VAL:HB	5:E:106:PRO:HD3	2.04	0.40
6:F:97:PHE:H	18:R:32:ARG:NH1	2.17	0.40
11:K:47:VAL:HG12	11:K:48:ILE:N	2.36	0.40
12:L:46:LYS:CG	12:L:47:LYS:H	2.35	0.40
17:Q:72:ARG:HH11	17:Q:72:ARG:HD2	1.70	0.40
1:A:7:G:H5'	1:A:298:A:O4'	2.22	0.40
1:A:389:A:H2'	1:A:390:C:H5'	2.03	0.40
1:A:448:A:C2	1:A:449:C:C5	3.10	0.40
1:A:734:G:H21	18:R:75:ILE:CD1	2.35	0.40
1:A:735:C:O2'	1:A:736:C:H5'	2.21	0.40
1:A:810:C:O2	1:A:899:C:N4	2.54	0.40
1:A:1248:A:C6	1:A:1249:C:N4	2.90	0.40
2:B:16:HIS:O	2:B:17:PHE:C	2.64	0.40
2:B:60:ASP:O	2:B:64:ARG:HG3	2.21	0.40
2:B:69:LEU:HB3	2:B:162:ILE:HD12	2.03	0.40
9:I:28:VAL:O	9:I:31:GLN:N	2.54	0.40
16:P:59:TRP:O	16:P:60:LEU:C	2.64	0.40
20:T:73:HIS:HB3	20:T:74:LYS:H	1.48	0.40
1:A:357:G:C2	1:A:358:U:C5	3.09	0.40
1:A:451:A:OP1	1:A:451:A:C8	2.75	0.40
1:A:669:U:H2'	1:A:670:G:C8	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:803:G:H2'	1:A:804:U:O4'	2.22	0.40
1:A:1219:U:C4	1:A:1220:G:N7	2.89	0.40
1:A:1375:A:H4'	7:G:29:LYS:NZ	2.36	0.40
3:C:59:ARG:HG3	3:C:63:ASN:O	2.21	0.40
7:G:150:ALA:HA	11:K:59:TYR:CD2	2.56	0.40
9:I:112:LYS:HG3	9:I:117:HIS:O	2.22	0.40
12:L:110:VAL:HG13	12:L:111:LYS:HZ1	1.86	0.40
19:S:28:LYS:CD	19:S:31:ILE:HG12	2.51	0.40
20:T:53:LEU:HD12	20:T:102:GLY:H	1.86	0.40
1:A:179:A:H2'	1:A:180:U:C6	2.56	0.40
1:A:527:7MG:O2'	1:A:535:A:N1	2.48	0.40
1:A:542:G:O2'	1:A:543:C:H5'	2.21	0.40
1:A:981:U:H4'	14:N:21:TYR:CE2	2.56	0.40
1:A:1148:U:H4'	9:I:14:VAL:HG11	2.04	0.40
1:A:1162:C:C2	1:A:1175:G:C2	3.09	0.40
1:A:1297:C:H6	1:A:1297:C:OP2	2.05	0.40
1:A:1504:G:C4'	1:A:1505:G:H5'	2.51	0.40
2:B:27:LYS:HB3	2:B:27:LYS:HE2	1.78	0.40
4:D:70:ILE:HG23	4:D:71:SER:N	2.36	0.40
4:D:172:PRO:HD2	4:D:173:TRP:CE3	2.56	0.40
8:H:92:ARG:HH11	8:H:92:ARG:HG3	1.86	0.40
9:I:75:ASP:OD2	9:I:78:LYS:HE3	2.21	0.40
10:J:21:GLN:O	10:J:25:GLU:HG3	2.22	0.40
12:L:53:ARG:HD3	12:L:93:LEU:CD2	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	232/256 (91%)	203 (88%)	25 (11%)	4 (2%)	7 31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	204/239 (85%)	175 (86%)	28 (14%)	1 (0%)	24	55
4	D	206/209 (99%)	190 (92%)	14 (7%)	2 (1%)	12	41
5	E	148/162 (91%)	138 (93%)	9 (6%)	1 (1%)	18	48
6	F	99/101 (98%)	90 (91%)	9 (9%)	0	100	100
7	G	153/156 (98%)	133 (87%)	20 (13%)	0	100	100
8	H	136/138 (99%)	127 (93%)	9 (7%)	0	100	100
9	I	125/128 (98%)	113 (90%)	11 (9%)	1 (1%)	16	45
10	J	96/105 (91%)	73 (76%)	19 (20%)	4 (4%)	2	16
11	K	114/129 (88%)	104 (91%)	10 (9%)	0	100	100
12	L	121/135 (90%)	109 (90%)	10 (8%)	2 (2%)	7	31
13	M	116/126 (92%)	105 (90%)	10 (9%)	1 (1%)	14	43
14	N	58/61 (95%)	53 (91%)	5 (9%)	0	100	100
15	O	85/89 (96%)	75 (88%)	10 (12%)	0	100	100
16	P	81/88 (92%)	75 (93%)	5 (6%)	1 (1%)	10	38
17	Q	97/105 (92%)	88 (91%)	9 (9%)	0	100	100
18	R	68/88 (77%)	62 (91%)	6 (9%)	0	100	100
19	S	78/93 (84%)	70 (90%)	7 (9%)	1 (1%)	9	36
20	T	97/106 (92%)	79 (81%)	17 (18%)	1 (1%)	12	41
21	U	22/27 (82%)	19 (86%)	3 (14%)	0	100	100
All	All	2336/2541 (92%)	2081 (89%)	236 (10%)	19 (1%)	16	45

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	21	ARG
2	B	24	TRP
3	C	15	THR
12	L	28	LYS
19	S	31	ILE
10	J	79	ARG
10	J	86	MET
4	D	156	GLU
20	T	99	LEU
2	B	12	GLU
9	I	119	ALA

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Mol	Chain	Res	Type
4	D	5	ILE
12	L	25	PRO
10	J	34	VAL
5	E	70	PRO
2	B	229	VAL
13	M	84	ILE
16	P	53	VAL
10	J	72	VAL

5.3.2 Protein sidechains [i](#)

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%)	161 (80%)	41 (20%)	1	7
3	C	160/188 (85%)	119 (74%)	41 (26%)	0	4
4	D	180/181 (99%)	142 (79%)	38 (21%)	1	7
5	E	115/123 (94%)	80 (70%)	35 (30%)	0	2
6	F	90/90 (100%)	69 (77%)	21 (23%)	1	5
7	G	126/127 (99%)	99 (79%)	27 (21%)	1	7
8	H	119/119 (100%)	76 (64%)	43 (36%)	0	0
9	I	98/99 (99%)	79 (81%)	19 (19%)	1	8
10	J	87/92 (95%)	65 (75%)	22 (25%)	0	4
11	K	88/99 (89%)	63 (72%)	25 (28%)	0	2
12	L	103/110 (94%)	68 (66%)	35 (34%)	0	1
13	M	94/101 (93%)	68 (72%)	26 (28%)	0	3
14	N	49/50 (98%)	36 (74%)	13 (26%)	0	3
15	O	79/80 (99%)	59 (75%)	20 (25%)	0	4
16	P	72/74 (97%)	58 (81%)	14 (19%)	1	8
17	Q	94/97 (97%)	68 (72%)	26 (28%)	0	3
18	R	61/77 (79%)	40 (66%)	21 (34%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	S	71/80 (89%)	50 (70%)	21 (30%)	0	2
20	T	76/82 (93%)	51 (67%)	25 (33%)	0	1
21	U	19/22 (86%)	15 (79%)	4 (21%)	1	7
All	All	1983/2111 (94%)	1466 (74%)	517 (26%)	0	4

All (517) 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	17	PHE
2	B	19	HIS
2	B	23	ARG
2	B	39	ILE
2	B	47	THR
2	B	51	LEU
2	B	53	ARG
2	B	55	PHE
2	B	63	MET
2	B	75	LYS
2	B	109	SER
2	B	110	GLN
2	B	112	VAL
2	B	121	LEU
2	B	127	ILE
2	B	140	HIS
2	B	142	LEU
2	B	157	ARG
2	B	160	ASP
2	B	162	ILE
2	B	164	VAL
2	B	168	THR
2	B	170	GLU
2	B	178	ARG
2	B	187	LEU
2	B	190	THR
2	B	195	ASP
2	B	196	LEU

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Mol	Chain	Res	Type
2	B	206	ASP
2	B	208	ILE
2	B	209	ARG
2	B	212	GLN
2	B	214	ILE
2	B	215	LEU
2	B	217	ARG
2	B	236	TYR
3	C	3	ASN
3	C	5	ILE
3	C	10	PHE
3	C	14	ILE
3	C	19	GLU
3	C	21	ARG
3	C	30	ARG
3	C	31	HIS
3	C	32	LEU
3	C	34	LEU
3	C	46	GLU
3	C	56	ASP
3	C	58	GLU
3	C	59	ARG
3	C	68	VAL
3	C	70	VAL
3	C	76	VAL
3	C	84	ILE
3	C	91	LEU
3	C	95	THR
3	C	101	LEU
3	C	103	VAL
3	C	111	LEU
3	C	116	VAL
3	C	130	VAL
3	C	143	GLU
3	C	144	SER
3	C	157	ILE
3	C	162	GLN
3	C	167	TRP
3	C	172	ARG
3	C	175	LEU
3	C	176	HIS
3	C	188	LEU

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Mol	Chain	Res	Type
3	C	190	ARG
3	C	192	THR
3	C	195	VAL
3	C	196	LEU
3	C	198	VAL
3	C	204	LEU
3	C	207	VAL
4	D	5	ILE
4	D	9	CYS
4	D	17	VAL
4	D	19	LEU
4	D	21	LEU
4	D	22	LYS
4	D	25	ARG
4	D	26	CYS
4	D	34	GLU
4	D	50	ARG
4	D	58	LEU
4	D	59	ARG
4	D	61	LYS
4	D	64	LEU
4	D	70	ILE
4	D	71	SER
4	D	78	LEU
4	D	85	LYS
4	D	89	THR
4	D	108	LEU
4	D	115	ARG
4	D	122	ARG
4	D	135	LEU
4	D	137	SER
4	D	140	VAL
4	D	150	GLU
4	D	156	GLU
4	D	158	ILE
4	D	162	LEU
4	D	170	VAL
4	D	176	LEU
4	D	186	LEU
4	D	187	ARG
4	D	192	GLU
4	D	194	LEU

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Mol	Chain	Res	Type
4	D	196	LEU
4	D	200	GLU
4	D	208	SER
5	E	10	MET
5	E	12	LEU
5	E	14	ARG
5	E	15	ARG
5	E	16	THR
5	E	18	ARG
5	E	24	ARG
5	E	26	PHE
5	E	31	LEU
5	E	37	ARG
5	E	38	GLN
5	E	41	VAL
5	E	43	LEU
5	E	53	LEU
5	E	55	VAL
5	E	56	GLN
5	E	65	ASN
5	E	68	GLU
5	E	71	LEU
5	E	75	THR
5	E	76	ILE
5	E	79	GLU
5	E	80	ILE
5	E	82	VAL
5	E	100	VAL
5	E	105	VAL
5	E	118	ILE
5	E	121	LYS
5	E	123	LEU
5	E	125	SER
5	E	135	THR
5	E	144	THR
5	E	148	VAL
5	E	149	GLU
5	E	151	LEU
6	F	3	ARG
6	F	9	VAL
6	F	10	LEU
6	F	14	LEU

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Mol	Chain	Res	Type
6	F	16	GLN
6	F	19	LEU
6	F	21	LEU
6	F	23	LYS
6	F	25	ILE
6	F	28	ARG
6	F	32	ASN
6	F	43	LEU
6	F	47	ARG
6	F	55	ASP
6	F	75	LEU
6	F	79	LEU
6	F	81	ILE
6	F	87	ARG
6	F	89	MET
6	F	93	SER
6	F	95	GLU
7	G	6	ARG
7	G	8	GLU
7	G	16	LEU
7	G	21	VAL
7	G	23	VAL
7	G	33	ASP
7	G	42	ILE
7	G	67	GLU
7	G	70	LYS
7	G	74	GLU
7	G	77	SER
7	G	80	VAL
7	G	87	VAL
7	G	97	GLN
7	G	99	LEU
7	G	104	LEU
7	G	106	GLN
7	G	111	ARG
7	G	113	GLU
7	G	114	ARG
7	G	124	LEU
7	G	125	MET
7	G	129	GLU
7	G	141	VAL
7	G	142	GLU

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Mol	Chain	Res	Type
7	G	149	ARG
7	G	155	ARG
8	H	3	THR
8	H	5	PRO
8	H	9	MET
8	H	11	THR
8	H	14	ARG
8	H	15	ASN
8	H	18	ARG
8	H	19	VAL
8	H	24	THR
8	H	26	VAL
8	H	29	SER
8	H	35	ILE
8	H	38	ILE
8	H	39	LEU
8	H	41	ARG
8	H	45	ILE
8	H	46	LYS
8	H	49	GLU
8	H	54	ASP
8	H	64	LYS
8	H	68	ARG
8	H	82	HIS
8	H	83	ILE
8	H	84	ARG
8	H	85	ARG
8	H	86	ILE
8	H	88	LYS
8	H	91	ARG
8	H	92	ARG
8	H	97	VAL
8	H	98	LYS
8	H	100	ILE
8	H	102	ARG
8	H	104	ARG
8	H	105	ARG
8	H	109	ILE
8	H	112	LEU
8	H	114	THR
8	H	120	THR
8	H	123	GLU

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Mol	Chain	Res	Type
8	H	127	LEU
8	H	129	VAL
8	H	133	LEU
9	I	3	GLN
9	I	16	ARG
9	I	19	LEU
9	I	38	GLN
9	I	40	LEU
9	I	51	ARG
9	I	53	VAL
9	I	65	VAL
9	I	66	ARG
9	I	79	LEU
9	I	83	ARG
9	I	85	LEU
9	I	86	VAL
9	I	89	ASN
9	I	93	ARG
9	I	97	LYS
9	I	99	LEU
9	I	109	VAL
9	I	110	GLU
10	J	3	LYS
10	J	8	LEU
10	J	16	LEU
10	J	19	SER
10	J	21	GLN
10	J	24	VAL
10	J	30	SER
10	J	38	ILE
10	J	44	VAL
10	J	47	PHE
10	J	48	THR
10	J	57	LYS
10	J	62	HIS
10	J	63	PHE
10	J	70	ARG
10	J	74	ILE
10	J	75	ILE
10	J	80	LYS
10	J	87	THR
10	J	89	ASP

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Mol	Chain	Res	Type
10	J	90	LEU
10	J	96	ILE
11	K	11	LYS
11	K	14	VAL
11	K	18	ARG
11	K	21	ILE
11	K	24	SER
11	K	29	ILE
11	K	33	THR
11	K	36	ASP
11	K	40	ILE
11	K	47	VAL
11	K	48	ILE
11	K	51	LYS
11	K	53	SER
11	K	62	GLN
11	K	75	TYR
11	K	78	GLN
11	K	79	SER
11	K	91	ARG
11	K	95	ILE
11	K	98	LEU
11	K	114	VAL
11	K	119	CYS
11	K	122	LYS
11	K	124	LYS
11	K	126	ARG
12	L	6	THR
12	L	7	ILE
12	L	10	LEU
12	L	11	VAL
12	L	18	VAL
12	L	19	ARG
12	L	20	LYS
12	L	21	LYS
12	L	24	VAL
12	L	33	ARG
12	L	34	ARG
12	L	36	VAL
12	L	41	ARG
12	L	42	THR
12	L	43	VAL

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Mol	Chain	Res	Type
12	L	47	LYS
12	L	52	LEU
12	L	55	VAL
12	L	60	LEU
12	L	61	THR
12	L	64	TYR
12	L	65	GLU
12	L	66	VAL
12	L	70	ILE
12	L	79	GLU
12	L	80	HIS
12	L	82	VAL
12	L	89	ARG
12	L	93	LEU
12	L	96	VAL
12	L	111	LYS
12	L	116	SER
12	L	119	LYS
12	L	122	THR
12	L	123	LYS
13	M	9	ILE
13	M	11	ARG
13	M	14	ARG
13	M	22	ILE
13	M	27	LYS
13	M	32	GLU
13	M	43	THR
13	M	46	LYS
13	M	48	LEU
13	M	50	GLU
13	M	53	VAL
13	M	56	LEU
13	M	60	VAL
13	M	63	THR
13	M	73	GLU
13	M	80	ARG
13	M	91	ARG
13	M	94	ARG
13	M	102	ARG
13	M	103	THR
13	M	105	THR
13	M	106	ASN

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Mol	Chain	Res	Type
13	M	108	ARG
13	M	109	THR
13	M	110	ARG
13	M	115	LYS
14	N	11	LYS
14	N	12	ARG
14	N	18	VAL
14	N	21	TYR
14	N	22	THR
14	N	33	VAL
14	N	36	PHE
14	N	41	ARG
14	N	42	ILE
14	N	47	LEU
14	N	53	LEU
14	N	56	VAL
14	N	58	LYS
15	O	4	THR
15	O	9	GLN
15	O	12	ILE
15	O	13	GLN
15	O	22	THR
15	O	28	GLN
15	O	32	LEU
15	O	34	LEU
15	O	39	LEU
15	O	47	LYS
15	O	59	MET
15	O	65	ARG
15	O	66	LEU
15	O	67	LEU
15	O	70	LEU
15	O	71	GLN
15	O	73	GLU
15	O	76	GLU
15	O	79	ARG
15	O	81	LEU
16	P	1	MET
16	P	2	VAL
16	P	3	LYS
16	P	29	ASP
16	P	31	LYS

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Mol	Chain	Res	Type
16	P	44	THR
16	P	49	LEU
16	P	53	VAL
16	P	54	GLU
16	P	62	VAL
16	P	68	ASP
16	P	75	ARG
16	P	82	GLN
16	P	83	GLU
17	Q	3	LYS
17	Q	6	LEU
17	Q	7	THR
17	Q	9	VAL
17	Q	10	VAL
17	Q	13	ASP
17	Q	15	MET
17	Q	22	LEU
17	Q	23	VAL
17	Q	30	PRO
17	Q	35	VAL
17	Q	37	LYS
17	Q	38	ARG
17	Q	41	LYS
17	Q	53	LEU
17	Q	57	VAL
17	Q	59	ILE
17	Q	73	VAL
17	Q	74	LEU
17	Q	75	ARG
17	Q	76	LEU
17	Q	85	VAL
17	Q	86	GLU
17	Q	87	LYS
17	Q	92	ARG
17	Q	100	LYS
18	R	19	LYS
18	R	21	LYS
18	R	22	VAL
18	R	26	LEU
18	R	28	GLU
18	R	32	ARG
18	R	38	GLU

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Mol	Chain	Res	Type
18	R	46	GLU
18	R	47	THR
18	R	50	ILE
18	R	51	LEU
18	R	64	ARG
18	R	65	ILE
18	R	68	LYS
18	R	69	THR
18	R	75	ILE
18	R	78	LEU
18	R	82	THR
18	R	86	VAL
18	R	87	ARG
18	R	88	LYS
19	S	4	SER
19	S	7	LYS
19	S	15	LEU
19	S	22	LEU
19	S	29	ARG
19	S	30	LEU
19	S	31	ILE
19	S	32	LYS
19	S	33	THR
19	S	36	ARG
19	S	41	VAL
19	S	43	GLU
19	S	49	ILE
19	S	55	LYS
19	S	57	HIS
19	S	58	VAL
19	S	63	THR
19	S	64	GLU
19	S	71	LEU
19	S	79	THR
19	S	81	ARG
20	T	10	LEU
20	T	13	LEU
20	T	15	ARG
20	T	19	SER
20	T	20	LEU
20	T	23	ARG
20	T	27	LYS

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Mol	Chain	Res	Type
20	T	29	LYS
20	T	33	ILE
20	T	35	THR
20	T	36	LEU
20	T	41	ILE
20	T	45	GLN
20	T	50	GLU
20	T	51	GLU
20	T	53	LEU
20	T	56	MET
20	T	62	LEU
20	T	72	LEU
20	T	75	ASN
20	T	84	LEU
20	T	87	LYS
20	T	92	LEU
20	T	93	GLU
20	T	104	LEU
21	U	8	THR
21	U	10	ARG
21	U	12	LYS
21	U	13	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	19	HIS
2	B	212	GLN
3	C	3	ASN
3	C	6	HIS
3	C	63	ASN
3	C	98	ASN
3	C	102	ASN
3	C	110	ASN
3	C	123	GLN
3	C	181	ASN
4	D	77	ASN
6	F	27	GLN
6	F	84	ASN
6	F	94	GLN
7	G	28	ASN
8	H	78	GLN

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Mol	Chain	Res	Type
8	H	82	HIS
9	I	73	GLN
9	I	117	HIS
11	K	13	GLN
13	M	101	GLN
15	O	9	GLN
15	O	53	HIS
16	P	82	GLN
17	Q	29	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1511/1522 (99%)	417 (27%)	57 (3%)

All (417) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	G
1	A	7	G
1	A	9	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	51	A
1	A	54	C
1	A	55	A
1	A	59	A
1	A	66	G
1	A	67	C
1	A	69	G
1	A	73	C
1	A	81	U
1	A	88	A
1	A	91	C
1	A	92	C
1	A	98	U
1	A	113	G

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Mol	Chain	Res	Type
1	A	114	U
1	A	115	G
1	A	116	A
1	A	120	A
1	A	121	C
1	A	122	G
1	A	129(A)	G
1	A	130	A
1	A	131	C
1	A	135	C
1	A	151	A
1	A	160	A
1	A	161	A
1	A	163	C
1	A	164	U
1	A	166	G
1	A	173	U
1	A	181	G
1	A	182	U
1	A	183	G
1	A	190(C)	C
1	A	190(E)	U
1	A	190(F)	G
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	220	G
1	A	226	G
1	A	227	G
1	A	231	G
1	A	243	A
1	A	244	U
1	A	247	G
1	A	250	A
1	A	251	G
1	A	252	U
1	A	253	U
1	A	254	G
1	A	266	G

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Mol	Chain	Res	Type
1	A	267	C
1	A	269	C
1	A	289	G
1	A	292	G
1	A	293	G
1	A	299	G
1	A	319	G
1	A	321	A
1	A	323	U
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	349	A
1	A	350	G
1	A	351	G
1	A	352	C
1	A	353	A
1	A	354	G
1	A	356	A
1	A	367	U
1	A	370	C
1	A	371	G
1	A	373	A
1	A	379	C
1	A	384	G
1	A	390	C
1	A	398	C
1	A	406	G
1	A	411	A
1	A	412	A
1	A	413	G
1	A	415	A
1	A	421	U
1	A	422	C
1	A	428	G
1	A	429	U
1	A	430	A
1	A	439	A

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Mol	Chain	Res	Type
1	A	445	G
1	A	450	G
1	A	452	A
1	A	455	C
1	A	456	C
1	A	460	A
1	A	461	C
1	A	477	G
1	A	479	C
1	A	481	G
1	A	482	A
1	A	484	G
1	A	485	G
1	A	497	A
1	A	498	U
1	A	499	A
1	A	503	C
1	A	505	G
1	A	509	A
1	A	510	A
1	A	511	C
1	A	513	C
1	A	516	PSU
1	A	517	G
1	A	518	C
1	A	519	C
1	A	531	U
1	A	532	A
1	A	533	A
1	A	547	A
1	A	559	A
1	A	560	U
1	A	564	C
1	A	566	G
1	A	568	G
1	A	571	U
1	A	572	A
1	A	573	A
1	A	576	G
1	A	577	G
1	A	579	G
1	A	581	G

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Mol	Chain	Res	Type
1	A	582	U
1	A	587	G
1	A	588	G
1	A	597	G
1	A	598	U
1	A	609	A
1	A	616	G
1	A	618	C
1	A	645	C
1	A	653	A
1	A	661	G
1	A	665	A
1	A	670	G
1	A	673	G
1	A	686	U
1	A	687	A
1	A	688	G
1	A	697	U
1	A	701	C
1	A	702	A
1	A	718	G
1	A	719	C
1	A	721	G
1	A	722	A
1	A	723	U
1	A	731	G
1	A	748	C
1	A	749	C
1	A	751	U
1	A	755	G
1	A	770	C
1	A	777	A
1	A	781	A
1	A	782	A
1	A	787	A
1	A	792	A
1	A	793	U
1	A	794	A
1	A	813	U
1	A	814	A
1	A	815	A
1	A	817	C

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Mol	Chain	Res	Type
1	A	819	A
1	A	820	U
1	A	821	G
1	A	828	A
1	A	837	G
1	A	839	U
1	A	840	C
1	A	841	U
1	A	848	C
1	A	849	C
1	A	858	G
1	A	859	A
1	A	865	A
1	A	869	G
1	A	872	A
1	A	876	G
1	A	889	A
1	A	895	G
1	A	902	G
1	A	914	A
1	A	917	G
1	A	922	G
1	A	926	G
1	A	927	G
1	A	934	C
1	A	935	A
1	A	939	G
1	A	940	C
1	A	941	G
1	A	942	G
1	A	943	U
1	A	960	U
1	A	961	U
1	A	963	G
1	A	964	A
1	A	966	M2G
1	A	968	A
1	A	969	A
1	A	971	G
1	A	974	A
1	A	975	A
1	A	976	G

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Mol	Chain	Res	Type
1	A	977	A
1	A	981	U
1	A	982	U
1	A	984	C
1	A	989	C
1	A	990	C
1	A	991	U
1	A	992	U
1	A	993	G
1	A	994	A
1	A	1000	U
1	A	1003(A)	G
1	A	1004	A
1	A	1005	A
1	A	1006	C
1	A	1008	C
1	A	1010	G
1	A	1011	G
1	A	1016	A
1	A	1018	C
1	A	1020	U
1	A	1023	G
1	A	1024	G
1	A	1025	U
1	A	1026	G
1	A	1027	C
1	A	1030(B)	C
1	A	1031	G
1	A	1044	A
1	A	1045	C
1	A	1046	A
1	A	1052	U
1	A	1054	C
1	A	1055	A
1	A	1060	C
1	A	1061	G
1	A	1065	U
1	A	1066	C
1	A	1068	G
1	A	1073	U
1	A	1078	U
1	A	1085	U

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Mol	Chain	Res	Type
1	A	1090	U
1	A	1092	A
1	A	1094	G
1	A	1095	U
1	A	1101	A
1	A	1120	G
1	A	1122	U
1	A	1123	A
1	A	1125	U
1	A	1126	U
1	A	1127	G
1	A	1128	C
1	A	1129	C
1	A	1130	A
1	A	1136	U
1	A	1137	C
1	A	1138	G
1	A	1139	G
1	A	1140	C
1	A	1146	A
1	A	1152	A
1	A	1154	G
1	A	1159	U
1	A	1160	G
1	A	1167	A
1	A	1168	A
1	A	1169	A
1	A	1171	G
1	A	1174	G
1	A	1178	G
1	A	1181	G
1	A	1183	A
1	A	1184	G
1	A	1185	G
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

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Mol	Chain	Res	Type
1	A	1202	G
1	A	1206	G
1	A	1207	2MG
1	A	1212	U
1	A	1214	C
1	A	1215	G
1	A	1224	G
1	A	1225	A
1	A	1227	A
1	A	1238	A
1	A	1241	G
1	A	1245	A
1	A	1250	A
1	A	1251	A
1	A	1256	A
1	A	1257	U
1	A	1258	G
1	A	1260	C
1	A	1270	C
1	A	1277	C
1	A	1278	U
1	A	1279	A
1	A	1280	A
1	A	1281	U
1	A	1282	C
1	A	1286	A
1	A	1287	A
1	A	1297	C
1	A	1298	C
1	A	1300	G
1	A	1301	U
1	A	1302	U
1	A	1303	C
1	A	1304	G
1	A	1305	G
1	A	1306	A
1	A	1307	U
1	A	1310	G
1	A	1312	G
1	A	1315	U
1	A	1319	A
1	A	1320	C

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Mol	Chain	Res	Type
1	A	1322	C
1	A	1326	C
1	A	1335	C
1	A	1336	C
1	A	1338	G
1	A	1339	A
1	A	1340	A
1	A	1346	A
1	A	1347	G
1	A	1348	U
1	A	1351	U
1	A	1353	G
1	A	1359	C
1	A	1362	C
1	A	1364	U
1	A	1370	G
1	A	1379	G
1	A	1381	U
1	A	1398	A
1	A	1399	C
1	A	1400	5MC
1	A	1401	G
1	A	1411	C
1	A	1419	G
1	A	1437	C
1	A	1440	C
1	A	1441	G
1	A	1442	G
1	A	1443	G
1	A	1446	A
1	A	1447	G
1	A	1451	A
1	A	1452	C
1	A	1453	G
1	A	1454	G
1	A	1485	U
1	A	1487	G
1	A	1493	A
1	A	1494	G
1	A	1496	C
1	A	1497	G
1	A	1498	UR3

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Mol	Chain	Res	Type
1	A	1499	A
1	A	1500	A
1	A	1501	C
1	A	1502	A
1	A	1504	G
1	A	1505	G
1	A	1506	U
1	A	1509	C
1	A	1518	MA6
1	A	1519	MA6
1	A	1520	G
1	A	1529	G
1	A	1530	G
1	A	1531	A
1	A	1533	C
1	A	1542	U

All (57) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	5	U
1	A	91	C
1	A	115	G
1	A	129(A)	G
1	A	150	C
1	A	160	A
1	A	181	G
1	A	202	U
1	A	203	U
1	A	204	U
1	A	243	A
1	A	246	A
1	A	250	A
1	A	251	G
1	A	329	A
1	A	350	G
1	A	372	C
1	A	428	G
1	A	429	U
1	A	484	G
1	A	509	A
1	A	518	C

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Mol	Chain	Res	Type
1	A	532	A
1	A	559	A
1	A	686	U
1	A	687	A
1	A	701	C
1	A	718	G
1	A	733	A
1	A	748	C
1	A	777	A
1	A	792	A
1	A	812	C
1	A	819	A
1	A	913	A
1	A	960	U
1	A	975	A
1	A	992	U
1	A	1004	A
1	A	1065	U
1	A	1067	A
1	A	1139	G
1	A	1145	C
1	A	1190	G
1	A	1196	U
1	A	1201	A
1	A	1256	A
1	A	1257	U
1	A	1279	A
1	A	1285	A
1	A	1300	G
1	A	1305	G
1	A	1346	A
1	A	1347	G
1	A	1358	U
1	A	1380	U
1	A	1505	G

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

15 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	1518	1	23,26,27	2.56	12 (52%)	33,38,41	1.79	11 (33%)
1	5MC	A	1400	1	19,22,23	1.51	1 (5%)	26,32,35	1.30	4 (15%)
1	PSU	A	1540	1	18,21,22	1.06	1 (5%)	21,30,33	1.55	4 (19%)
1	UR3	A	1498	1	19,22,23	2.02	7 (36%)	26,32,35	1.20	2 (7%)
1	7MG	A	527	1	23,26,27	3.89	5 (21%)	27,39,42	2.64	9 (33%)
1	MA6	A	1519	1	23,26,27	3.11	10 (43%)	33,38,41	1.09	3 (9%)
1	PSU	A	516	23,1	18,21,22	1.60	3 (16%)	21,30,33	1.54	4 (19%)
1	PSU	A	1541	1	18,21,22	1.28	1 (5%)	21,30,33	1.75	5 (23%)
12	0TD	L	92	12	8,9,10	4.17	1 (12%)	6,11,13	3.80	3 (50%)
1	5MC	A	1404	1	19,22,23	1.57	2 (10%)	26,32,35	1.10	1 (3%)
1	4OC	A	1402	1	20,23,24	1.47	2 (10%)	25,32,35	0.77	0
1	5MC	A	967	1	19,22,23	1.47	2 (10%)	26,32,35	0.76	0
1	M2G	A	966	1	24,27,28	1.38	4 (16%)	33,40,43	0.99	2 (6%)
1	5MC	A	1407	1	19,22,23	1.99	3 (15%)	26,32,35	1.81	9 (34%)
1	2MG	A	1207	1	23,26,27	1.53	4 (17%)	33,38,41	1.27	3 (9%)

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	1518	1	-	2/11/29/30	0/3/3/3
1	5MC	A	1400	1	-	2/7/25/26	0/2/2/2
1	PSU	A	1540	1	-	0/7/25/26	0/2/2/2
1	UR3	A	1498	1	-	2/7/25/26	0/2/2/2
1	7MG	A	527	1	-	2/7/37/38	0/3/3/3
1	MA6	A	1519	1	-	6/11/29/30	0/3/3/3
1	PSU	A	516	23,1	-	2/7/25/26	0/2/2/2
1	PSU	A	1541	1	-	0/7/25/26	0/2/2/2
12	0TD	L	92	12	-	3/7/12/14	-
1	5MC	A	1404	1	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	4OC	A	1402	1	-	3/9/29/30	0/2/2/2
1	5MC	A	967	1	-	1/7/25/26	0/2/2/2
1	M2G	A	966	1	-	5/11/29/30	0/3/3/3
1	5MC	A	1407	1	-	0/7/25/26	0/2/2/2
1	2MG	A	1207	1	-	2/9/27/28	0/3/3/3

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	527	7MG	C8-N9	-15.63	1.35	1.45
12	L	92	0TD	CB-CA	-11.29	1.51	1.54
1	A	1519	MA6	C4-N3	7.21	1.47	1.34
1	A	527	7MG	C5-N7	6.55	1.43	1.35
1	A	1519	MA6	C5-N7	6.16	1.50	1.39
1	A	1519	MA6	C6-N1	6.04	1.45	1.34
1	A	1518	MA6	C8-N9	5.88	1.47	1.37
1	A	1407	5MC	C5-C4	5.75	1.48	1.44
1	A	516	PSU	C6-C5	5.37	1.41	1.35
1	A	1400	5MC	C2-N1	5.22	1.51	1.40
1	A	1519	MA6	C8-N9	5.18	1.46	1.37
1	A	1498	UR3	C6-N1	-5.08	1.26	1.38
1	A	1407	5MC	C2-N1	5.07	1.50	1.40
1	A	1402	4OC	C2-N3	4.90	1.46	1.36
1	A	967	5MC	C5-C4	-4.90	1.40	1.44
1	A	527	7MG	C2-N2	4.84	1.45	1.34
1	A	1518	MA6	C5-C4	4.79	1.47	1.39
1	A	1518	MA6	C2-N1	4.67	1.42	1.33
1	A	1541	PSU	C6-C5	4.60	1.40	1.35
1	A	1519	MA6	C5-C4	4.50	1.47	1.39
1	A	1498	UR3	C4-N3	-4.35	1.31	1.40
1	A	1404	5MC	C2-N1	4.27	1.49	1.40
1	A	1404	5MC	C2-N3	3.96	1.44	1.36
1	A	1518	MA6	C5-N7	3.91	1.46	1.39
1	A	1207	2MG	C2-N1	3.81	1.42	1.36
1	A	1540	PSU	C6-C5	3.65	1.39	1.35
1	A	1518	MA6	C5-C6	3.55	1.50	1.41
1	A	966	M2G	C4-N3	3.52	1.42	1.34
1	A	1498	UR3	C2-N1	-3.20	1.34	1.38
1	A	1207	2MG	C8-N9	3.19	1.44	1.37
1	A	1519	MA6	C5-C6	3.14	1.49	1.41
1	A	527	7MG	O6-C6	-3.12	1.17	1.23
1	A	1519	MA6	C2-N1	3.11	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1518	MA6	C9-N6	3.08	1.52	1.45
1	A	966	M2G	C8-N9	2.94	1.44	1.37
1	A	1519	MA6	C9-N6	2.93	1.52	1.45
1	A	1207	2MG	C6-N1	2.92	1.44	1.38
1	A	516	PSU	C2-N1	2.77	1.40	1.36
1	A	1207	2MG	C2-N2	2.76	1.39	1.33
1	A	1402	4OC	CM4-N4	2.75	1.50	1.45
1	A	527	7MG	C4-N3	2.70	1.40	1.34
1	A	966	M2G	C4-N9	2.66	1.44	1.38
1	A	1518	MA6	C8-N7	2.43	1.36	1.31
1	A	1518	MA6	C6-N6	2.43	1.43	1.36
1	A	1519	MA6	C4-N9	2.42	1.42	1.37
1	A	1498	UR3	C1'-N1	-2.36	1.40	1.47
1	A	1407	5MC	O2-C2	-2.28	1.19	1.23
1	A	1498	UR3	C3U-N3	-2.24	1.43	1.47
1	A	1518	MA6	C4-N9	-2.23	1.33	1.37
1	A	516	PSU	O4'-C1'	-2.18	1.40	1.43
1	A	966	M2G	C2-N2	2.17	1.39	1.35
1	A	1518	MA6	C4-N3	2.16	1.38	1.34
1	A	1518	MA6	C10-N6	2.15	1.50	1.45
1	A	1518	MA6	C6-N1	2.13	1.38	1.34
1	A	1498	UR3	C5-C4	-2.09	1.38	1.43
1	A	967	5MC	C2-N3	2.09	1.40	1.36
1	A	1498	UR3	O3'-C3'	2.08	1.48	1.43
1	A	1519	MA6	C8-N7	2.02	1.35	1.31

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	527	7MG	C5-C6-N1	6.86	123.00	110.94
12	L	92	0TD	CSB-SB-CB	-6.54	90.61	102.36
12	L	92	0TD	CB-CA-N	-5.16	98.64	109.10
1	A	527	7MG	C2-N3-C4	5.14	121.16	112.30
1	A	527	7MG	C6-C5-N7	4.33	138.65	131.93
1	A	1518	MA6	C4-N9-C1'	-4.30	116.57	126.63
1	A	527	7MG	C6-C5-C4	-4.18	115.04	122.40
1	A	1541	PSU	N1-C2-N3	4.08	119.47	115.17
1	A	1407	5MC	C1'-N1-C6	-4.08	114.44	121.15
1	A	527	7MG	N9-C4-N3	4.03	131.37	125.46
1	A	527	7MG	C5-C4-N3	-3.96	120.70	128.13
1	A	1541	PSU	C4-N3-C2	-3.76	121.19	126.37
1	A	527	7MG	C2-N1-C6	-3.71	118.39	125.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1541	PSU	O2-C2-N1	-3.68	118.99	122.79
1	A	516	PSU	N1-C2-N3	3.66	119.03	115.17
1	A	1518	MA6	N1-C6-N6	-3.64	112.42	116.86
1	A	1518	MA6	C1'-N9-C8	3.56	135.00	127.09
1	A	1400	5MC	C5-C4-N3	3.45	125.30	121.75
1	A	1207	2MG	N2-C2-N3	-3.42	116.15	120.51
1	A	1540	PSU	O2-C2-N1	-3.41	119.27	122.79
1	A	1540	PSU	N1-C2-N3	3.32	118.67	115.17
1	A	1540	PSU	C4-N3-C2	-3.32	121.80	126.37
12	L	92	0TD	OD1-CG-CB	-3.19	115.76	122.44
1	A	527	7MG	N9-C8-N7	3.18	107.87	103.37
1	A	516	PSU	C4-N3-C2	-3.15	122.03	126.37
1	A	1407	5MC	C1'-N1-C2	3.07	125.22	118.44
1	A	1541	PSU	C6-N1-C2	-3.06	119.86	122.69
1	A	1404	5MC	C1'-N1-C6	-2.98	116.24	121.15
1	A	1407	5MC	C5-C4-N3	2.97	124.80	121.75
1	A	1407	5MC	C4-N3-C2	-2.96	116.70	120.81
1	A	516	PSU	C6-N1-C2	-2.95	119.95	122.69
1	A	527	7MG	O6-C6-C5	-2.94	120.41	127.62
1	A	1407	5MC	N4-C4-N3	-2.93	113.20	118.51
1	A	1400	5MC	N4-C4-N3	-2.84	113.37	118.51
1	A	1407	5MC	CM5-C5-C6	-2.82	119.03	122.85
1	A	1518	MA6	C5-C6-N6	2.79	129.74	125.33
1	A	1407	5MC	O2-C2-N3	-2.74	118.02	122.33
1	A	966	M2G	C5-C4-N3	-2.70	124.09	128.39
1	A	1207	2MG	C2-N1-C6	-2.70	121.29	124.55
1	A	1518	MA6	C6-C5-N7	2.68	137.71	133.43
1	A	1519	MA6	C2-N1-C6	2.53	118.01	111.83
1	A	1518	MA6	C4-C5-N7	-2.52	107.71	110.58
1	A	1518	MA6	C2-N1-C6	2.50	117.94	111.83
1	A	1400	5MC	O2-C2-N1	2.48	123.75	118.90
1	A	1519	MA6	C4-N9-C8	2.42	108.28	105.74
1	A	516	PSU	O2-C2-N3	-2.32	117.75	121.86
1	A	966	M2G	N9-C4-N3	2.27	130.50	125.95
1	A	1207	2MG	C5-C4-N3	-2.24	124.83	128.39
1	A	1407	5MC	O2-C2-N1	2.18	123.16	118.90
1	A	1400	5MC	O2-C2-N3	-2.15	118.94	122.33
1	A	1519	MA6	C4-N9-C1'	-2.14	121.63	126.63
1	A	1518	MA6	C5-C4-N9	2.14	108.14	105.81
1	A	1518	MA6	N9-C8-N7	-2.13	110.91	113.94
1	A	1518	MA6	C4-N9-C8	2.13	107.97	105.74
1	A	1541	PSU	O4'-C1'-C2'	2.11	108.07	105.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1540	PSU	C6-N1-C2	-2.08	120.76	122.69
1	A	1518	MA6	N1-C2-N3	2.07	131.72	128.58
1	A	1407	5MC	CM5-C5-C4	2.07	123.91	120.51
1	A	1498	UR3	C6-C5-C4	2.07	124.69	120.73
1	A	1498	UR3	C5-C4-N3	-2.01	112.38	115.04

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	966	M2G	N1-C2-N2-CM1
1	A	966	M2G	N3-C2-N2-CM1
1	A	966	M2G	N3-C2-N2-CM2
1	A	1207	2MG	O4'-C4'-C5'-O5'
1	A	1519	MA6	O4'-C4'-C5'-O5'
1	A	1519	MA6	C3'-C4'-C5'-O5'
1	A	1519	MA6	C5-C6-N6-C9
1	A	1519	MA6	C5-C6-N6-C10
1	A	1519	MA6	N1-C6-N6-C9
1	A	1519	MA6	N1-C6-N6-C10
1	A	516	PSU	O4'-C4'-C5'-O5'
1	A	1207	2MG	C3'-C4'-C5'-O5'
1	A	1400	5MC	O4'-C4'-C5'-O5'
1	A	1518	MA6	O4'-C4'-C5'-O5'
1	A	527	7MG	O4'-C4'-C5'-O5'
1	A	527	7MG	C3'-C4'-C5'-O5'
1	A	1400	5MC	C3'-C4'-C5'-O5'
1	A	516	PSU	C3'-C4'-C5'-O5'
1	A	1518	MA6	C3'-C4'-C5'-O5'
1	A	966	M2G	N1-C2-N2-CM2
1	A	1402	4OC	C3'-C4'-C5'-O5'
1	A	1498	UR3	O4'-C4'-C5'-O5'
1	A	1402	4OC	O4'-C4'-C5'-O5'
1	A	1404	5MC	C3'-C4'-C5'-O5'
12	L	92	0TD	CG-CB-SB-CSB
12	L	92	0TD	SB-CB-CG-OD1
1	A	1404	5MC	O4'-C4'-C5'-O5'
1	A	966	M2G	C4'-C5'-O5'-P
1	A	1498	UR3	C3'-C4'-C5'-O5'
1	A	967	5MC	O4'-C4'-C5'-O5'
12	L	92	0TD	SB-CB-CG-OD2
1	A	1402	4OC	C2'-C1'-N1-C2

There are no ring outliers.

12 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1518	MA6	2	0
1	A	1400	5MC	4	0
1	A	1540	PSU	2	0
1	A	1498	UR3	3	0
1	A	527	7MG	2	0
1	A	1519	MA6	4	0
12	L	92	0TD	3	0
1	A	1404	5MC	3	0
1	A	1402	4OC	1	0
1	A	967	5MC	4	0
1	A	966	M2G	4	0
1	A	1207	2MG	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 270 ligands modelled in this entry, 269 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
22	SRY	A	1601	-	40,42,42	2.35	9 (22%)	49,63,63	2.17	17 (34%)

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
22	SRY	A	1601	-	-	1/20/87/87	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	1601	SRY	CD1-N31	8.89	1.48	1.33
22	A	1601	SRY	CA1-N11	7.07	1.45	1.33
22	A	1601	SRY	O53-C53	-3.32	1.36	1.44
22	A	1601	SRY	CA1-NB1	3.21	1.46	1.34
22	A	1601	SRY	C23-N23	-3.12	1.42	1.47
22	A	1601	SRY	O32-C32	-2.74	1.40	1.44
22	A	1601	SRY	CD1-NE1	2.73	1.44	1.34
22	A	1601	SRY	O51-C51	-2.40	1.37	1.43
22	A	1601	SRY	C21-C11	-2.33	1.48	1.53

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1601	SRY	C12-O42-C42	-7.34	96.63	108.48
22	A	1601	SRY	C13-O53-C53	-4.33	105.25	113.72
22	A	1601	SRY	C61-C11-N11	-3.92	103.40	110.62
22	A	1601	SRY	C13-O13-C22	-3.67	110.01	116.26
22	A	1601	SRY	C33-C43-C53	-3.35	104.16	110.23
22	A	1601	SRY	O13-C13-C23	3.23	113.32	108.07
22	A	1601	SRY	O42-C12-C22	-3.16	103.92	107.31
22	A	1601	SRY	CI3-N23-C23	-3.14	110.17	114.23
22	A	1601	SRY	O41-C41-C51	3.00	114.85	107.23
22	A	1601	SRY	C63-C53-C43	2.55	119.28	113.02
22	A	1601	SRY	C43-C33-C23	-2.53	106.72	110.40
22	A	1601	SRY	O33-C33-C23	2.51	114.58	109.58
22	A	1601	SRY	O42-C42-CH2	2.46	115.04	110.17
22	A	1601	SRY	O13-C13-O53	-2.40	104.37	110.69
22	A	1601	SRY	O13-C22-C32	2.27	116.81	111.79
22	A	1601	SRY	O43-C43-C53	2.20	114.75	109.32
22	A	1601	SRY	C11-N11-CA1	-2.20	119.03	123.39

There are no chirality outliers.

All (1) torsion outliers are listed below:

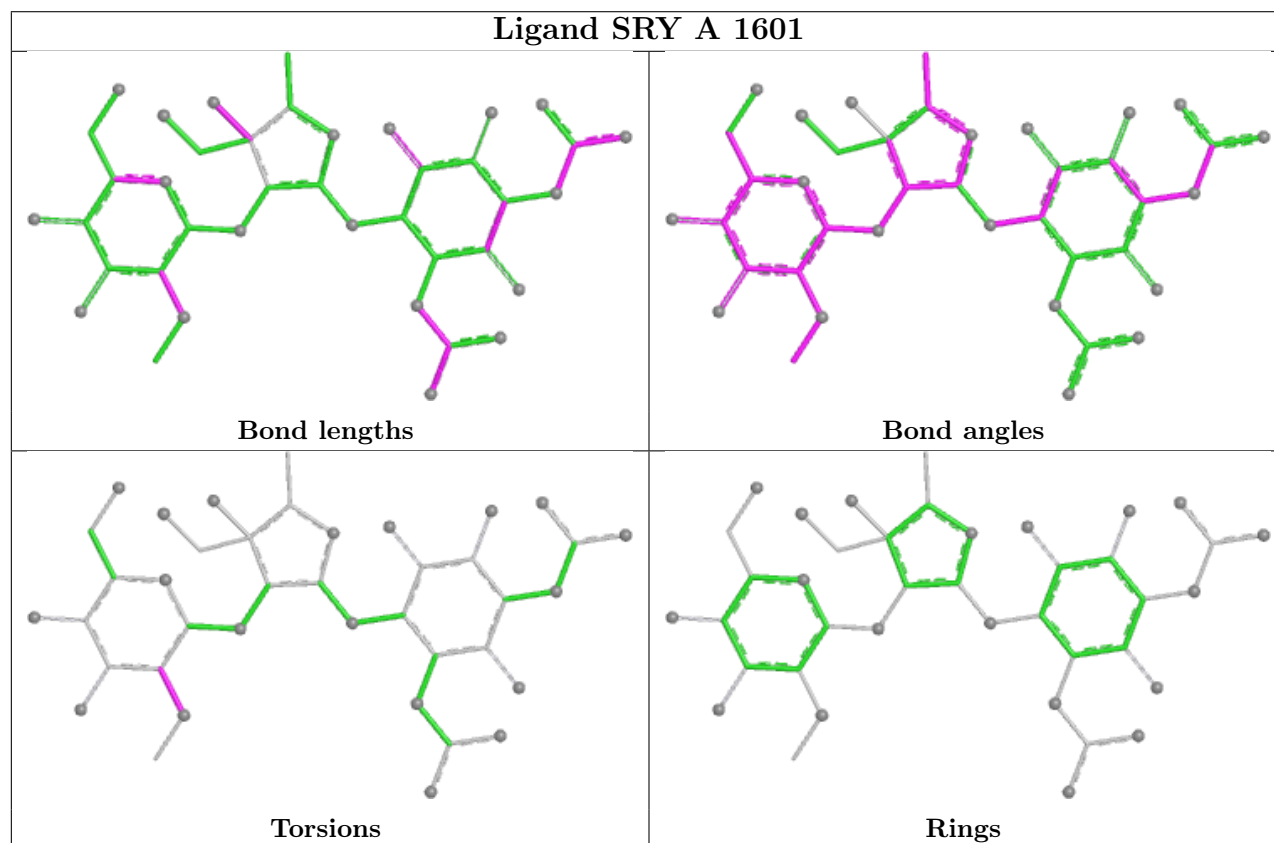
Mol	Chain	Res	Type	Atoms
22	A	1601	SRY	C13-C23-N23-CI3

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A	1601	SRY	6	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1498/1522 (98%)	-0.48	12 (0%) 82 59	91, 154, 301, 391	0
2	B	234/256 (91%)	-0.55	1 (0%) 88 71	125, 174, 266, 283	0
3	C	206/239 (86%)	-0.31	0 100 100	181, 240, 279, 300	0
4	D	208/209 (99%)	-0.34	4 (1%) 66 40	112, 159, 214, 231	0
5	E	150/162 (92%)	-0.70	0 100 100	80, 126, 173, 210	0
6	F	101/101 (100%)	-0.56	0 100 100	123, 174, 206, 235	0
7	G	155/156 (99%)	-0.40	0 100 100	151, 198, 247, 296	0
8	H	138/138 (100%)	-0.80	0 100 100	81, 110, 145, 193	0
9	I	127/128 (99%)	-0.25	3 (2%) 59 35	154, 229, 263, 300	0
10	J	98/105 (93%)	-0.25	0 100 100	217, 246, 300, 348	0
11	K	116/129 (89%)	-0.61	1 (0%) 81 57	117, 150, 194, 234	0
12	L	123/135 (91%)	-0.40	2 (1%) 70 43	87, 145, 186, 245	0
13	M	118/126 (93%)	-0.35	0 100 100	136, 183, 220, 242	0
14	N	60/61 (98%)	0.03	2 (3%) 49 29	184, 226, 269, 294	0
15	O	87/89 (97%)	-0.69	0 100 100	87, 137, 178, 199	0
16	P	83/88 (94%)	-0.39	0 100 100	117, 152, 181, 207	0
17	Q	99/105 (94%)	-0.62	0 100 100	89, 128, 163, 183	0
18	R	70/88 (79%)	-0.67	0 100 100	113, 150, 199, 218	0
19	S	80/93 (86%)	-0.13	3 (3%) 44 27	180, 242, 278, 303	0
20	T	99/106 (93%)	-0.25	1 (1%) 79 54	117, 155, 206, 236	0
21	U	24/27 (88%)	0.26	1 (4%) 40 24	154, 205, 230, 236	0
All	All	3874/4063 (95%)	-0.46	30 (0%) 82 59	80, 165, 269, 391	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
20	T	106	ALA	6.5
4	D	2	GLY	4.9
1	A	985	C	4.5
1	A	984	C	3.8
12	L	115	LYS	3.5
19	S	35	SER	3.2
4	D	9	CYS	3.2
4	D	31	CYS	3.2
14	N	25	VAL	3.1
1	A	793	U	3.1
1	A	1129	C	3.0
1	A	202	U	2.9
19	S	3	ARG	2.8
9	I	128	ARG	2.8
19	S	34	TRP	2.8
14	N	2	ALA	2.6
9	I	90	PRO	2.6
21	U	6	ARG	2.5
1	A	1220	G	2.5
1	A	1222	G	2.4
12	L	73	GLU	2.4
11	K	51	LYS	2.4
1	A	532	A	2.3
4	D	26	CYS	2.3
1	A	91	C	2.3
1	A	80	G	2.3
1	A	92	C	2.2
9	I	127	LYS	2.1
1	A	792	A	2.1
2	B	214	ILE	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	PSU	A	1541	20/21	0.64	0.12	257,268,323,323	0
1	PSU	A	1540	20/21	0.84	0.14	251,258,331,332	0
1	MA6	A	1518	24/25	0.87	0.11	138,166,194,200	0
1	MA6	A	1519	24/25	0.92	0.11	126,149,157,161	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	UR3	A	1498	21/22	0.93	0.17	130,151,177,185	0
1	5MC	A	1407	21/22	0.95	0.08	163,173,184,184	0
1	PSU	A	516	20/21	0.95	0.07	126,162,186,188	0
1	2MG	A	1207	24/25	0.96	0.13	233,253,259,266	0
1	5MC	A	1400	21/22	0.96	0.07	123,161,167,168	0
1	5MC	A	1404	21/22	0.96	0.09	140,150,159,171	0
1	4OC	A	1402	22/23	0.97	0.09	130,148,159,165	0
1	M2G	A	966	25/26	0.97	0.07	141,169,180,185	0
1	7MG	A	527	24/25	0.98	0.07	118,132,143,146	0
1	5MC	A	967	21/22	0.99	0.05	145,164,179,184	0
12	0TD	L	92	10/11	0.99	0.09	111,148,156,269	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	MG	A	1624	1/1	0.34	0.30	214,214,214,214	0
23	MG	A	1850	1/1	0.57	0.08	314,314,314,314	0
23	MG	A	1797	1/1	0.59	0.26	140,140,140,140	0
23	MG	A	1657	1/1	0.64	0.18	177,177,177,177	0
23	MG	B	301	1/1	0.66	0.18	159,159,159,159	0
23	MG	S	101	1/1	0.66	0.39	130,130,130,130	0
23	MG	A	1776	1/1	0.67	0.17	135,135,135,135	0
23	MG	A	1793	1/1	0.67	0.22	139,139,139,139	0
23	MG	A	1696	1/1	0.69	0.35	138,138,138,138	0
23	MG	A	1661	1/1	0.71	0.69	118,118,118,118	0
23	MG	A	1741	1/1	0.72	0.32	105,105,105,105	0
23	MG	A	1794	1/1	0.72	0.61	117,117,117,117	0
23	MG	A	1665	1/1	0.72	0.12	247,247,247,247	0
23	MG	A	1762	1/1	0.73	0.31	172,172,172,172	0
23	MG	A	1782	1/1	0.73	0.28	123,123,123,123	0
23	MG	A	1785	1/1	0.73	0.19	137,137,137,137	0
23	MG	A	1791	1/1	0.75	0.35	138,138,138,138	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	MG	A	1750	1/1	0.76	0.11	158,158,158,158	0
23	MG	A	1684	1/1	0.76	0.17	242,242,242,242	0
23	MG	J	201	1/1	0.76	0.16	128,128,128,128	0
23	MG	A	1743	1/1	0.76	0.28	129,129,129,129	0
23	MG	A	1679	1/1	0.77	0.31	125,125,125,125	0
23	MG	A	1742	1/1	0.80	0.25	151,151,151,151	0
23	MG	A	1763	1/1	0.80	0.19	290,290,290,290	0
23	MG	A	1783	1/1	0.80	0.32	91,91,91,91	0
23	MG	A	1747	1/1	0.81	0.35	104,104,104,104	0
23	MG	A	1704	1/1	0.81	0.10	97,97,97,97	0
23	MG	A	1758	1/1	0.81	0.26	106,106,106,106	0
23	MG	A	1697	1/1	0.81	0.10	260,260,260,260	0
23	MG	A	1796	1/1	0.81	0.16	137,137,137,137	0
23	MG	A	1769	1/1	0.82	0.42	157,157,157,157	0
23	MG	A	1716	1/1	0.83	0.16	111,111,111,111	0
23	MG	A	1764	1/1	0.83	0.15	122,122,122,122	0
23	MG	B	302	1/1	0.83	0.09	112,112,112,112	0
23	MG	A	1733	1/1	0.83	0.60	124,124,124,124	0
23	MG	M	201	1/1	0.83	0.27	139,139,139,139	0
23	MG	A	1602	1/1	0.83	0.18	198,198,198,198	0
23	MG	A	1660	1/1	0.84	0.10	211,211,211,211	0
23	MG	A	1755	1/1	0.84	0.15	122,122,122,122	0
23	MG	A	1819	1/1	0.84	0.14	309,309,309,309	0
23	MG	A	1799	1/1	0.85	0.24	117,117,117,117	0
23	MG	A	1737	1/1	0.85	0.11	158,158,158,158	0
23	MG	A	1746	1/1	0.85	0.09	145,145,145,145	0
23	MG	A	1774	1/1	0.85	0.08	496,496,496,496	0
23	MG	A	1618	1/1	0.86	0.14	139,139,139,139	0
23	MG	A	1706	1/1	0.86	0.78	167,167,167,167	0
23	MG	A	1789	1/1	0.86	0.16	137,137,137,137	0
23	MG	Q	201	1/1	0.86	0.17	118,118,118,118	0
23	MG	A	1710	1/1	0.86	0.23	98,98,98,98	0
23	MG	P	102	1/1	0.87	0.12	115,115,115,115	0
23	MG	A	1671	1/1	0.87	0.15	135,135,135,135	0
23	MG	A	1695	1/1	0.87	0.11	146,146,146,146	0
23	MG	A	1714	1/1	0.88	0.13	112,112,112,112	0
23	MG	A	1659	1/1	0.88	0.05	154,154,154,154	0
23	MG	A	1607	1/1	0.88	0.07	183,183,183,183	0
23	MG	A	1757	1/1	0.88	0.59	122,122,122,122	0
23	MG	A	1744	1/1	0.88	0.54	115,115,115,115	0
23	MG	A	1668	1/1	0.88	0.31	191,191,191,191	0
23	MG	A	1772	1/1	0.89	0.11	243,243,243,243	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	MG	A	1667	1/1	0.89	0.26	114,114,114,114	0
23	MG	A	1740	1/1	0.89	0.20	112,112,112,112	0
23	MG	A	1779	1/1	0.89	0.52	119,119,119,119	0
23	MG	A	1795	1/1	0.89	0.23	127,127,127,127	0
23	MG	A	1727	1/1	0.89	0.23	116,116,116,116	0
23	MG	A	1765	1/1	0.89	0.17	139,139,139,139	0
23	MG	A	1707	1/1	0.89	0.23	117,117,117,117	0
23	MG	A	1811	1/1	0.89	0.15	226,226,226,226	0
23	MG	A	1673	1/1	0.90	0.24	99,99,99,99	0
23	MG	A	1817	1/1	0.90	0.12	354,354,354,354	0
23	MG	A	1788	1/1	0.90	0.17	112,112,112,112	0
23	MG	A	1821	1/1	0.90	0.12	315,315,315,315	0
23	MG	A	1833	1/1	0.90	0.10	189,189,189,189	0
23	MG	A	1620	1/1	0.90	0.09	166,166,166,166	0
23	MG	A	1756	1/1	0.90	0.10	120,120,120,120	0
23	MG	A	1718	1/1	0.90	0.18	145,145,145,145	0
23	MG	H	204	1/1	0.90	0.17	125,125,125,125	0
23	MG	A	1651	1/1	0.90	0.10	144,144,144,144	0
23	MG	A	1777	1/1	0.90	0.05	132,132,132,132	0
23	MG	A	1732	1/1	0.90	0.46	101,101,101,101	0
23	MG	A	1698	1/1	0.90	0.18	115,115,115,115	0
23	MG	Q	202	1/1	0.90	0.10	89,89,89,89	0
23	MG	A	1713	1/1	0.90	0.46	110,110,110,110	0
23	MG	A	1724	1/1	0.91	0.20	128,128,128,128	0
23	MG	A	1652	1/1	0.91	0.26	126,126,126,126	0
23	MG	A	1700	1/1	0.91	0.11	144,144,144,144	0
23	MG	A	1800	1/1	0.91	0.09	105,105,105,105	0
23	MG	A	1801	1/1	0.91	0.18	105,105,105,105	0
23	MG	A	1787	1/1	0.92	0.11	145,145,145,145	0
23	MG	A	1729	1/1	0.92	0.26	162,162,162,162	0
23	MG	A	1670	1/1	0.92	0.22	130,130,130,130	0
23	MG	A	1822	1/1	0.92	0.12	265,265,265,265	0
23	MG	A	1771	1/1	0.92	0.05	348,348,348,348	0
23	MG	A	1705	1/1	0.92	0.14	127,127,127,127	0
23	MG	A	1681	1/1	0.92	0.09	226,226,226,226	0
23	MG	A	1739	1/1	0.92	0.21	117,117,117,117	0
23	MG	D	302	1/1	0.92	0.16	124,124,124,124	0
23	MG	A	1639	1/1	0.92	0.10	139,139,139,139	0
23	MG	A	1720	1/1	0.92	0.21	115,115,115,115	0
23	MG	A	1798	1/1	0.92	0.11	131,131,131,131	0
23	MG	M	202	1/1	0.92	0.12	137,137,137,137	0
23	MG	A	1722	1/1	0.92	0.12	117,117,117,117	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	MG	A	1708	1/1	0.92	0.21	115,115,115,115	0
23	MG	A	1784	1/1	0.92	0.28	125,125,125,125	0
23	MG	A	1615	1/1	0.92	0.08	121,121,121,121	0
23	MG	A	1654	1/1	0.93	0.25	176,176,176,176	0
23	MG	A	1835	1/1	0.93	0.08	166,166,166,166	0
23	MG	A	1844	1/1	0.93	0.12	199,199,199,199	0
23	MG	A	1846	1/1	0.93	0.14	228,228,228,228	0
23	MG	A	1632	1/1	0.93	0.15	103,103,103,103	0
23	MG	A	1662	1/1	0.93	0.12	148,148,148,148	0
23	MG	A	1786	1/1	0.93	0.15	155,155,155,155	0
23	MG	A	1725	1/1	0.93	0.12	89,89,89,89	0
23	MG	A	1775	1/1	0.93	0.15	135,135,135,135	0
23	MG	A	1803	1/1	0.93	0.32	103,103,103,103	0
23	MG	A	1809	1/1	0.93	0.11	118,118,118,118	0
23	MG	A	1644	1/1	0.93	0.22	127,127,127,127	0
23	MG	A	1748	1/1	0.93	0.33	144,144,144,144	0
23	MG	A	1778	1/1	0.93	0.16	180,180,180,180	0
23	MG	A	1686	1/1	0.93	0.10	184,184,184,184	0
23	MG	A	1752	1/1	0.93	0.06	148,148,148,148	0
23	MG	A	1701	1/1	0.94	0.24	133,133,133,133	0
23	MG	A	1719	1/1	0.94	0.27	143,143,143,143	0
23	MG	A	1634	1/1	0.94	0.06	101,101,101,101	0
23	MG	A	1638	1/1	0.94	0.41	136,136,136,136	0
23	MG	A	1658	1/1	0.94	0.15	148,148,148,148	0
23	MG	A	1694	1/1	0.94	0.39	141,141,141,141	0
23	MG	A	1610	1/1	0.94	0.17	106,106,106,106	0
23	MG	A	1766	1/1	0.94	0.07	114,114,114,114	0
23	MG	H	202	1/1	0.94	0.09	83,83,83,83	0
23	MG	A	1802	1/1	0.94	0.10	139,139,139,139	0
23	MG	A	1767	1/1	0.94	0.20	132,132,132,132	0
23	MG	A	1621	1/1	0.94	0.10	109,109,109,109	0
23	MG	A	1616	1/1	0.94	0.20	95,95,95,95	0
23	MG	A	1675	1/1	0.94	0.29	113,113,113,113	0
23	MG	A	1735	1/1	0.94	0.12	112,112,112,112	0
23	MG	A	1792	1/1	0.94	0.16	136,136,136,136	0
23	MG	A	1611	1/1	0.94	0.09	174,174,174,174	0
23	MG	A	1832	1/1	0.95	0.22	148,148,148,148	0
23	MG	A	1643	1/1	0.95	0.08	85,85,85,85	0
23	MG	A	1693	1/1	0.95	0.12	134,134,134,134	0
23	MG	A	1841	1/1	0.95	0.08	274,274,274,274	0
23	MG	A	1612	1/1	0.95	0.10	128,128,128,128	0
23	MG	A	1648	1/1	0.95	0.06	144,144,144,144	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	MG	A	1711	1/1	0.95	0.16	121,121,121,121	0
23	MG	A	1712	1/1	0.95	0.09	128,128,128,128	0
23	MG	A	1613	1/1	0.95	0.16	177,177,177,177	0
23	MG	A	1804	1/1	0.95	0.20	146,146,146,146	0
23	MG	H	201	1/1	0.95	0.10	85,85,85,85	0
23	MG	A	1808	1/1	0.95	0.12	139,139,139,139	0
23	MG	A	1636	1/1	0.95	0.08	167,167,167,167	0
23	MG	A	1676	1/1	0.95	0.18	109,109,109,109	0
23	MG	A	1812	1/1	0.95	0.10	202,202,202,202	0
23	MG	A	1663	1/1	0.95	0.17	141,141,141,141	0
23	MG	P	101	1/1	0.95	0.19	93,93,93,93	0
23	MG	A	1818	1/1	0.95	0.27	423,423,423,423	0
23	MG	A	1623	1/1	0.95	0.08	100,100,100,100	0
23	MG	A	1683	1/1	0.95	0.12	272,272,272,272	0
23	MG	A	1614	1/1	0.95	0.12	94,94,94,94	0
23	MG	A	1768	1/1	0.96	0.15	118,118,118,118	0
23	MG	A	1745	1/1	0.96	0.07	179,179,179,179	0
23	MG	A	1770	1/1	0.96	0.07	215,215,215,215	0
23	MG	A	1666	1/1	0.96	0.21	168,168,168,168	0
23	MG	A	1637	1/1	0.96	0.14	177,177,177,177	0
23	MG	A	1836	1/1	0.96	0.07	201,201,201,201	0
23	MG	A	1625	1/1	0.96	0.33	206,206,206,206	0
23	MG	A	1709	1/1	0.96	0.11	102,102,102,102	0
23	MG	A	1627	1/1	0.96	0.22	130,130,130,130	0
23	MG	A	1848	1/1	0.96	0.07	278,278,278,278	0
23	MG	A	1640	1/1	0.96	0.14	107,107,107,107	0
23	MG	A	1734	1/1	0.96	0.11	145,145,145,145	0
23	MG	A	1629	1/1	0.96	0.10	97,97,97,97	0
23	MG	A	1780	1/1	0.96	0.13	105,105,105,105	0
23	MG	A	1781	1/1	0.96	0.07	101,101,101,101	0
23	MG	A	1609	1/1	0.96	0.14	126,126,126,126	0
23	MG	A	1806	1/1	0.96	0.16	128,128,128,128	0
23	MG	A	1759	1/1	0.96	0.17	161,161,161,161	0
23	MG	A	1647	1/1	0.96	0.10	146,146,146,146	0
23	MG	A	1699	1/1	0.96	0.13	130,130,130,130	0
23	MG	A	1619	1/1	0.96	0.18	150,150,150,150	0
23	MG	A	1813	1/1	0.96	0.18	371,371,371,371	0
23	MG	A	1680	1/1	0.96	0.26	190,190,190,190	0
23	MG	A	1649	1/1	0.96	0.08	206,206,206,206	0
23	MG	A	1604	1/1	0.96	0.26	103,103,103,103	0
23	MG	T	1201	1/1	0.96	0.07	81,81,81,81	0
24	ZN	N	101	1/1	0.96	0.06	395,395,395,395	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	MG	A	1738	1/1	0.97	0.07	112,112,112,112	0
23	MG	A	1664	1/1	0.97	0.18	180,180,180,180	0
23	MG	A	1838	1/1	0.97	0.25	427,427,427,427	0
23	MG	A	1760	1/1	0.97	0.15	139,139,139,139	0
23	MG	A	1688	1/1	0.97	0.10	116,116,116,116	0
23	MG	A	1691	1/1	0.97	0.19	331,331,331,331	0
23	MG	A	1847	1/1	0.97	0.20	418,418,418,418	0
23	MG	A	1641	1/1	0.97	0.13	149,149,149,149	0
23	MG	A	1630	1/1	0.97	0.06	116,116,116,116	0
23	MG	A	1677	1/1	0.97	0.14	149,149,149,149	0
23	MG	A	1626	1/1	0.97	0.15	162,162,162,162	0
23	MG	A	1622	1/1	0.97	0.13	156,156,156,156	0
23	MG	A	1810	1/1	0.97	0.05	190,190,190,190	0
23	MG	A	1731	1/1	0.97	0.16	118,118,118,118	0
23	MG	H	203	1/1	0.97	0.09	111,111,111,111	0
23	MG	A	1669	1/1	0.97	0.08	131,131,131,131	0
23	MG	A	1790	1/1	0.97	0.10	133,133,133,133	0
23	MG	A	1749	1/1	0.97	0.05	142,142,142,142	0
23	MG	A	1656	1/1	0.97	0.09	143,143,143,143	0
23	MG	A	1773	1/1	0.97	0.08	334,334,334,334	0
23	MG	A	1603	1/1	0.97	0.07	135,135,135,135	0
23	MG	A	1715	1/1	0.97	0.14	134,134,134,134	0
23	MG	A	1823	1/1	0.97	0.12	307,307,307,307	0
23	MG	A	1826	1/1	0.97	0.12	366,366,366,366	0
23	MG	A	1736	1/1	0.97	0.05	109,109,109,109	0
23	MG	T	1202	1/1	0.97	0.19	330,330,330,330	0
23	MG	A	1685	1/1	0.97	0.06	127,127,127,127	0
23	MG	A	1642	1/1	0.98	0.04	249,249,249,249	0
23	MG	A	1702	1/1	0.98	0.08	116,116,116,116	0
23	MG	A	1837	1/1	0.98	0.21	350,350,350,350	0
23	MG	A	1703	1/1	0.98	0.09	121,121,121,121	0
23	MG	A	1840	1/1	0.98	0.09	100,100,100,100	0
23	MG	A	1721	1/1	0.98	0.05	98,98,98,98	0
23	MG	A	1843	1/1	0.98	0.11	380,380,380,380	0
23	MG	A	1805	1/1	0.98	0.15	105,105,105,105	0
23	MG	A	1845	1/1	0.98	0.23	341,341,341,341	0
23	MG	A	1672	1/1	0.98	0.10	167,167,167,167	0
23	MG	A	1723	1/1	0.98	0.16	102,102,102,102	0
23	MG	A	1687	1/1	0.98	0.07	114,114,114,114	0
23	MG	A	1849	1/1	0.98	0.10	399,399,399,399	0
23	MG	A	1617	1/1	0.98	0.07	92,92,92,92	0
23	MG	A	1690	1/1	0.98	0.24	138,138,138,138	0

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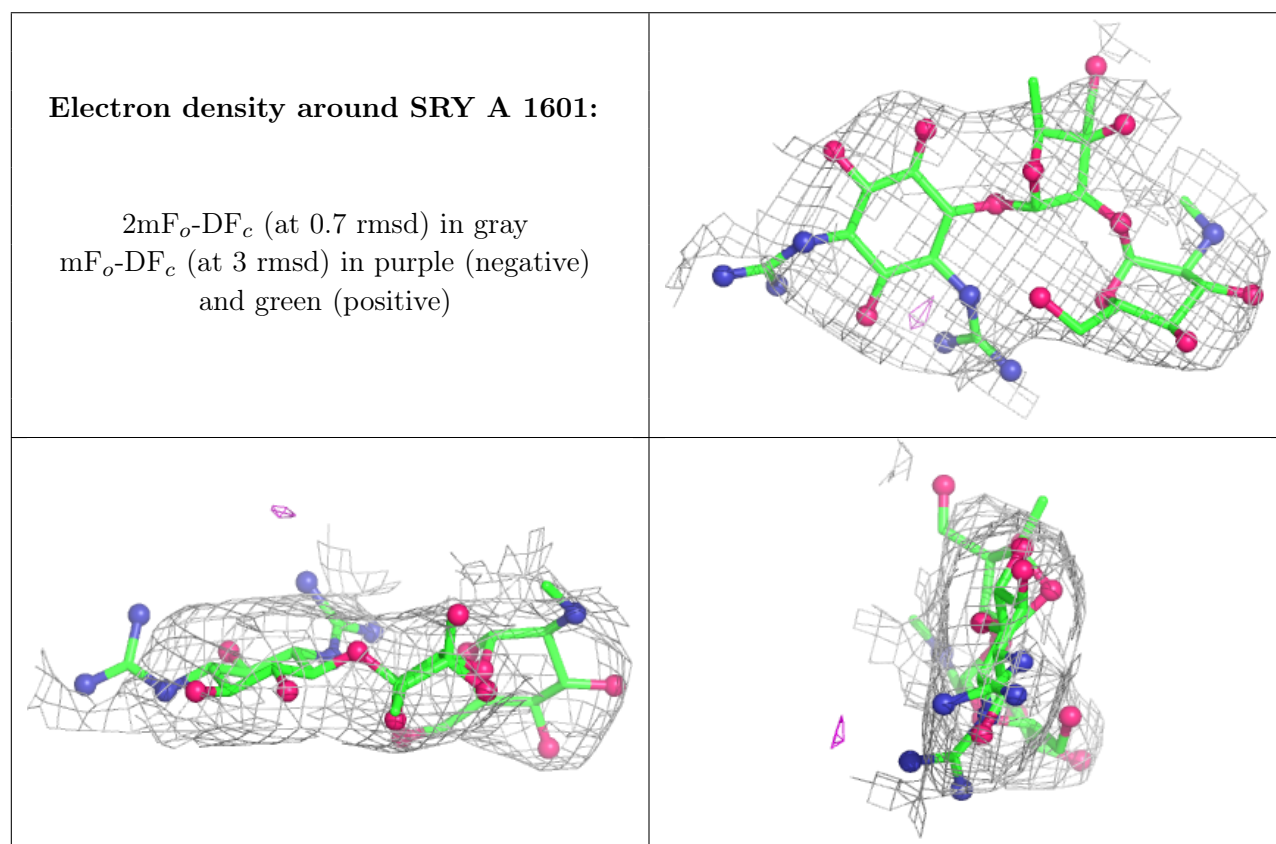
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	MG	A	1653	1/1	0.98	0.07	124,124,124,124	0
23	MG	A	1631	1/1	0.98	0.07	102,102,102,102	0
23	MG	E	201	1/1	0.98	0.03	167,167,167,167	0
23	MG	A	1814	1/1	0.98	0.12	254,254,254,254	0
23	MG	A	1815	1/1	0.98	0.19	406,406,406,406	0
23	MG	A	1655	1/1	0.98	0.18	161,161,161,161	0
23	MG	A	1751	1/1	0.98	0.19	257,257,257,257	0
23	MG	A	1678	1/1	0.98	0.06	146,146,146,146	0
23	MG	A	1754	1/1	0.98	0.06	122,122,122,122	0
23	MG	A	1646	1/1	0.98	0.07	148,148,148,148	0
23	MG	A	1608	1/1	0.98	0.10	112,112,112,112	0
23	MG	A	1824	1/1	0.98	0.13	485,485,485,485	0
23	MG	A	1606	1/1	0.98	0.25	117,117,117,117	0
23	MG	A	1828	1/1	0.98	0.11	409,409,409,409	0
23	MG	A	1829	1/1	0.98	0.07	180,180,180,180	0
22	SRY	A	1601	40/40	0.98	0.06	103,141,162,165	0
23	MG	A	1650	1/1	0.98	0.05	138,138,138,138	0
23	MG	A	1834	1/1	0.98	0.06	204,204,204,204	0
23	MG	A	1827	1/1	0.99	0.06	134,134,134,134	0
23	MG	A	1728	1/1	0.99	0.15	156,156,156,156	0
23	MG	A	1753	1/1	0.99	0.08	265,265,265,265	0
23	MG	A	1830	1/1	0.99	0.09	114,114,114,114	0
23	MG	A	1831	1/1	0.99	0.08	114,114,114,114	0
23	MG	A	1674	1/1	0.99	0.06	113,113,113,113	0
23	MG	A	1730	1/1	0.99	0.13	144,144,144,144	0
23	MG	A	1628	1/1	0.99	0.14	131,131,131,131	0
23	MG	A	1633	1/1	0.99	0.05	91,91,91,91	0
23	MG	A	1682	1/1	0.99	0.08	185,185,185,185	0
23	MG	A	1816	1/1	0.99	0.07	179,179,179,179	0
23	MG	A	1689	1/1	0.99	0.21	336,336,336,336	0
23	MG	A	1605	1/1	0.99	0.06	107,107,107,107	0
23	MG	A	1761	1/1	0.99	0.22	163,163,163,163	0
23	MG	A	1842	1/1	0.99	0.06	159,159,159,159	0
23	MG	A	1645	1/1	0.99	0.11	144,144,144,144	0
23	MG	A	1692	1/1	0.99	0.11	117,117,117,117	0
23	MG	A	1726	1/1	0.99	0.14	121,121,121,121	0
23	MG	A	1807	1/1	0.99	0.08	99,99,99,99	0
23	MG	A	1825	1/1	0.99	0.14	314,314,314,314	0
24	ZN	D	301	1/1	0.99	0.18	125,125,125,125	0
23	MG	A	1717	1/1	0.99	0.03	107,107,107,107	0
23	MG	A	1820	1/1	1.00	0.04	176,176,176,176	0
23	MG	A	1839	1/1	1.00	0.04	116,116,116,116	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	MG	A	1635	1/1	1.00	0.04	89,89,89,89	0

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



6.5 Other polymers [i](#)

There are no such residues in this entry.