



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 08:21 AM UTC

PDB ID : 4DV5 / pdb_00004dv5
Title : Crystal structure of the *Thermus thermophilus* 30S ribosomal subunit with a 16S rRNA mutation, A914G, 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 : 3.68 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

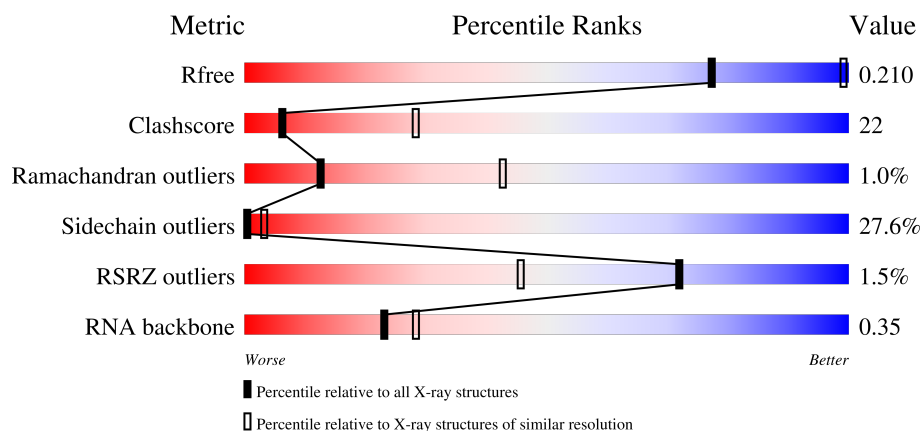
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.68 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.



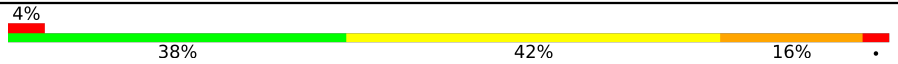
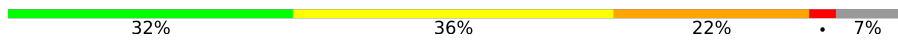
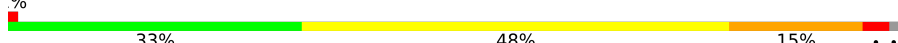
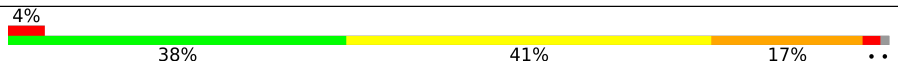
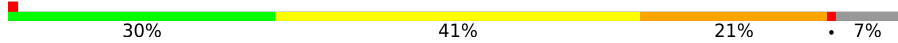
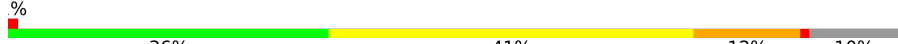
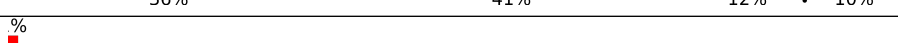
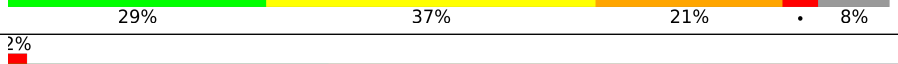
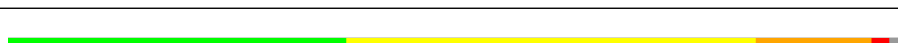
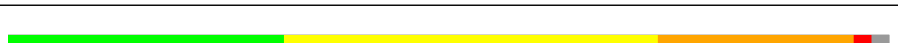
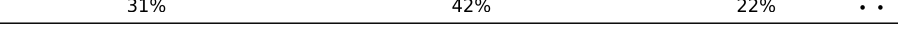
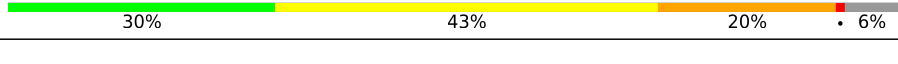
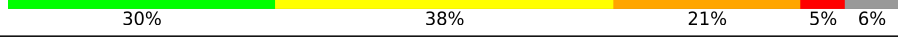
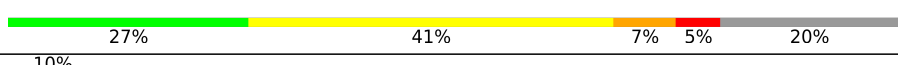
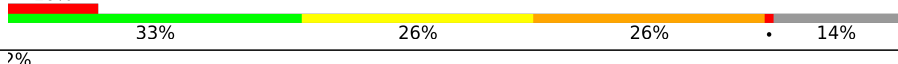
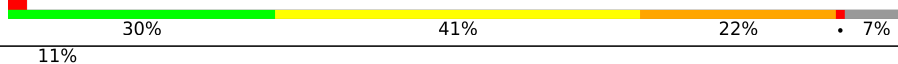
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1263 (3.80-3.56)
Clashscore	190562	1305 (3.80-3.56)
Ramachandran outliers	187476	1259 (3.80-3.56)
Sidechain outliers	187428	1256 (3.80-3.56)
RSRZ outliers	180081	1262 (3.80-3.56)
RNA backbone	3983	1000 (4.26-3.08)

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	2% 38% 41% 19% ..
2	B	256	29% 41% 19% . 9%
3	C	239	2% 34% 34% 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	1796	-	-	-	X

2 Entry composition

There are 25 unique types of molecules in this entry. The entry contains 52300 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
			32508	14477	6011	10508	1512			

There are 3 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is a protein called ribosomal protein S2.

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

- Molecule 3 is a protein called ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	1			

- Molecule 4 is a protein called ribosomal protein S4.

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

- Molecule 5 is a protein called ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	150	Total	C	N	O	S	0	0	0
			1146	724	217	201	4			

- Molecule 6 is a protein called ribosomal protein S6.

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

- Molecule 7 is a protein called ribosomal protein S7.

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

- Molecule 8 is a protein called ribosomal protein S8.

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

- Molecule 9 is a protein called ribosomal protein S9.

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

- Molecule 10 is a protein called ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	98	Total	C	N	O	S	0	0	0
			792	498	156	137	1			

- Molecule 11 is a protein called ribosomal protein S11.

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

- Molecule 12 is a protein called ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	124	Total	C	N	O	S	0	0	0
			972	612	195	163	2			

- Molecule 13 is a protein called ribosomal protein S13.

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

- Molecule 14 is a protein called ribosomal protein S14.

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

- Molecule 15 is a protein called ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	O	87	Total	C	N	O	S	0	0	0
			729	457	146	124	2			

- Molecule 16 is a protein called ribosomal protein S16.

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

- Molecule 17 is a protein called ribosomal protein S17.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 18 is a protein called ribosomal protein S18.

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

- Molecule 19 is a protein called ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	S	80	Total	C	N	O	S	0	0	0
			647	414	119	112	2			

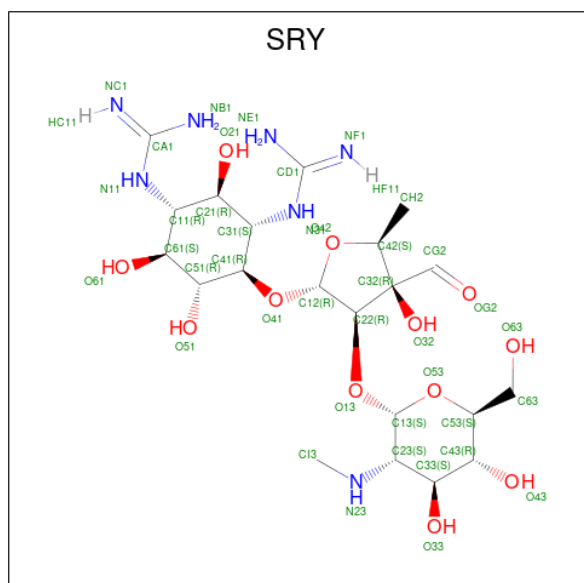
- Molecule 20 is a protein called ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	T	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

- Molecule 21 is a protein called ribosomal protein THX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	U	24	Total	C	N	O	0	0	0
			208	128	50	30			

- Molecule 22 is 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	253	Total 253	Mg 253	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	2	Total 2	Mg 2	0	0
23	M	2	Total 2	Mg 2	0	0
23	N	1	Total 1	Mg 1	0	0
23	P	3	Total 3	Mg 3	0	0
23	Q	1	Total 1	Mg 1	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	374	Total 374	O 374	0	0
25	B	1	Total 1	O 1	0	0
25	D	1	Total 1	O 1	0	0

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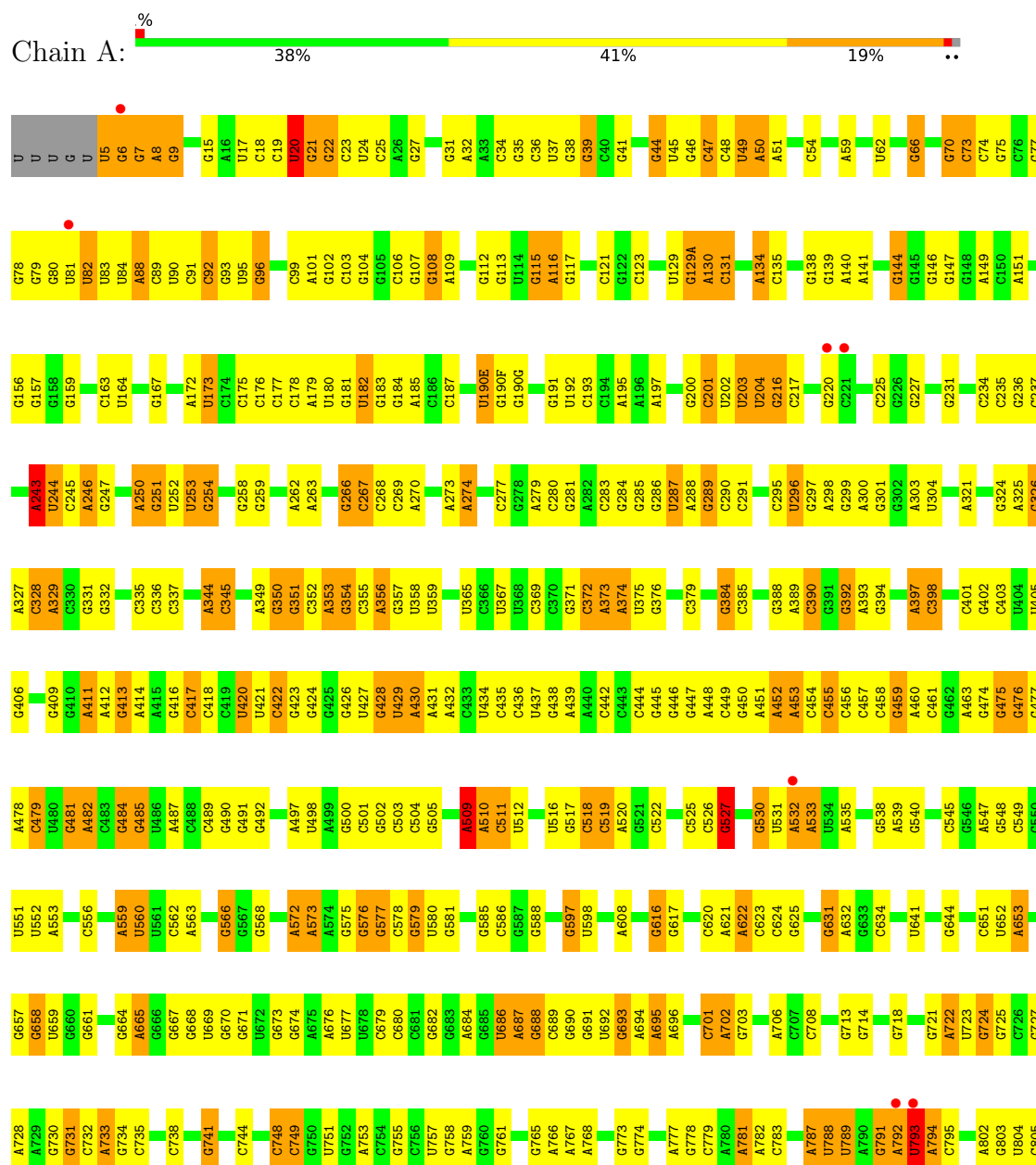
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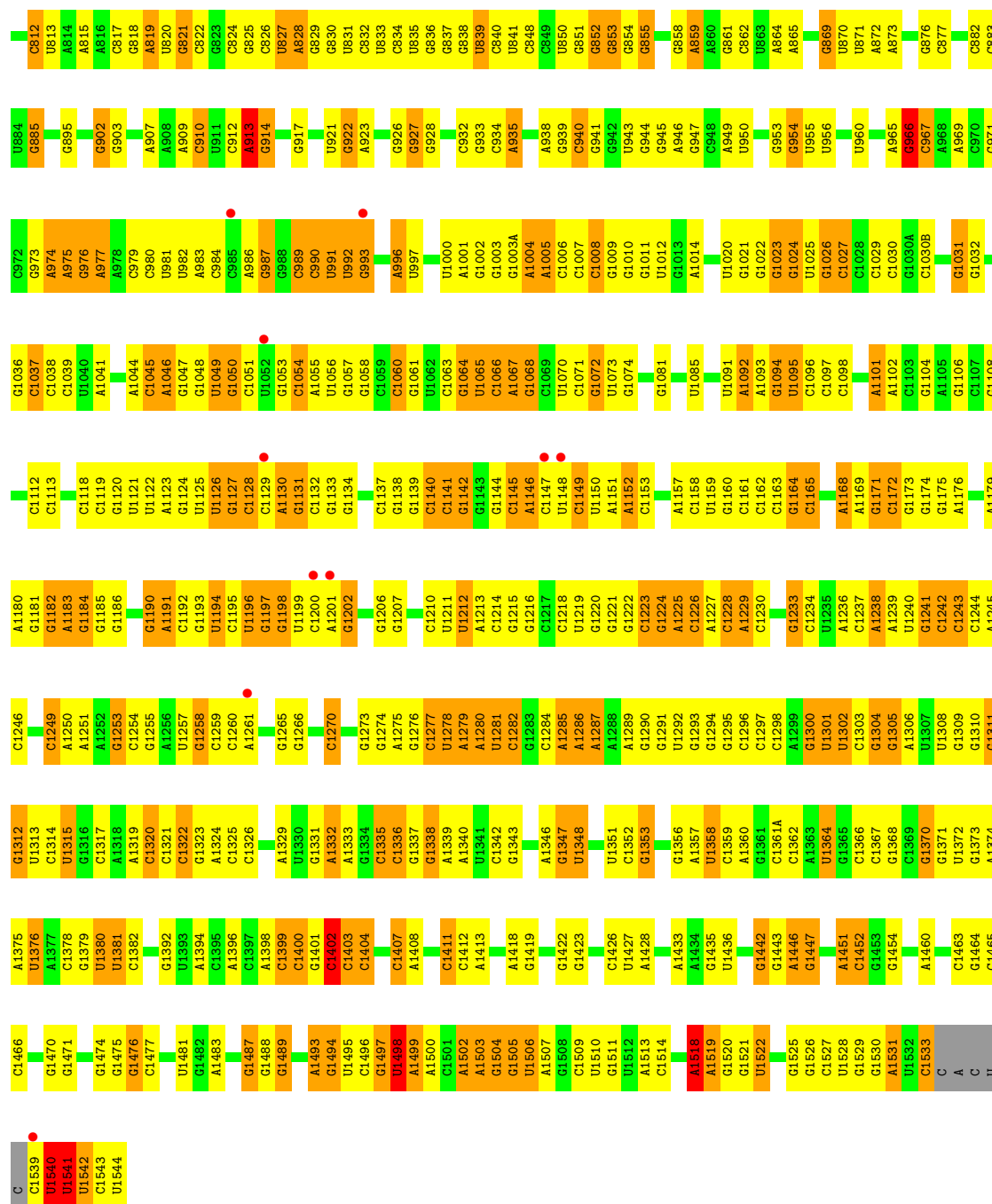
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	E	7	Total	O	0	0
			7	7		
25	L	1	Total	O	0	0
			1	1		
25	N	1	Total	O	0	0
			1	1		
25	P	2	Total	O	0	0
			2	2		
25	T	2	Total	O	0	0
			2	2		

3 Residue-property plots

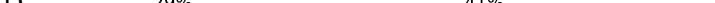
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

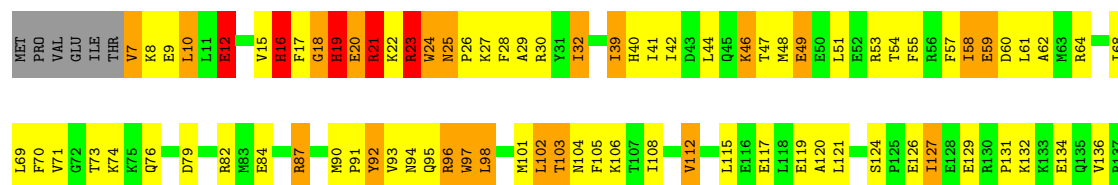
• Molecule 1: 16S rRNA

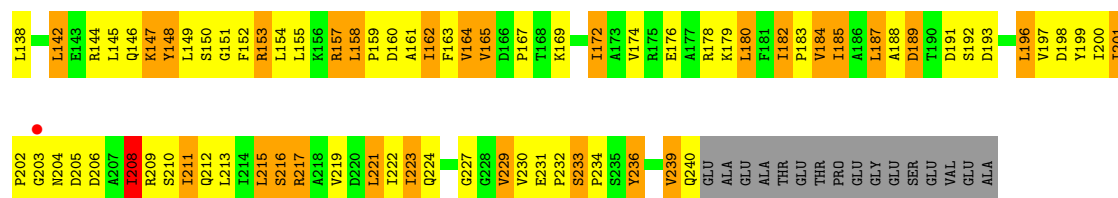




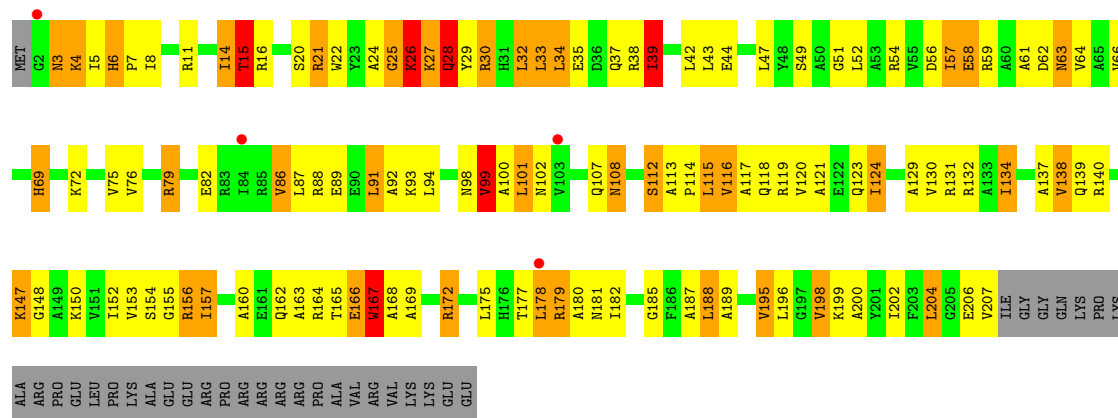
- Molecule 2: ribosomal protein S2

Chain B:  29% 41% 19% 1% 10%

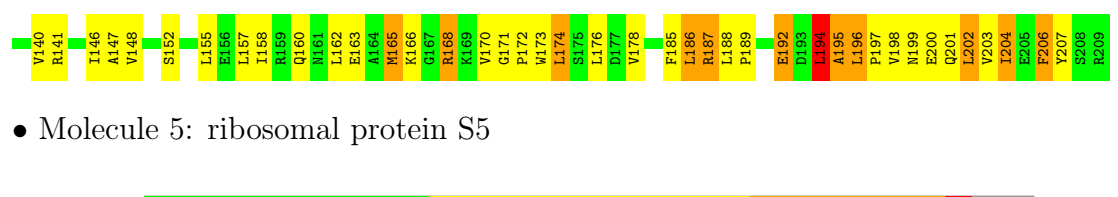
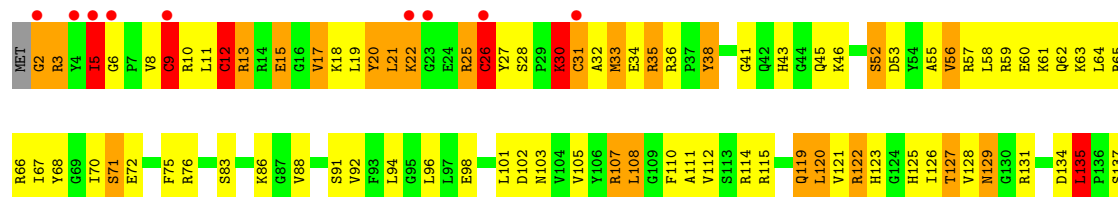




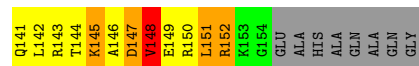
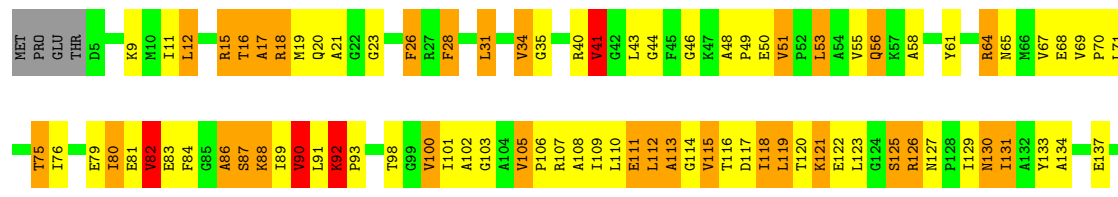
• Molecule 3: ribosomal protein S3



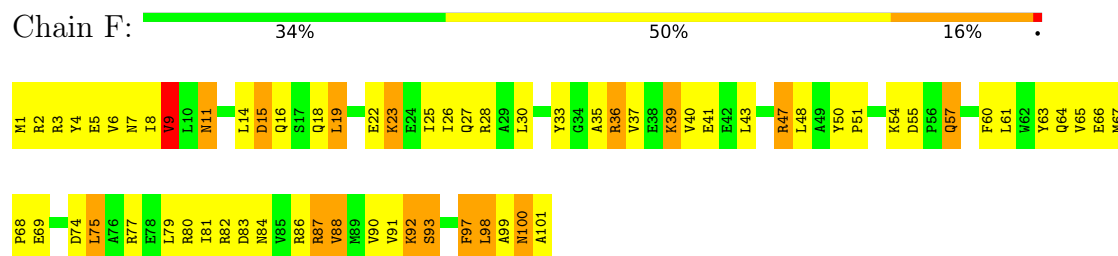
• Molecule 4: ribosomal protein S4



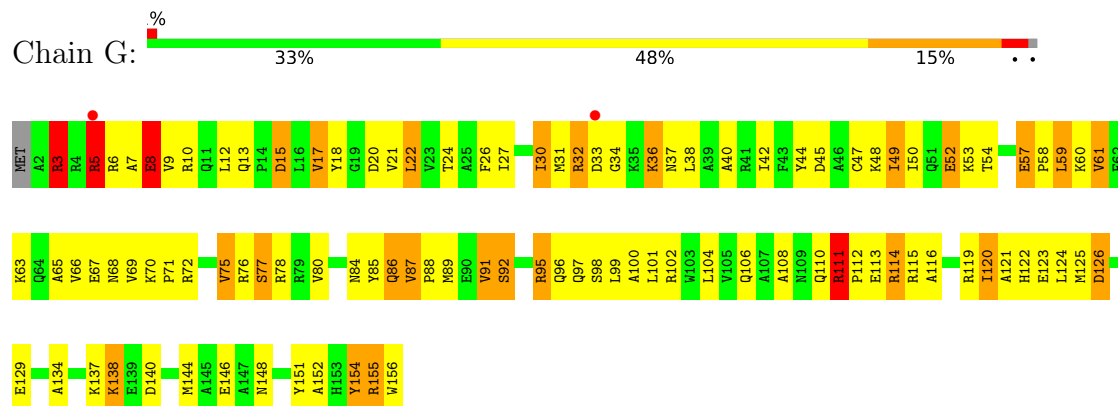
• Molecule 5: ribosomal protein S5



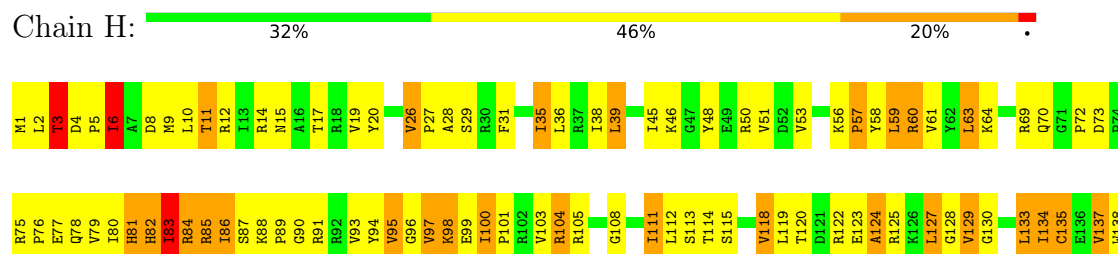
- Molecule 6: ribosomal protein S6



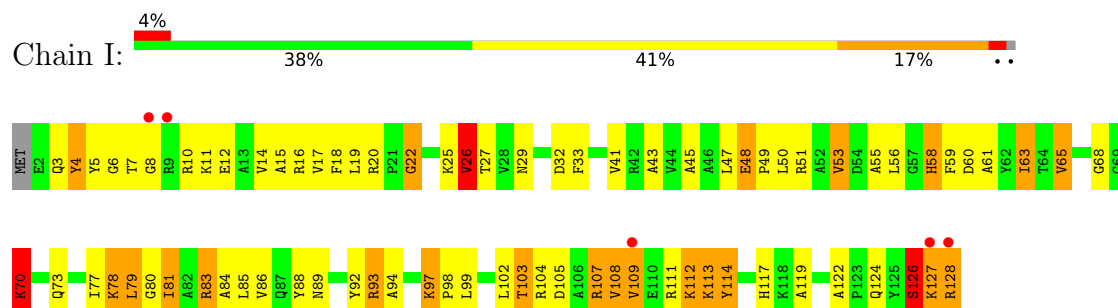
- Molecule 7: ribosomal protein S7



- Molecule 8: ribosomal protein S8

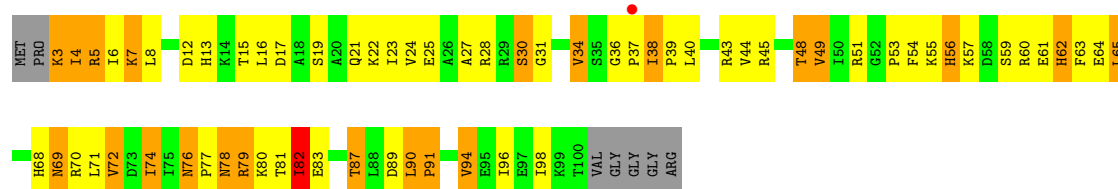


- Molecule 9: ribosomal protein S9

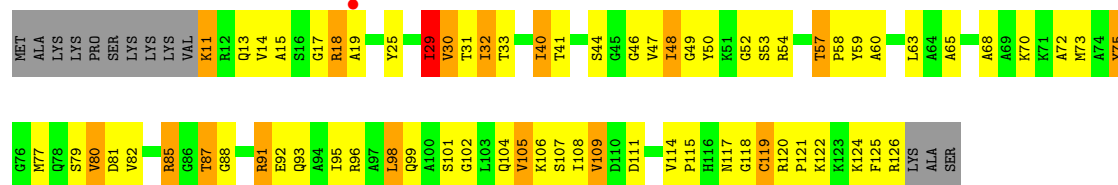


- Molecule 10: ribosomal protein S10

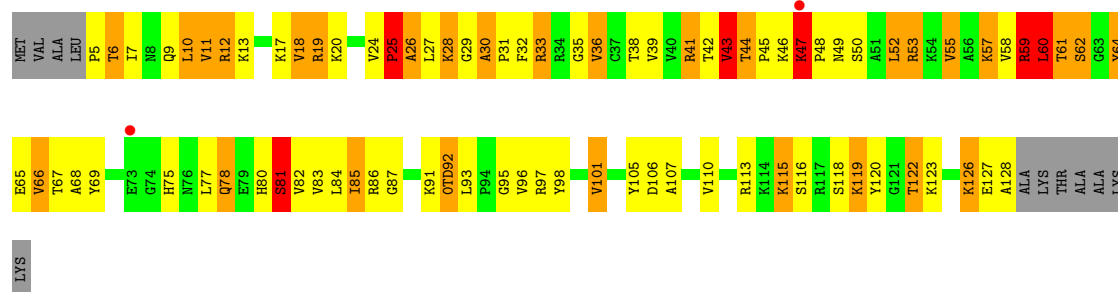




- Molecule 11: ribosomal protein S11



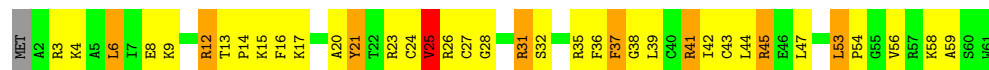
- Molecule 12: ribosomal protein S12



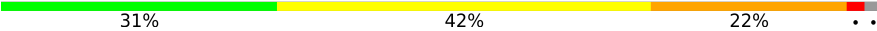
- Molecule 13: ribosomal protein S13

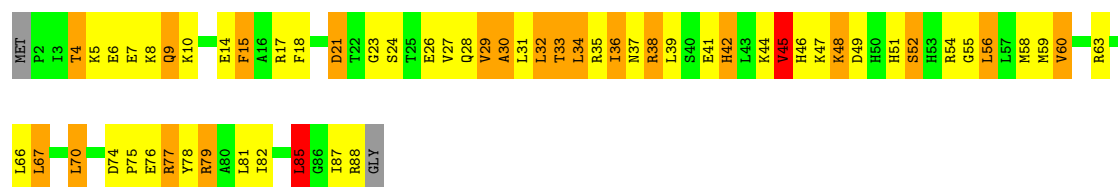


- Molecule 14: ribosomal protein S14

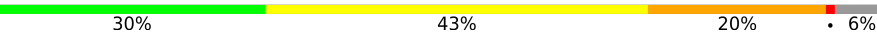


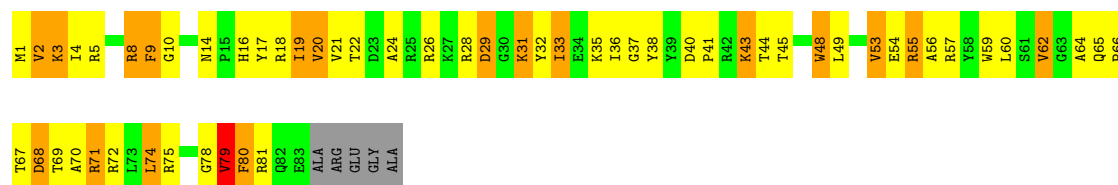
- Molecule 15: ribosomal protein S15

Chain O:  31% 42% 22% . .

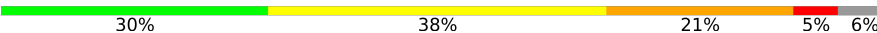


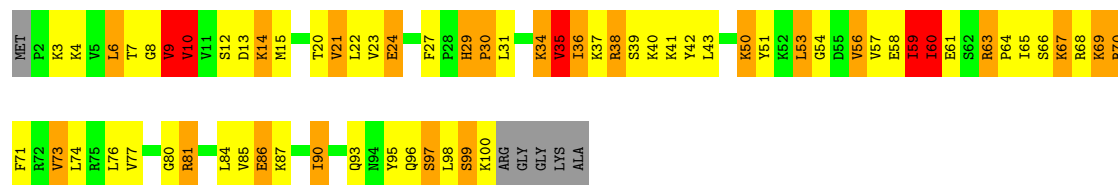
• Molecule 16: ribosomal protein S16

Chain P:  30% 43% 20% . 6%

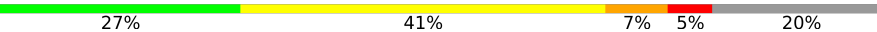


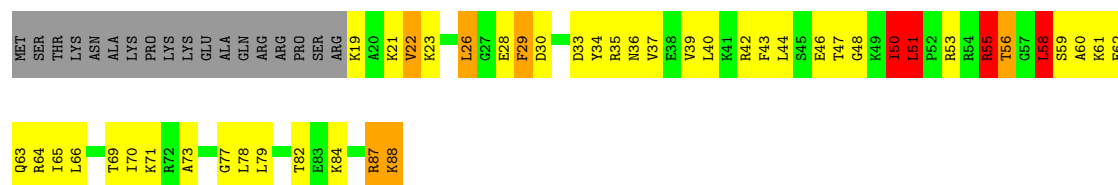
• Molecule 17: ribosomal protein S17

Chain Q:  30% 38% 21% 5% 6%

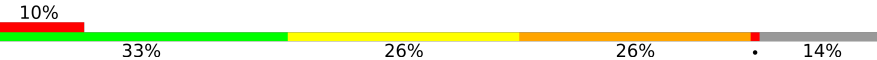


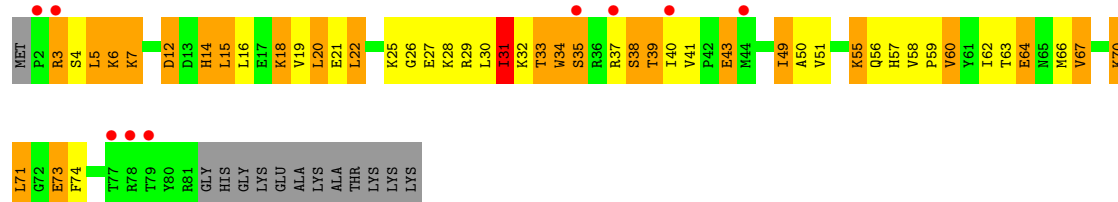
• Molecule 18: ribosomal protein S18

Chain R:  27% 41% 7% 5% 20%

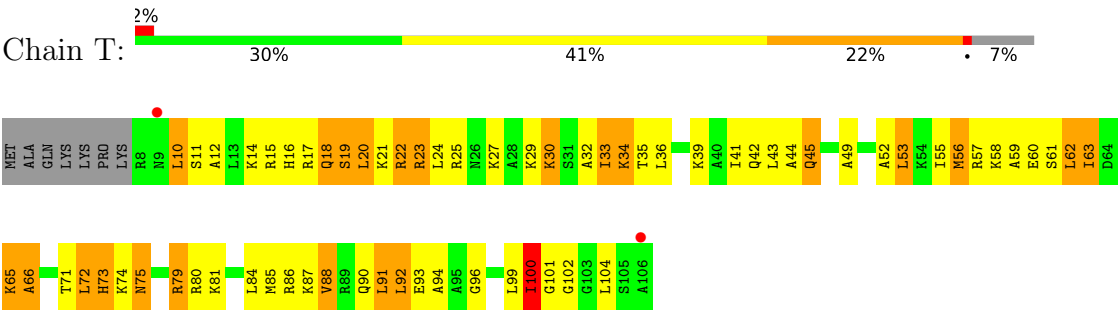


• Molecule 19: ribosomal protein S19

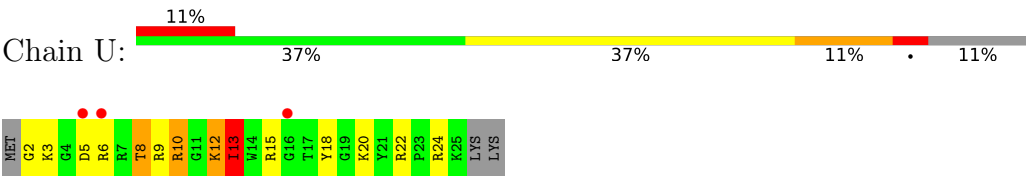
Chain S:  10% 33% 26% 26% . 14%



• 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	402.13Å 402.13Å 172.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.55 – 3.68 34.55 – 3.68	Depositor EDS
% Data completeness (in resolution range)	98.1 (34.55-3.68) 97.7 (34.55-3.68)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 3.66Å)	Xtriage
Refinement program	PHENIX dev_978	Depositor
R, R_{free}	0.156 , 0.211 0.155 , 0.210	Depositor DCC
R_{free} test set	7392 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	122.3	Xtriage
Anisotropy	0.371	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 122.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	52300	wwPDB-VP
Average B, all atoms (Å ²)	148.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.44% 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: MA6, ZN, SRY, 0TD, UR3, 2MG, 7MG, 5MC, M2G, MG, 4OC, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.74	2/36041 (0.0%)	0.70	8/56245 (0.0%)
2	B	1.18	8/1935 (0.4%)	1.45	24/2609 (0.9%)
3	C	0.96	1/1636 (0.1%)	1.38	21/2205 (1.0%)
4	D	1.10	6/1733 (0.3%)	1.64	34/2318 (1.5%)
5	E	1.49	10/1162 (0.9%)	1.72	31/1564 (2.0%)
6	F	0.94	2/856 (0.2%)	1.30	5/1154 (0.4%)
7	G	0.93	0/1276	1.35	15/1709 (0.9%)
8	H	1.51	11/1136 (1.0%)	1.66	26/1527 (1.7%)
9	I	0.94	0/1029	1.42	13/1379 (0.9%)
10	J	1.00	2/805 (0.2%)	1.45	16/1082 (1.5%)
11	K	1.07	1/879 (0.1%)	1.53	15/1187 (1.3%)
12	L	1.31	8/977 (0.8%)	1.86	35/1306 (2.7%)
13	M	0.95	2/947 (0.2%)	1.47	12/1270 (0.9%)
14	N	0.86	0/501	1.43	7/664 (1.1%)
15	O	1.15	4/740 (0.5%)	1.36	10/987 (1.0%)
16	P	1.24	5/716 (0.7%)	1.54	9/963 (0.9%)
17	Q	1.46	10/836 (1.2%)	1.75	19/1117 (1.7%)
18	R	0.98	0/579	1.49	9/768 (1.2%)
19	S	0.92	0/661	1.27	8/890 (0.9%)
20	T	1.10	1/765 (0.1%)	1.50	10/1007 (1.0%)
21	U	0.78	0/212	1.18	2/277 (0.7%)
All	All	0.90	73/55422 (0.1%)	1.03	329/82228 (0.4%)

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
3	C	0	2
4	D	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
7	G	0	1
8	H	0	1
9	I	0	1
10	J	0	2
12	L	0	1
17	Q	0	1
20	T	0	1
All	All	0	11

All (73) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	5	ILE	CA-CB	9.56	1.67	1.54
17	Q	35	VAL	CA-CB	-9.06	1.43	1.53
2	B	201	ILE	CA-CB	-8.99	1.44	1.53
5	E	148	VAL	CA-CB	-8.73	1.42	1.54
16	P	36	ILE	CA-CB	-8.67	1.43	1.54
8	H	111	ILE	CA-CB	-8.49	1.44	1.53
17	Q	99	SER	CA-C	7.99	1.63	1.52
5	E	90	VAL	CA-CB	-7.92	1.44	1.54
2	B	172	ILE	CA-CB	-7.89	1.44	1.54
5	E	115	VAL	CA-CB	-7.69	1.45	1.54
8	H	61	VAL	CA-CB	-7.60	1.45	1.54
12	L	85	ILE	CA-CB	-7.55	1.45	1.54
5	E	82	VAL	CA-CB	-7.54	1.44	1.54
12	L	68	ALA	CA-CB	-7.45	1.41	1.53
17	Q	10	VAL	CA-CB	-7.41	1.45	1.54
17	Q	9	VAL	CA-CB	-7.20	1.45	1.54
8	H	124	ALA	CA-CB	-7.09	1.41	1.53
1	A	1498	UR3	O3'-P	6.92	1.63	1.56
17	Q	60	ILE	CA-CB	-6.76	1.45	1.54
8	H	89	PRO	CA-C	-6.65	1.45	1.52
17	Q	21	VAL	CA-CB	-6.61	1.45	1.53
10	J	82	ILE	CA-CB	6.59	1.62	1.54
17	Q	69	LYS	CA-C	-6.48	1.46	1.53
12	L	66	VAL	CA-CB	-6.45	1.48	1.55
2	B	58	ILE	CA-CB	-6.42	1.46	1.54
8	H	59	LEU	CA-C	-6.23	1.45	1.52
2	B	182	ILE	CA-CB	-6.16	1.46	1.54
2	B	19	HIS	CA-C	6.13	1.60	1.52
15	O	60	VAL	CA-CB	-6.10	1.46	1.54
16	P	20	VAL	CA-CB	-6.08	1.46	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	83	ILE	CA-CB	-6.07	1.46	1.54
6	F	90	VAL	CA-CB	-6.00	1.47	1.54
4	D	9	CYS	CA-C	5.95	1.60	1.52
2	B	174	VAL	CA-CB	-5.93	1.47	1.54
1	A	793	U	C1'-N1	5.91	1.56	1.47
12	L	26	ALA	CA-CB	5.88	1.62	1.53
12	L	25	PRO	CA-C	5.87	1.60	1.52
8	H	134	ILE	CA-CB	-5.85	1.46	1.54
17	Q	90	ILE	CA-CB	-5.84	1.46	1.54
6	F	9	VAL	CA-CB	-5.83	1.47	1.54
5	E	41	VAL	CA-CB	-5.81	1.45	1.54
16	P	19	ILE	CA-CB	-5.80	1.47	1.54
4	D	204	ILE	CA-CB	-5.76	1.48	1.54
17	Q	73	VAL	CA-CB	-5.74	1.47	1.53
2	B	41	ILE	CA-CB	-5.72	1.47	1.54
4	D	31	CYS	N-CA	5.72	1.53	1.46
15	O	45	VAL	CA-CB	-5.72	1.46	1.54
8	H	93	VAL	CA-CB	-5.71	1.47	1.54
12	L	36	VAL	CA-CB	-5.64	1.47	1.54
4	D	185	PHE	CA-C	-5.59	1.45	1.53
13	M	7	VAL	CA-C	5.55	1.59	1.52
16	P	33	ILE	CA-CB	-5.47	1.47	1.54
3	C	138	VAL	CA-CB	-5.44	1.48	1.54
5	E	28	PHE	CA-C	-5.41	1.46	1.52
15	O	30	ALA	CA-C	-5.40	1.47	1.53
15	O	30	ALA	CA-CB	-5.39	1.46	1.53
5	E	108	ALA	CA-CB	-5.38	1.45	1.53
5	E	34	VAL	CA-CB	-5.37	1.46	1.55
13	M	7	VAL	CA-CB	5.37	1.61	1.54
17	Q	56	VAL	CA-CB	-5.34	1.48	1.54
10	J	90	LEU	CA-C	5.30	1.59	1.52
20	T	63	ILE	CA-CB	-5.29	1.48	1.54
4	D	12	CYS	CB-SG	5.27	1.98	1.81
11	K	29	ILE	CA-CB	5.25	1.61	1.54
12	L	13	LYS	C-O	-5.24	1.17	1.23
16	P	36	ILE	CA-C	-5.17	1.46	1.52
8	H	6	ILE	CA-CB	-5.16	1.48	1.54
8	H	135	CYS	CB-SG	-5.12	1.64	1.81
8	H	137	VAL	CA-CB	-5.09	1.47	1.54
5	E	109	ILE	CA-CB	-5.08	1.48	1.54
2	B	103	THR	CA-CB	-5.05	1.45	1.53
5	E	86	ALA	CA-CB	-5.04	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	L	13	LYS	CA-C	-5.02	1.47	1.53

All (329) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	171	GLY	CA-C-N	14.60	134.45	119.56
4	D	171	GLY	C-N-CA	14.60	134.45	119.56
12	L	24	VAL	CA-C-N	-13.75	102.65	119.84
12	L	24	VAL	C-N-CA	-13.75	102.65	119.84
12	L	26	ALA	N-CA-C	-12.58	97.56	111.28
4	D	26	CYS	N-CA-C	-12.03	98.59	113.02
4	D	30	LYS	N-CA-C	11.46	128.62	113.72
17	Q	29	HIS	CA-C-N	11.32	130.91	119.82
17	Q	29	HIS	C-N-CA	11.32	130.91	119.82
4	D	3	ARG	N-CA-C	10.75	124.01	111.11
18	R	79	LEU	CA-C-N	10.46	130.22	119.76
18	R	79	LEU	C-N-CA	10.46	130.22	119.76
12	L	66	VAL	CB-CA-C	-10.31	96.86	111.40
16	P	80	PHE	N-CA-C	10.29	126.76	112.45
20	T	94	ALA	N-CA-C	-10.19	90.65	108.69
14	N	53	LEU	CA-C-N	10.18	130.83	119.83
14	N	53	LEU	C-N-CA	10.18	130.83	119.83
3	C	167	TRP	N-CA-C	10.04	122.08	108.23
11	K	49	GLY	N-CA-C	9.99	125.02	112.83
17	Q	35	VAL	CB-CA-C	-9.69	97.74	111.31
3	C	179	ARG	N-CA-C	-9.48	90.60	110.80
7	G	111	ARG	CA-C-N	9.48	128.83	118.97
7	G	111	ARG	C-N-CA	9.48	128.83	118.97
12	L	119	LYS	N-CA-C	-9.45	95.27	110.20
12	L	30	ALA	CA-C-N	9.29	128.94	119.56
12	L	30	ALA	C-N-CA	9.29	128.94	119.56
13	M	9	ILE	CA-C-N	9.27	129.63	119.90
13	M	9	ILE	C-N-CA	9.27	129.63	119.90
16	P	45	THR	CA-C-N	-9.24	109.36	118.97
16	P	45	THR	C-N-CA	-9.24	109.36	118.97
3	C	138	VAL	CB-CA-C	-9.22	100.08	111.88
17	Q	21	VAL	CB-CA-C	-9.20	98.41	111.19
4	D	12	CYS	N-CA-C	-9.02	96.57	111.37
5	E	41	VAL	CB-CA-C	-8.82	98.19	110.90
2	B	23	ARG	N-CA-C	-8.80	92.06	110.80
16	P	79	VAL	N-CA-C	-8.80	99.72	112.04
4	D	38	TYR	CA-C-N	8.79	129.44	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	38	TYR	C-N-CA	8.79	129.44	120.38
8	H	100	ILE	CA-C-N	8.71	128.77	119.89
8	H	100	ILE	C-N-CA	8.71	128.77	119.89
11	K	114	VAL	CA-C-N	-8.53	111.95	120.31
11	K	114	VAL	C-N-CA	-8.53	111.95	120.31
12	L	66	VAL	N-CA-C	8.42	119.70	107.75
2	B	12	GLU	N-CA-C	8.27	122.80	112.87
12	L	18	VAL	N-CA-C	8.19	119.49	107.37
3	C	26	LYS	N-CA-C	-8.16	101.31	111.11
13	M	84	ILE	N-CA-C	-8.11	101.04	110.21
21	U	13	ILE	N-CA-C	-7.95	102.78	110.42
12	L	44	THR	CA-C-N	7.93	129.75	119.84
12	L	44	THR	C-N-CA	7.93	129.75	119.84
3	C	25	GLY	N-CA-C	7.89	127.64	115.72
4	D	33	MET	N-CA-C	-7.88	102.38	110.97
8	H	122	ARG	N-CA-C	-7.87	102.69	111.82
13	M	108	ARG	N-CA-C	7.83	121.77	111.75
5	E	113	ALA	N-CA-C	-7.72	103.75	113.02
8	H	134	ILE	CB-CA-C	-7.71	101.95	112.04
5	E	109	ILE	CB-CA-C	-7.70	102.18	111.81
5	E	92	LYS	CA-C-N	7.62	128.22	120.14
5	E	92	LYS	C-N-CA	7.62	128.22	120.14
4	D	196	LEU	N-CA-C	7.61	118.35	109.60
12	L	78	GLN	N-CA-C	7.54	118.19	108.24
7	G	13	GLN	CA-C-N	-7.51	112.95	120.98
7	G	13	GLN	C-N-CA	-7.51	112.95	120.98
5	E	120	THR	N-CA-C	7.45	120.62	108.26
2	B	172	ILE	CB-CA-C	-7.41	102.00	112.22
3	C	27	LYS	N-CA-C	7.40	120.42	111.40
7	G	36	LYS	N-CA-C	-7.37	102.95	112.23
2	B	16	HIS	N-CA-C	7.35	124.82	110.56
3	C	39	ILE	CB-CA-C	-7.34	102.57	111.97
2	B	16	HIS	CB-CA-C	-7.34	98.87	112.00
4	D	12	CYS	CA-CB-SG	7.30	131.18	114.40
19	S	67	VAL	N-CA-C	7.29	118.05	110.62
4	D	6	GLY	CA-C-N	7.29	128.27	120.11
4	D	6	GLY	C-N-CA	7.29	128.27	120.11
8	H	82	HIS	N-CA-C	7.27	119.91	108.79
10	J	36	GLY	CA-C-N	7.25	131.19	120.96
10	J	36	GLY	C-N-CA	7.25	131.19	120.96
17	Q	99	SER	N-CA-C	7.24	126.21	110.80
12	L	85	ILE	CB-CA-C	-7.21	100.43	110.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	21	LEU	N-CA-C	-7.20	104.10	113.17
17	Q	14	LYS	N-CA-C	7.19	120.03	111.33
4	D	13	ARG	N-CA-C	7.19	120.03	111.33
4	D	56	VAL	CB-CA-C	-7.19	102.60	112.02
14	N	37	PHE	N-CA-C	7.16	122.40	112.45
4	D	107	ARG	N-CA-C	-7.13	103.20	110.97
10	J	77	PRO	N-CA-C	-7.10	99.45	110.95
2	B	165	VAL	N-CA-C	7.10	119.10	111.58
5	E	15	ARG	N-CA-C	7.08	120.37	111.24
10	J	62	HIS	N-CA-C	7.04	120.44	110.23
8	H	89	PRO	CA-C-N	-7.02	112.60	122.86
8	H	89	PRO	C-N-CA	-7.02	112.60	122.86
12	L	49	ASN	N-CA-C	7.02	120.06	109.95
3	C	108	ASN	CA-C-N	7.01	126.64	119.56
3	C	108	ASN	C-N-CA	7.01	126.64	119.56
11	K	91	ARG	N-CA-C	-6.98	103.11	111.69
2	B	189	ASP	N-CA-C	6.95	117.16	108.19
9	I	58	HIS	N-CA-C	-6.92	104.71	113.02
18	R	51	LEU	CA-C-N	6.91	127.32	119.92
18	R	51	LEU	C-N-CA	6.91	127.32	119.92
5	E	64	ARG	N-CA-C	-6.90	100.77	110.50
6	F	9	VAL	CB-CA-C	-6.87	100.38	110.62
2	B	18	GLY	N-CA-C	6.87	121.03	112.79
14	N	8	GLU	N-CA-C	6.84	120.50	111.75
8	H	80	ILE	CB-CA-C	-6.83	102.45	111.81
2	B	19	HIS	N-CA-C	6.83	119.14	108.96
5	E	23	GLY	N-CA-C	6.81	118.42	111.95
12	L	110	VAL	N-CA-C	6.80	118.20	109.30
14	N	6	LEU	N-CA-C	6.78	121.27	112.92
11	K	119	CYS	CA-C-N	-6.78	111.59	120.67
11	K	119	CYS	C-N-CA	-6.78	111.59	120.67
11	K	80	VAL	N-CA-C	6.77	118.06	108.17
18	R	55	ARG	N-CA-C	6.77	121.70	113.17
6	F	57	GLN	N-CA-C	6.76	118.07	108.74
9	I	122	ALA	N-CA-C	-6.74	100.76	110.40
4	D	30	LYS	CA-C-O	-6.72	111.66	119.05
2	B	148	TYR	N-CA-C	6.71	118.67	111.36
5	E	120	THR	CA-C-N	-6.71	113.66	123.05
5	E	120	THR	C-N-CA	-6.71	113.66	123.05
15	O	85	LEU	N-CA-C	6.68	121.03	113.01
8	H	12	ARG	NE-CZ-NH1	-6.62	114.88	121.50
3	C	6	HIS	CA-C-N	6.62	126.13	119.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	6	HIS	C-N-CA	6.62	126.13	119.24
10	J	90	LEU	N-CA-C	6.62	124.44	109.81
3	C	58	GLU	N-CA-C	6.61	119.47	109.95
9	I	59	PHE	N-CA-C	6.61	119.18	108.41
8	H	3	THR	CA-C-N	-6.60	113.94	122.98
8	H	3	THR	C-N-CA	-6.60	113.94	122.98
8	H	135	CYS	N-CA-C	6.57	118.84	108.79
4	D	34	GLU	N-CA-C	-6.57	100.11	109.96
10	J	56	HIS	N-CA-C	-6.57	102.81	111.02
7	G	61	VAL	N-CA-C	-6.55	103.95	110.30
16	P	2	VAL	N-CA-C	-6.54	102.81	110.21
18	R	29	PHE	N-CA-C	6.53	119.64	109.52
11	K	17	GLY	N-CA-C	6.52	119.99	110.80
7	G	152	ALA	N-CA-C	6.52	120.09	111.75
19	S	33	THR	N-CA-C	6.49	118.99	108.34
8	H	12	ARG	N-CA-C	-6.47	104.15	111.07
1	A	20	U	C4'-C3'-O3'	6.45	122.68	113.00
5	E	17	ALA	N-CA-C	6.45	120.33	109.76
5	E	109	ILE	N-CA-C	6.41	116.52	110.30
2	B	21	ARG	N-CA-C	6.38	124.38	110.80
4	D	2	GLY	CA-C-N	6.37	129.14	120.54
4	D	2	GLY	C-N-CA	6.37	129.14	120.54
14	N	25	VAL	N-CA-C	6.35	117.86	110.62
4	D	204	ILE	CB-CA-C	-6.33	103.60	111.70
11	K	50	TYR	N-CA-C	6.30	118.69	110.43
13	M	103	THR	N-CA-C	6.28	121.72	113.30
7	G	66	VAL	N-CA-C	6.25	116.42	110.42
16	P	5	ARG	N-CA-C	6.24	116.81	108.38
17	Q	63	ARG	N-CA-C	-6.23	101.73	109.64
2	B	174	VAL	CB-CA-C	-6.23	104.03	111.81
8	H	45	ILE	N-CA-C	-6.22	98.57	108.90
16	P	29	ASP	N-CA-C	6.18	120.52	112.92
12	L	59	ARG	N-CA-C	-6.17	99.64	109.76
9	I	22	GLY	N-CA-C	6.17	118.91	110.58
8	H	57	PRO	CB-CA-C	-6.15	103.89	111.64
5	E	148	VAL	CB-CA-C	-6.14	104.00	112.24
10	J	78	ASN	N-CA-C	6.14	116.39	108.34
12	L	25	PRO	N-CA-C	6.12	125.09	112.47
5	E	111	GLU	N-CA-C	-6.10	104.71	111.36
20	T	23	ARG	N-CA-C	-6.10	103.79	111.11
5	E	115	VAL	CB-CA-C	-6.09	101.66	111.59
14	N	12	ARG	CB-CA-C	-6.09	108.95	117.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	O	74	ASP	CA-C-N	6.09	125.57	119.24
15	O	74	ASP	C-N-CA	6.09	125.57	119.24
17	Q	67	LYS	N-CA-C	-6.08	101.67	110.24
7	G	92	SER	N-CA-C	-6.07	101.21	110.07
1	A	20	U	C3'-C2'-C1'	-6.07	95.23	101.30
9	I	97	LYS	CA-C-N	6.04	125.74	119.82
9	I	97	LYS	C-N-CA	6.04	125.74	119.82
12	L	25	PRO	CA-C-N	6.03	128.36	120.28
12	L	25	PRO	C-N-CA	6.03	128.36	120.28
20	T	73	HIS	CB-CA-C	-6.03	108.62	115.79
3	C	28	GLN	N-CA-C	6.02	120.76	113.17
5	E	105	VAL	CA-C-N	-6.02	112.66	119.28
5	E	105	VAL	C-N-CA	-6.02	112.66	119.28
11	K	46	GLY	N-CA-C	-6.02	107.20	114.66
17	Q	23	VAL	CB-CA-C	-6.01	102.83	111.19
10	J	76	ASN	CA-C-N	-6.00	113.01	119.98
10	J	76	ASN	C-N-CA	-6.00	113.01	119.98
15	O	60	VAL	CB-CA-C	-6.00	104.04	112.14
5	E	49	PRO	N-CA-C	5.99	121.70	113.98
4	D	31	CYS	N-CA-CB	5.98	120.60	110.49
8	H	94	TYR	N-CA-C	-5.97	100.06	109.50
10	J	94	VAL	CB-CA-C	-5.96	102.26	110.96
12	L	118	SER	N-CA-C	-5.95	104.49	110.97
17	Q	70	ARG	N-CA-C	5.93	120.53	112.88
2	B	103	THR	CB-CA-C	-5.93	100.95	110.79
5	E	50	GLU	N-CA-C	-5.87	100.13	109.23
12	L	17	LYS	CA-C-N	-5.87	115.13	123.11
12	L	17	LYS	C-N-CA	-5.87	115.13	123.11
19	S	73	GLU	N-CA-C	-5.87	104.96	111.71
4	D	17	VAL	CA-C-N	-5.84	114.65	122.42
4	D	17	VAL	C-N-CA	-5.84	114.65	122.42
11	K	87	THR	N-CA-C	-5.84	100.54	109.41
2	B	158	LEU	CA-CB-CG	-5.82	95.92	116.30
17	Q	21	VAL	N-CA-C	5.82	115.98	107.37
7	G	8	GLU	N-CA-C	5.81	118.44	110.24
13	M	62	ASN	CA-C-N	5.80	132.61	121.54
13	M	62	ASN	C-N-CA	5.80	132.61	121.54
6	F	11	ASN	CA-C-N	5.80	125.48	119.05
6	F	11	ASN	C-N-CA	5.80	125.48	119.05
10	J	89	ASP	N-CA-C	5.79	118.64	109.96
8	H	73	ASP	CA-C-N	5.79	125.32	119.19
8	H	73	ASP	C-N-CA	5.79	125.32	119.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	48	GLU	CA-C-N	5.79	125.65	119.28
9	I	48	GLU	C-N-CA	5.79	125.65	119.28
12	L	105	TYR	CB-CA-C	-5.79	109.92	116.63
10	J	91	PRO	N-CA-C	5.79	120.31	111.34
15	O	79	ARG	N-CA-C	-5.79	104.17	111.11
20	T	34	LYS	N-CA-C	-5.77	104.18	111.11
19	S	12	ASP	N-CA-C	5.77	118.20	110.35
15	O	47	LYS	N-CA-C	-5.75	104.37	111.33
2	B	103	THR	N-CA-C	5.75	117.55	111.28
15	O	15	PHE	N-CA-C	5.74	120.41	113.17
3	C	99	VAL	N-CA-C	5.74	115.86	107.37
17	Q	80	GLY	CA-C-N	-5.73	114.88	122.85
17	Q	80	GLY	C-N-CA	-5.73	114.88	122.85
9	I	26	VAL	N-CA-C	5.72	116.30	107.78
3	C	86	VAL	N-CA-C	5.72	116.49	110.72
6	F	6	VAL	CB-CA-C	-5.70	103.74	111.15
2	B	211	ILE	CB-CA-C	-5.68	104.70	111.97
7	G	155	ARG	N-CA-C	5.67	122.87	110.80
19	S	14	HIS	N-CA-C	5.67	117.26	111.14
12	L	75	HIS	N-CA-C	5.66	118.01	109.23
2	B	20	GLU	N-CA-C	5.65	122.84	110.80
21	U	20	LYS	N-CA-C	-5.65	105.27	111.82
17	Q	59	ILE	N-CA-C	-5.63	100.38	108.48
8	H	12	ARG	NE-CZ-NH2	5.62	124.26	119.20
8	H	83	ILE	N-CA-C	-5.62	100.08	108.46
16	P	9	PHE	N-CA-C	5.62	120.83	113.30
5	E	103	GLY	N-CA-C	-5.61	105.48	111.93
4	D	135	LEU	CB-CA-C	-5.61	104.62	110.17
19	S	6	LYS	N-CA-C	5.57	122.66	110.80
16	P	48	TRP	N-CA-C	-5.57	106.26	113.16
13	M	64	TRP	N-CA-C	5.56	118.69	110.46
8	H	81	HIS	N-CA-C	-5.55	105.24	112.23
5	E	92	LYS	N-CA-C	-5.54	101.59	109.62
5	E	102	ALA	N-CA-C	5.53	117.25	108.79
12	L	43	VAL	N-CA-C	5.53	117.61	108.99
9	I	63	ILE	CB-CA-C	-5.52	103.81	110.99
9	I	70	LYS	N-CA-C	5.52	117.38	111.36
2	B	233	SER	CA-C-N	5.50	125.17	119.56
2	B	233	SER	C-N-CA	5.50	125.17	119.56
7	G	5	ARG	N-CA-C	5.50	115.54	108.34
18	R	46	GLU	N-CA-C	-5.49	104.32	111.02
2	B	12	GLU	CA-CB-CG	-5.49	103.13	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	67	ILE	CB-CA-C	-5.48	104.85	112.02
15	O	66	LEU	N-CA-C	-5.47	105.39	111.36
11	K	118	GLY	N-CA-C	5.46	126.11	113.18
12	L	127	GLU	N-CA-C	-5.44	99.64	108.41
4	D	168	ARG	N-CA-C	-5.44	102.22	110.28
5	E	12	LEU	N-CA-C	5.44	117.53	108.99
9	I	126	SER	N-CA-C	5.44	122.39	110.80
8	H	38	ILE	CB-CA-C	-5.43	104.90	112.02
3	C	116	VAL	CB-CA-C	-5.43	105.02	111.97
12	L	60	LEU	N-CA-C	5.43	118.42	109.85
10	J	5	ARG	N-CA-C	-5.42	101.70	110.32
3	C	5	ILE	CB-CA-C	-5.40	102.43	111.29
19	S	38	SER	N-CA-C	5.38	118.42	110.46
10	J	44	VAL	N-CA-C	5.37	116.27	107.24
2	B	239	VAL	N-CA-C	5.36	115.56	110.42
15	O	36	ILE	CB-CA-C	-5.36	104.84	111.70
9	I	3	GLN	N-CA-C	5.35	117.91	108.75
10	J	74	ILE	N-CA-C	5.35	114.45	106.85
4	D	53	ASP	N-CA-C	-5.35	104.69	111.11
17	Q	3	LYS	N-CA-C	-5.35	101.99	109.96
5	E	145	LYS	N-CA-C	-5.35	105.35	111.07
3	C	124	ILE	N-CA-C	5.34	116.12	110.72
4	D	43	HIS	N-CA-C	5.34	119.49	112.92
7	G	3	ARG	N-CA-C	5.33	118.25	111.69
15	O	30	ALA	N-CA-C	-5.33	102.78	111.04
12	L	52	LEU	CA-C-N	-5.32	114.72	122.65
12	L	52	LEU	C-N-CA	-5.32	114.72	122.65
2	B	208	ILE	N-CA-C	5.30	118.49	111.17
20	T	19	SER	N-CA-C	-5.29	104.76	111.11
11	K	57	THR	CA-C-N	5.29	124.92	119.05
11	K	57	THR	C-N-CA	5.29	124.92	119.05
18	R	50	ILE	CB-CA-C	-5.28	103.46	111.33
5	E	48	ALA	CA-C-N	5.28	124.99	119.82
5	E	48	ALA	C-N-CA	5.28	124.99	119.82
8	H	114	THR	N-CA-C	5.28	116.30	108.86
3	C	69	HIS	N-CA-C	5.27	117.31	107.99
13	M	25	ILE	N-CA-C	5.24	115.44	108.11
12	L	81	SER	N-CA-C	5.24	117.62	110.24
17	Q	35	VAL	N-CA-C	5.23	115.30	107.51
20	T	88	VAL	CB-CA-C	-5.23	105.01	111.70
18	R	58	LEU	N-CA-C	5.23	117.94	109.79
1	A	1498	UR3	P-O3'-C3'	5.22	125.97	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	112	GLY	CA-C-N	5.22	125.22	119.90
13	M	112	GLY	C-N-CA	5.22	125.22	119.90
12	L	95	GLY	CA-C-N	-5.22	116.48	122.95
12	L	95	GLY	C-N-CA	-5.22	116.48	122.95
20	T	15	ARG	N-CA-C	-5.20	105.69	111.36
2	B	25	ASN	N-CA-C	-5.20	98.33	109.81
8	H	89	PRO	N-CA-C	-5.19	102.96	110.80
2	B	119	GLU	N-CA-C	-5.19	105.74	111.71
17	Q	30	PRO	CB-CA-C	-5.18	104.05	111.62
12	L	47	LYS	N-CA-C	5.18	119.98	113.25
12	L	57	LYS	N-CA-C	-5.18	103.20	110.50
4	D	206	PHE	CA-C-N	-5.17	113.02	122.38
4	D	206	PHE	C-N-CA	-5.17	113.02	122.38
17	Q	38	ARG	N-CA-C	-5.16	101.52	109.52
20	T	66	ALA	N-CA-C	-5.15	105.56	111.07
20	T	100	ILE	CB-CA-C	-5.15	103.92	112.26
10	J	94	VAL	N-CA-C	5.14	115.26	107.80
5	E	87	SER	N-CA-C	5.13	117.27	108.90
7	G	114	ARG	N-CA-C	5.13	116.73	111.03
11	K	102	GLY	N-CA-C	-5.13	107.91	114.37
5	E	100	VAL	CB-CA-C	-5.13	104.46	111.33
5	E	16	THR	N-CA-C	5.12	121.70	110.80
7	G	148	ASN	N-CA-C	5.12	119.22	112.92
19	S	34	TRP	N-CA-C	-5.08	106.92	113.02
5	E	75	THR	N-CA-C	5.07	116.94	108.99
8	H	111	ILE	N-CA-CB	-5.07	105.08	111.41
12	L	85	ILE	N-CA-C	5.06	115.14	107.80
4	D	194	LEU	N-CA-C	5.06	117.48	109.24
13	M	10	PRO	CA-C-O	-5.05	115.28	121.03
1	A	15	G	C4-N9-C1'	5.04	141.63	126.50
1	A	913	A	C2'-C3'-O3'	5.03	117.05	109.50
1	A	243	A	P-O3'-C3'	5.03	127.75	120.20
3	C	37	GLN	N-CA-C	5.03	116.76	111.28
8	H	60	ARG	CG-CD-NE	-5.02	100.95	112.00
1	A	15	G	C8-N9-C1'	-5.02	111.95	127.00
4	D	26	CYS	CB-CA-C	5.02	119.30	110.37
3	C	124	ILE	CB-CA-C	-5.02	105.30	112.22
1	A	509	A	C3'-C2'-C1'	-5.01	96.28	101.30
17	Q	15	MET	N-CA-C	5.01	117.00	110.53
20	T	59	ALA	N-CA-C	-5.01	104.78	111.24

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	166	GLU	Peptide
3	C	24	ALA	Peptide
4	D	195	ALA	Peptide
7	G	154	TYR	Peptide
8	H	90	GLY	Peptide
9	I	126	SER	Peptide
10	J	3	LYS	Peptide
10	J	87	THR	Peptide
12	L	25	PRO	Peptide
17	Q	13	ASP	Peptide
20	T	93	GLU	Peptide

5.2 Too-close contacts [i](#)

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	32508	0	16426	863	0
2	B	1900	0	1951	121	0
3	C	1612	0	1677	96	0
4	D	1703	0	1763	106	0
5	E	1146	0	1207	74	0
6	F	843	0	857	57	0
7	G	1257	0	1296	79	0
8	H	1116	0	1177	74	0
9	I	1010	0	1037	76	0
10	J	792	0	835	52	0
11	K	864	0	881	54	0
12	L	972	0	1058	69	0
13	M	937	0	995	57	0
14	N	492	0	529	52	0
15	O	729	0	768	49	0
16	P	700	0	720	49	0
17	Q	823	0	893	55	0
18	R	574	0	644	47	0
19	S	647	0	673	40	0
20	T	763	0	861	52	0
21	U	208	0	221	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	A	40	0	37	7	0
23	A	253	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	2	0	0	0	0
23	M	2	0	0	0	0
23	N	1	0	0	0	0
23	P	3	0	0	0	0
23	Q	1	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	374	0	0	14	0
25	B	1	0	0	0	0
25	D	1	0	0	0	0
25	E	7	0	0	0	0
25	L	1	0	0	0	0
25	N	1	0	0	0	0
25	P	2	0	0	0	0
25	T	2	0	0	1	0
All	All	52300	0	36506	1946	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 22.

All (1946) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:26:LEU:HD11	18:R:42:ARG:HD3	1.46	0.98
1:A:792:A:H1'	1:A:793:U:H2'	1.47	0.96
11:K:48:ILE:HD12	11:K:63:LEU:HB2	1.45	0.96
1:A:1326:C:OP2	21:U:6:ARG:NH2	2.00	0.93
12:L:87:GLY:HA2	12:L:98:TYR:HA	1.51	0.92
3:C:129:ALA:HB1	3:C:132:ARG:HB3	1.51	0.92
3:C:27:LYS:O	3:C:30:ARG:NH2	2.05	0.89
1:A:103:C:OP1	20:T:17:ARG:NH1	2.05	0.89
6:F:87:ARG:HH11	6:F:87:ARG:HG3	1.36	0.89
1:A:1030:C:O2	1:A:1031:G:N2	2.05	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:39:LEU:HD23	15:O:56:LEU:HB2	1.53	0.89
3:C:153:VAL:HG12	3:C:166:GLU:HB2	1.55	0.89
1:A:1373:G:H5''	7:G:36:LYS:HD2	1.55	0.88
11:K:91:ARG:HD2	18:R:88:LYS:HZ3	1.36	0.88
1:A:1496:C:O2'	1:A:1497:G:O5'	1.91	0.87
1:A:1126:U:H3'	1:A:1127:G:H8	1.36	0.87
1:A:1249:C:O2'	9:I:73:GLN:NE2	2.07	0.86
3:C:188:LEU:HD11	3:C:195:VAL:HG23	1.57	0.86
7:G:69:VAL:HG21	7:G:104:LEU:HD21	1.58	0.86
6:F:36:ARG:HB3	6:F:36:ARG:HH11	1.40	0.86
3:C:58:GLU:O	3:C:59:ARG:NH1	2.09	0.86
3:C:34:LEU:HD13	3:C:38:ARG:HH21	1.40	0.86
7:G:78:ARG:HD2	7:G:156:TRP:HB2	1.58	0.86
1:A:973:G:H3'	1:A:974:A:H5''	1.57	0.85
1:A:1442:G:N2	1:A:1447:G:N7	2.22	0.85
15:O:29:VAL:HG21	15:O:67:LEU:HD23	1.59	0.85
5:E:11:ILE:HG23	5:E:31:LEU:HB3	1.59	0.84
5:E:84:PHE:HB2	5:E:134:ALA:HB2	1.59	0.84
7:G:5:ARG:HH12	7:G:8:GLU:HG3	1.41	0.84
21:U:12:LYS:O	21:U:22:ARG:NH1	2.11	0.83
1:A:235:C:N4	25:A:1963:HOH:O	2.10	0.83
19:S:31:ILE:HG21	19:S:49:ILE:HD13	1.61	0.83
11:K:65:ALA:HB1	11:K:98:LEU:HD13	1.61	0.82
1:A:1366:C:H2'	1:A:1367:C:H6	1.44	0.82
1:A:1221:G:OP2	19:S:37:ARG:NH2	2.11	0.82
3:C:121:ALA:HA	3:C:124:ILE:HD12	1.61	0.82
1:A:1255:G:N2	1:A:1259:C:O2	2.13	0.82
1:A:1357:A:H2'	1:A:1358:U:C6	2.14	0.81
15:O:38:ARG:HB3	15:O:38:ARG:HH11	1.46	0.81
1:A:138:G:O6	1:A:225:C:N4	2.09	0.81
1:A:1238:A:H5'	1:A:1336:C:H41	1.45	0.81
1:A:1510:U:H2'	1:A:1511:G:C8	2.16	0.81
8:H:11:THR:OG1	8:H:14:ARG:NH1	2.11	0.81
17:Q:27:PHE:CE1	17:Q:36:ILE:HD11	2.15	0.81
18:R:53:ARG:HG2	18:R:63:GLN:HE21	1.46	0.81
5:E:126:ARG:HG2	5:E:126:ARG:HH11	1.46	0.81
13:M:10:PRO:HB2	13:M:18:ALA:HB1	1.60	0.81
1:A:996:A:N1	1:A:1046:A:O2'	2.13	0.81
1:A:1404:5MC:H1'	1:A:1499:A:C2	2.15	0.81
3:C:156:ARG:NH1	3:C:160:ALA:O	2.14	0.80
2:B:12:GLU:HG3	2:B:213:LEU:HD21	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:47:LYS:HG3	12:L:48:PRO:HD3	1.63	0.80
7:G:17:VAL:HG12	7:G:18:TYR:HD1	1.47	0.80
13:M:75:ALA:HA	13:M:78:ILE:HD12	1.64	0.80
1:A:1009:G:H1	1:A:1020:U:H3	1.27	0.80
7:G:5:ARG:HD3	7:G:7:ALA:H	1.47	0.79
8:H:100:ILE:O	8:H:125:ARG:NH2	2.16	0.79
12:L:59:ARG:HH12	12:L:65:GLU:HG3	1.47	0.79
1:A:989:C:O2	1:A:1216:G:N2	2.13	0.79
8:H:69:ARG:NH1	8:H:75:ARG:O	2.15	0.79
1:A:1047:G:OP1	14:N:4:LYS:NZ	2.13	0.79
3:C:134:ILE:HD11	3:C:153:VAL:HB	1.65	0.79
9:I:79:LEU:HD21	9:I:104:ARG:HA	1.65	0.79
9:I:108:VAL:HG12	9:I:109:VAL:H	1.48	0.79
1:A:1280:A:O2'	25:A:2104:HOH:O	2.01	0.78
16:P:67:THR:HB	16:P:70:ALA:H	1.47	0.78
1:A:1163:C:H2'	1:A:1164:G:H8	1.49	0.78
6:F:14:LEU:HB2	6:F:19:LEU:HD12	1.64	0.78
1:A:1101:A:H4'	1:A:1102:A:O5'	1.84	0.77
20:T:12:ALA:HA	25:T:302:HOH:O	1.82	0.77
1:A:130:A:H5'	17:Q:63:ARG:HE	1.50	0.77
7:G:20:ASP:OD1	7:G:22:LEU:N	2.16	0.77
1:A:992:U:H3	1:A:1044:A:H62	1.30	0.77
1:A:1347:G:H3'	9:I:108:VAL:O	1.85	0.77
3:C:167:TRP:HE3	3:C:168:ALA:H	1.32	0.77
1:A:457:C:O2	1:A:475:G:N2	2.11	0.76
1:A:1246:C:H42	1:A:1291:G:H1	1.32	0.76
1:A:1435:G:H2'	1:A:1436:U:C6	2.21	0.76
22:A:1601:SRY:OG2	12:L:91:LYS:NZ	2.17	0.76
10:J:53:PRO:HB3	14:N:42:ILE:HD11	1.68	0.76
3:C:147:LYS:NZ	3:C:206:GLU:OE2	2.18	0.75
9:I:17:VAL:HG11	9:I:81:ILE:HA	1.68	0.75
15:O:67:LEU:HD13	15:O:78:TYR:HE1	1.51	0.75
1:A:1380:U:O2'	1:A:1381:U:OP2	2.04	0.75
8:H:17:THR:O	8:H:78:GLN:NE2	2.20	0.75
12:L:5:PRO:HB2	12:L:10:LEU:HD23	1.68	0.75
4:D:8:VAL:HG11	4:D:21:LEU:HB2	1.68	0.75
12:L:53:ARG:NH1	12:L:92:0TD:OD2	2.20	0.75
1:A:1242:C:H42	1:A:1295:G:H1	1.34	0.74
1:A:448:A:OP2	1:A:485:G:N2	2.16	0.74
1:A:664:G:H22	1:A:741:G:H1	1.33	0.74
1:A:1356:G:H2'	1:A:1357:A:C8	2.23	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:532:A:O2'	1:A:533:A:OP1	2.06	0.73
4:D:28:SER:O	4:D:30:LYS:N	2.21	0.73
1:A:1118:C:H1'	1:A:1179:A:C4	2.23	0.73
1:A:1125:U:H3	10:J:5:ARG:HH21	1.36	0.73
1:A:617:G:H1	1:A:623:C:H42	1.35	0.73
1:A:975:A:H5'	1:A:975:A:H8	1.52	0.73
7:G:38:LEU:O	7:G:42:ILE:HG13	1.89	0.73
20:T:56:MET:HG3	20:T:88:VAL:HG21	1.69	0.72
8:H:82:HIS:CE1	8:H:138:TRP:NE1	2.57	0.72
17:Q:40:LYS:HD3	17:Q:42:TYR:CZ	2.24	0.72
1:A:869:G:N7	25:A:2218:HOH:O	2.21	0.72
1:A:794:A:H8	1:A:794:A:H3'	1.55	0.72
1:A:1195:C:H3'	1:A:1196:U:H5''	1.71	0.72
1:A:1493:A:H2'	1:A:1494:G:H8	1.53	0.72
1:A:914:G:OP1	22:A:1601:SRY:HI33	1.90	0.72
7:G:111:ARG:HD2	7:G:112:PRO:HD2	1.72	0.72
11:K:79:SER:HB3	11:K:106:LYS:HE2	1.71	0.72
1:A:701:C:H4'	1:A:702:A:H5''	1.72	0.72
3:C:25:GLY:HA2	3:C:28:GLN:H	1.54	0.72
1:A:18:C:H5''	5:E:127:ASN:HD21	1.53	0.72
1:A:113:G:H1'	1:A:354:G:H5'	1.72	0.72
2:B:55:PHE:HA	2:B:58:ILE:HD12	1.71	0.72
7:G:15:ASP:OD2	7:G:44:TYR:OH	2.07	0.72
1:A:794:A:H3'	1:A:794:A:C8	2.25	0.71
1:A:1412:C:H2'	1:A:1413:A:C8	2.24	0.71
2:B:184:VAL:HG23	2:B:198:ASP:H	1.55	0.71
1:A:1125:U:OP2	1:A:1145:C:N4	2.23	0.71
2:B:17:PHE:HA	2:B:44:LEU:HD11	1.72	0.71
5:E:147:ASP:OD1	5:E:147:ASP:N	2.12	0.71
12:L:27:LEU:C	12:L:29:GLY:H	1.97	0.71
20:T:56:MET:HE2	20:T:85:MET:HA	1.72	0.71
1:A:1357:A:H2'	1:A:1358:U:H6	1.56	0.71
4:D:152:SER:O	4:D:155:LEU:HG	1.90	0.71
1:A:74:C:O2	1:A:96:G:N2	2.20	0.71
1:A:384:G:H2'	1:A:385:C:H6	1.56	0.71
1:A:1368:G:H5''	9:I:112:LYS:HB3	1.73	0.71
13:M:23:TYR:CB	13:M:67:GLU:HA	2.20	0.71
1:A:1411:C:H42	1:A:1489:G:H1	1.38	0.71
1:A:73:C:H2'	1:A:74:C:H6	1.54	0.71
6:F:4:TYR:HE1	6:F:92:LYS:HG2	1.56	0.71
2:B:205:ASP:OD1	2:B:206:ASP:N	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:C:OP1	12:L:123:LYS:NZ	2.22	0.70
1:A:980:C:H5''	1:A:981:U:H5	1.56	0.70
4:D:187:ARG:HH22	4:D:188:LEU:HD12	1.56	0.70
15:O:4:THR:HG23	15:O:7:GLU:CD	2.15	0.70
1:A:858:G:N7	25:A:2220:HOH:O	2.24	0.70
1:A:1053:G:HO2'	1:A:1199:U:H5	1.39	0.70
1:A:200:G:H1	1:A:217:C:H42	1.38	0.70
20:T:56:MET:HE1	20:T:104:LEU:HD21	1.73	0.70
1:A:1004:A:O2'	1:A:1005:A:O5'	2.08	0.70
9:I:48:GLU:OE2	9:I:51:ARG:NH1	2.24	0.70
2:B:73:THR:HG21	2:B:96:ARG:HD2	1.74	0.70
8:H:95:VAL:HG23	8:H:99:GLU:HB2	1.73	0.70
15:O:87:ILE:HG22	15:O:88:ARG:H	1.54	0.70
2:B:87:ARG:HH21	2:B:233:SER:HB2	1.57	0.70
1:A:1255:G:O6	1:A:1282:C:N4	2.22	0.70
1:A:1518:MA6:H93	1:A:1519:MA6:N1	2.06	0.70
21:U:10:ARG:HD3	21:U:13:ILE:HD12	1.74	0.69
1:A:1168:A:H2'	1:A:1169:A:C8	2.28	0.69
1:A:1236:A:H4'	1:A:1304:G:H4'	1.74	0.69
3:C:155:GLY:HA3	3:C:163:ALA:HB1	1.73	0.69
6:F:4:TYR:HB2	6:F:65:VAL:HG22	1.71	0.69
7:G:92:SER:OG	7:G:95:ARG:N	2.21	0.69
1:A:103:C:P	20:T:17:ARG:HH12	2.15	0.69
1:A:353:A:H5'	1:A:353:A:H8	1.56	0.69
1:A:1358:U:H5''	14:N:35:ARG:HD2	1.73	0.69
1:A:993:G:O6	1:A:1045:C:N4	2.26	0.69
2:B:185:ILE:HA	2:B:199:TYR:O	1.92	0.69
5:E:143:ARG:HH12	8:H:77:GLU:CD	2.01	0.69
22:A:1601:SRV:O61	12:L:46:LYS:HD2	1.93	0.69
4:D:63:LYS:NZ	4:D:197:PRO:O	2.26	0.69
4:D:65:ARG:HG3	4:D:75:PHE:CD1	2.27	0.69
6:F:14:LEU:HD21	6:F:84:ASN:HD22	1.57	0.69
10:J:38:ILE:HG22	10:J:39:PRO:HD2	1.74	0.69
11:K:70:LYS:HA	11:K:73:MET:HE2	1.73	0.69
16:P:68:ASP:OD1	16:P:68:ASP:N	2.24	0.69
13:M:23:TYR:HB3	13:M:67:GLU:HA	1.73	0.69
19:S:22:LEU:HD11	19:S:28:LYS:HB2	1.75	0.69
1:A:36:C:H5''	12:L:123:LYS:HD3	1.75	0.68
1:A:250:A:H4'	1:A:251:G:O5'	1.93	0.68
1:A:827:U:H5''	1:A:828:A:OP2	1.93	0.68
3:C:120:VAL:HG12	3:C:124:ILE:HD11	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:677:U:H3	1:A:713:G:H22	1.40	0.68
1:A:390:C:H4'	16:P:28:ARG:HH21	1.58	0.68
1:A:1329:A:H5'	13:M:29:ARG:HD2	1.75	0.68
1:A:1290:G:H2'	1:A:1291:G:H8	1.58	0.68
19:S:40:ILE:HD11	19:S:62:ILE:HG23	1.75	0.68
1:A:1246:C:N4	1:A:1291:G:H1	1.91	0.68
3:C:89:GLU:HG3	3:C:93:LYS:HZ3	1.58	0.68
1:A:1124:G:H2'	1:A:1145:C:H41	1.59	0.68
3:C:14:ILE:HB	3:C:15:THR:HG23	1.75	0.68
1:A:758:G:C8	25:A:2216:HOH:O	2.47	0.68
17:Q:84:LEU:HD12	17:Q:84:LEU:H	1.59	0.68
1:A:452:A:O2'	1:A:453:A:O5'	2.12	0.68
1:A:501:C:H2'	1:A:502:G:C8	2.28	0.68
1:A:1022:G:N2	1:A:1023:G:O6	2.25	0.68
4:D:119:GLN:HG3	4:D:123:HIS:HD2	1.59	0.68
5:E:105:VAL:HB	5:E:106:PRO:HD3	1.75	0.68
1:A:1338:G:H2'	1:A:1339:A:C8	2.28	0.68
10:J:12:ASP:HB3	10:J:15:THR:HG22	1.76	0.68
13:M:11:ARG:HA	13:M:45:VAL:HG11	1.74	0.68
1:A:505:G:H1	1:A:526:C:H42	1.40	0.67
1:A:1058:G:OP1	3:C:199:LYS:NZ	2.27	0.67
14:N:26:ARG:HD2	14:N:47:LEU:HD11	1.76	0.67
1:A:1095:U:OP1	1:A:1108:G:N2	2.20	0.67
6:F:100:ASN:HB2	18:R:23:LYS:HD2	1.74	0.67
7:G:31:MET:HE1	7:G:36:LYS:HG3	1.75	0.67
1:A:1006:C:H42	1:A:1022:G:H1	1.39	0.67
5:E:145:LYS:O	5:E:148:VAL:HG23	1.94	0.67
10:J:34:VAL:HG13	10:J:74:ILE:HA	1.75	0.67
2:B:7:VAL:HG11	2:B:221:LEU:HD23	1.77	0.67
4:D:68:TYR:OH	4:D:98:GLU:OE1	2.09	0.67
5:E:91:LEU:HB3	5:E:118:ILE:HD11	1.75	0.67
9:I:50:LEU:HD23	9:I:85:LEU:HD13	1.76	0.67
2:B:16:HIS:CE1	2:B:210:SER:HB2	2.30	0.67
1:A:1195:C:H3'	1:A:1196:U:C5'	2.25	0.66
11:K:40:ILE:HG23	11:K:75:TYR:CD2	2.30	0.66
3:C:14:ILE:O	3:C:16:ARG:N	2.28	0.66
7:G:68:ASN:O	7:G:138:LYS:NZ	2.28	0.66
1:A:35:G:H2'	1:A:36:C:H6	1.60	0.66
1:A:1147:C:O2'	9:I:16:ARG:HD3	1.94	0.66
1:A:1164:G:N2	1:A:1172:C:N3	2.42	0.66
1:A:1305:G:OP1	21:U:2:GLY:N	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:187:ARG:NH2	4:D:188:LEU:HB2	2.10	0.66
5:E:118:ILE:C	5:E:119:LEU:HD23	2.21	0.66
1:A:258:G:H2'	1:A:259:G:H8	1.59	0.66
1:A:758:G:N7	25:A:2216:HOH:O	2.28	0.66
17:Q:58:GLU:HB2	17:Q:74:LEU:HB3	1.75	0.66
4:D:13:ARG:NH2	4:D:36:ARG:HH21	1.93	0.66
15:O:28:GLN:O	15:O:32:LEU:HB2	1.95	0.66
16:P:21:VAL:HG21	16:P:59:TRP:CD1	2.31	0.66
4:D:8:VAL:O	4:D:11:LEU:N	2.28	0.66
11:K:91:ARG:HD2	18:R:88:LYS:NZ	2.09	0.66
15:O:36:ILE:HG13	15:O:59:MET:HE2	1.78	0.66
7:G:18:TYR:OH	7:G:58:PRO:HB2	1.96	0.66
1:A:1057:G:H5''	3:C:154:SER:HB2	1.78	0.66
1:A:39:G:N2	1:A:403:C:O2	2.24	0.65
4:D:163:GLU:HG3	4:D:166:LYS:HD2	1.78	0.65
1:A:21:G:N2	1:A:885:G:O3'	2.29	0.65
9:I:114:TYR:HE1	10:J:61:GLU:H	1.44	0.65
12:L:27:LEU:C	12:L:29:GLY:N	2.50	0.65
2:B:162:ILE:HG22	2:B:164:VAL:HG23	1.78	0.65
21:U:10:ARG:HA	21:U:13:ILE:HB	1.79	0.65
18:R:43:PHE:C	18:R:51:LEU:HD12	2.22	0.65
1:A:620:C:H2'	1:A:621:A:O4'	1.97	0.65
1:A:1240:U:OP1	7:G:119:ARG:NH2	2.28	0.65
2:B:19:HIS:HB3	2:B:20:GLU:HG2	1.79	0.65
7:G:18:TYR:HE2	7:G:59:LEU:HA	1.60	0.65
4:D:8:VAL:O	4:D:10:ARG:N	2.29	0.65
5:E:71:LEU:HD21	5:E:115:VAL:HG22	1.78	0.65
11:K:15:ALA:HA	11:K:77:MET:HA	1.79	0.65
18:R:43:PHE:HD2	18:R:56:THR:HG22	1.61	0.65
1:A:532:A:HO2'	1:A:533:A:P	2.20	0.65
4:D:13:ARG:HD2	4:D:38:TYR:O	1.97	0.65
11:K:57:THR:HG23	11:K:60:ALA:H	1.62	0.65
14:N:26:ARG:HB2	14:N:43:CYS:SG	2.37	0.65
1:A:1060:C:OP1	14:N:45:ARG:NH2	2.30	0.65
1:A:1126:U:H3	1:A:1149:C:H1'	1.62	0.65
1:A:1413:A:H2	1:A:1487:G:H22	1.45	0.65
9:I:8:GLY:HA3	9:I:79:LEU:HB3	1.79	0.65
12:L:38:THR:HG22	12:L:39:VAL:HG13	1.78	0.65
8:H:123:GLU:O	8:H:127:LEU:HB2	1.97	0.64
18:R:87:ARG:HD3	18:R:87:ARG:N	2.12	0.64
1:A:1505:G:C8	1:A:1505:G:H3'	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:21:VAL:HG12	16:P:33:ILE:HD12	1.78	0.64
7:G:26:PHE:HD1	7:G:101:LEU:HD22	1.62	0.64
11:K:32:ILE:HD11	11:K:68:ALA:HB1	1.78	0.64
1:A:1255:G:O2'	1:A:1258:G:H1'	1.97	0.64
1:A:673:G:H2'	1:A:674:G:C8	2.33	0.64
9:I:22:GLY:N	9:I:58:HIS:O	2.25	0.64
1:A:1097:C:H2'	1:A:1098:C:C6	2.32	0.64
2:B:97:TRP:HZ2	2:B:102:LEU:HD22	1.62	0.64
9:I:4:TYR:CD1	9:I:88:TYR:HB2	2.33	0.64
1:A:691:G:H2'	1:A:692:U:C6	2.33	0.63
6:F:4:TYR:CE1	6:F:92:LYS:HG2	2.33	0.63
8:H:35:ILE:O	8:H:39:LEU:HD22	1.98	0.63
1:A:35:G:H2'	1:A:36:C:C6	2.33	0.63
12:L:113:ARG:HH11	12:L:113:ARG:HG3	1.61	0.63
7:G:91:VAL:HG12	7:G:95:ARG:HB3	1.78	0.63
1:A:1003(A):G:N2	1:A:1038:C:O2'	2.18	0.63
1:A:1305:G:N2	1:A:1331:G:H1'	2.14	0.63
3:C:25:GLY:HA2	3:C:28:GLN:N	2.14	0.63
2:B:95:GLN:HG3	2:B:148:TYR:HA	1.79	0.63
15:O:33:THR:HG21	15:O:85:LEU:HD13	1.81	0.63
20:T:71:THR:O	20:T:72:LEU:HD23	1.99	0.63
1:A:384:G:H2'	1:A:385:C:C6	2.33	0.63
1:A:451:A:N6	1:A:481:G:C4	2.67	0.63
5:E:17:ALA:HB2	5:E:26:PHE:HD2	1.64	0.63
4:D:107:ARG:HH21	4:D:194:LEU:HD11	1.63	0.63
13:M:40:ASN:HB3	13:M:43:THR:HG23	1.80	0.63
1:A:62:U:O2'	1:A:379:C:O2	2.15	0.62
1:A:953:G:H5'	1:A:965:A:H61	1.64	0.62
3:C:88:ARG:HE	3:C:100:ALA:HB1	1.63	0.62
9:I:51:ARG:HG2	9:I:56:LEU:HG	1.81	0.62
4:D:173:TRP:CE2	4:D:189:PRO:HB3	2.34	0.62
10:J:61:GLU:OE1	14:N:45:ARG:NH1	2.27	0.62
1:A:691:G:H2'	1:A:692:U:H6	1.65	0.62
1:A:1183:A:O2'	1:A:1184:G:OP1	2.16	0.62
2:B:97:TRP:CZ2	2:B:102:LEU:HD22	2.34	0.62
3:C:148:GLY:HA3	3:C:172:ARG:O	2.00	0.62
12:L:126:LYS:HB2	12:L:126:LYS:HZ2	1.63	0.62
5:E:84:PHE:CE1	5:E:133:TYR:HB3	2.35	0.62
8:H:10:LEU:HD22	8:H:83:ILE:HD13	1.82	0.62
10:J:76:ASN:O	10:J:78:ASN:HB2	2.00	0.62
6:F:8:ILE:HD12	6:F:26:ILE:HD13	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:40:ILE:HG23	11:K:75:TYR:HD2	1.64	0.62
12:L:87:GLY:HA2	12:L:98:TYR:CA	2.26	0.62
12:L:82:VAL:HG12	12:L:106:ASP:OD1	2.00	0.62
1:A:413:G:O2'	1:A:428:G:N2	2.32	0.62
1:A:980:C:H5''	1:A:981:U:C5	2.34	0.62
3:C:120:VAL:O	3:C:124:ILE:HG13	2.00	0.62
1:A:191:G:O2'	20:T:101:GLY:O	2.17	0.61
1:A:826:C:O2	8:H:15:ASN:ND2	2.32	0.61
3:C:202:ILE:HG22	3:C:204:LEU:HD23	1.82	0.61
19:S:14:HIS:CE1	19:S:35:SER:HB2	2.35	0.61
1:A:328:C:O2	1:A:328:C:H2'	2.00	0.61
1:A:375:U:OP1	16:P:69:THR:HG21	2.00	0.61
1:A:129:U:O3'	1:A:129(A):G:H3'	2.00	0.61
1:A:838:G:H2'	1:A:839:U:H5''	1.82	0.61
10:J:76:ASN:HB3	10:J:78:ASN:CG	2.26	0.61
1:A:9:G:OP1	5:E:122:GLU:HG3	2.00	0.61
1:A:345:C:OP2	1:A:345:C:H6	1.84	0.61
5:E:80:ILE:HD12	5:E:80:ILE:H	1.65	0.61
13:M:16:ASP:OD1	13:M:16:ASP:N	2.33	0.61
2:B:87:ARG:HB3	2:B:87:ARG:HH11	1.66	0.61
9:I:51:ARG:NH1	9:I:51:ARG:HB2	2.15	0.61
15:O:26:GLU:HA	15:O:81:LEU:HD11	1.83	0.61
1:A:344:A:H5'	1:A:345:C:C5	2.35	0.61
1:A:560:U:H5'	1:A:566:G:N2	2.16	0.61
1:A:682:G:H1	1:A:708:C:H42	1.47	0.61
1:A:1300:G:O2'	1:A:1301:U:OP2	2.10	0.61
3:C:89:GLU:HG3	3:C:93:LYS:NZ	2.15	0.61
6:F:35:ALA:HA	6:F:67:MET:HB3	1.82	0.61
16:P:74:LEU:HD13	16:P:79:VAL:HG21	1.83	0.61
1:A:551:U:O2'	12:L:86:ARG:HD2	2.01	0.61
1:A:975:A:H5'	1:A:975:A:C8	2.34	0.60
1:A:1381:U:H2'	1:A:1382:C:H6	1.66	0.60
1:A:427:U:OP1	4:D:13:ARG:NH2	2.34	0.60
1:A:757:U:H2'	1:A:758:G:O4'	2.01	0.60
8:H:20:TYR:CE1	8:H:76:PRO:HG2	2.36	0.60
12:L:27:LEU:HG	12:L:28:LYS:H	1.66	0.60
1:A:981:U:H5'	14:N:21:TYR:CZ	2.36	0.60
1:A:695:A:OP2	11:K:53:SER:N	2.32	0.60
1:A:269:C:H2'	1:A:270:A:C8	2.36	0.60
1:A:789:U:O2'	1:A:791:G:N7	2.33	0.60
7:G:20:ASP:OD1	7:G:21:VAL:N	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:G:O2'	1:A:22:G:OP1	2.12	0.60
1:A:671:G:H1	1:A:735:C:H42	1.49	0.60
6:F:80:ARG:NH1	6:F:88:VAL:O	2.30	0.60
8:H:9:MET:HG3	8:H:26:VAL:HG21	1.84	0.60
1:A:1238:A:H5'	1:A:1336:C:N4	2.16	0.60
2:B:61:LEU:HD11	2:B:160:ASP:HB3	1.82	0.60
2:B:87:ARG:NH1	2:B:230:VAL:HG21	2.17	0.60
7:G:60:LYS:HZ3	7:G:63:LYS:HD2	1.66	0.60
8:H:82:HIS:HE1	8:H:138:TRP:HE1	1.50	0.60
9:I:53:VAL:HG21	9:I:85:LEU:HD11	1.84	0.60
18:R:56:THR:HB	18:R:58:LEU:HG	1.84	0.60
1:A:1191:A:OP1	3:C:3:ASN:HB2	2.02	0.60
2:B:70:PHE:HE1	2:B:90:MET:HG3	1.67	0.60
18:R:53:ARG:HG2	18:R:63:GLN:NE2	2.13	0.60
6:F:7:ASN:HD21	18:R:34:TYR:HE1	1.49	0.60
7:G:70:LYS:HD3	7:G:96:GLN:HB3	1.84	0.60
13:M:23:TYR:HB2	13:M:67:GLU:HG2	1.82	0.60
1:A:665:A:N3	1:A:732:C:H2'	2.17	0.60
1:A:1182:G:H4'	1:A:1183:A:H5''	1.81	0.60
3:C:153:VAL:HG23	3:C:198:VAL:HG13	1.84	0.60
9:I:114:TYR:HD1	10:J:60:ARG:HB2	1.66	0.60
1:A:73:C:H2'	1:A:74:C:C6	2.35	0.59
1:A:279:A:OP1	1:A:280:C:O2'	2.13	0.59
2:B:117:GLU:O	2:B:120:ALA:HB3	2.01	0.59
3:C:34:LEU:HD13	3:C:38:ARG:NH2	2.15	0.59
4:D:31:CYS:C	4:D:33:MET:H	2.08	0.59
4:D:165:MET:HA	4:D:165:MET:HE3	1.83	0.59
5:E:118:ILE:O	5:E:119:LEU:HD23	2.02	0.59
15:O:55:GLY:HA2	15:O:58:MET:HE2	1.84	0.59
16:P:43:LYS:HA	16:P:48:TRP:HB3	1.84	0.59
1:A:279:A:OP2	17:Q:95:TYR:OH	2.06	0.59
17:Q:27:PHE:CZ	17:Q:36:ILE:HD11	2.36	0.59
8:H:97:VAL:HA	8:H:100:ILE:HD11	1.83	0.59
18:R:39:VAL:HG13	18:R:40:LEU:HD23	1.84	0.59
1:A:349:A:H2'	1:A:350:G:H5''	1.85	0.59
2:B:82:ARG:HG2	2:B:92:TYR:HE1	1.65	0.59
3:C:88:ARG:CG	3:C:101:LEU:HB2	2.32	0.59
9:I:70:LYS:NZ	9:I:73:GLN:OE1	2.36	0.59
1:A:179:A:H2'	1:A:180:U:C6	2.38	0.59
1:A:1150:U:O4	1:A:1151:A:N6	2.35	0.59
1:A:653:A:P	8:H:56:LYS:HZ1	2.25	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:26:GLU:OE1	15:O:77:ARG:HD2	2.01	0.59
20:T:14:LYS:O	20:T:18:GLN:HG2	2.03	0.59
1:A:552:U:H2'	1:A:553:A:C8	2.38	0.59
1:A:1026:G:O2'	1:A:1027:C:OP1	2.18	0.59
1:A:1376:U:OP1	7:G:98:SER:OG	2.16	0.59
2:B:82:ARG:HA	2:B:92:TYR:CE1	2.38	0.59
15:O:42:HIS:C	15:O:42:HIS:CD2	2.79	0.59
18:R:26:LEU:HD23	18:R:29:PHE:CE2	2.37	0.59
1:A:200:G:H2'	1:A:201:C:O4'	2.02	0.59
1:A:1121:U:H2'	1:A:1122:U:H6	1.68	0.59
1:A:1180:A:OP1	9:I:103:THR:OG1	2.21	0.59
20:T:75:ASN:N	20:T:75:ASN:OD1	2.35	0.59
12:L:11:VAL:HG22	17:Q:29:HIS:CD2	2.38	0.59
16:P:69:THR:HA	16:P:72:ARG:HG2	1.83	0.59
1:A:489:C:H2'	1:A:490:G:H8	1.67	0.58
1:A:1255:G:H2'	1:A:1279:A:H61	1.68	0.58
2:B:15:VAL:HG13	2:B:209:ARG:HB3	1.83	0.58
5:E:43:LEU:HD23	5:E:44:GLY:N	2.17	0.58
1:A:5:U:H4'	1:A:6:G:O5'	2.02	0.58
1:A:509:A:C8	1:A:509:A:H3'	2.38	0.58
1:A:1004:A:H4'	1:A:1005:A:OP1	2.03	0.58
1:A:1541:PSU:H3'	1:A:1541:PSU:H6	1.68	0.58
4:D:170:VAL:HG22	4:D:174:LEU:HD12	1.85	0.58
9:I:26:VAL:HG12	9:I:61:ALA:HB3	1.85	0.58
11:K:124:LYS:HG3	11:K:125:PHE:CD2	2.39	0.58
18:R:43:PHE:O	18:R:51:LEU:HD12	2.03	0.58
1:A:353:A:H5'	1:A:353:A:C8	2.38	0.58
1:A:526:C:O3'	22:A:1601:SRY:HI31	2.03	0.58
7:G:122:HIS:O	7:G:126:ASP:HB2	2.02	0.58
6:F:48:LEU:HG	6:F:57:GLN:HA	1.84	0.58
12:L:42:THR:HA	12:L:53:ARG:O	2.04	0.58
14:N:39:LEU:HB3	14:N:43:CYS:HB3	1.86	0.58
1:A:89:C:O2'	1:A:90:U:H5'	2.02	0.58
1:A:945:G:O6	1:A:1236:A:N1	2.36	0.58
1:A:1240:U:C2	7:G:32:ARG:HD2	2.37	0.58
4:D:65:ARG:HD2	4:D:72:GLU:HA	1.86	0.58
7:G:70:LYS:HG2	7:G:100:ALA:HB2	1.84	0.58
12:L:84:LEU:HD23	12:L:101:VAL:HG21	1.86	0.58
1:A:1029:C:N4	1:A:1032:G:H1	2.01	0.58
1:A:1474:G:H2'	1:A:1475:G:H8	1.67	0.58
4:D:30:LYS:O	4:D:32:ALA:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:55:ALA:O	4:D:59:ARG:HG2	2.04	0.58
5:E:90:VAL:C	5:E:91:LEU:HD23	2.28	0.58
17:Q:4:LYS:HG2	17:Q:6:LEU:HD21	1.86	0.58
2:B:18:GLY:HA3	2:B:42:ILE:H	1.69	0.58
9:I:48:GLU:N	9:I:49:PRO:HD2	2.19	0.58
15:O:38:ARG:HB3	15:O:38:ARG:NH1	2.16	0.58
1:A:1225:A:H2'	1:A:1225:A:N3	2.18	0.57
1:A:1242:C:N4	1:A:1295:G:H1	2.01	0.57
5:E:83:GLU:HG2	5:E:88:LYS:HG3	1.86	0.57
8:H:100:ILE:HG23	8:H:112:LEU:HD11	1.85	0.57
20:T:45:GLN:HB3	20:T:91:LEU:HD13	1.86	0.57
6:F:15:ASP:HB3	6:F:18:GLN:NE2	2.19	0.57
10:J:12:ASP:OD2	10:J:15:THR:N	2.31	0.57
16:P:28:ARG:HD2	16:P:29:ASP:OD2	2.04	0.57
1:A:616:G:H1	1:A:624:C:H42	1.52	0.57
1:A:859:A:OP2	1:A:869:G:N1	2.33	0.57
1:A:1493:A:H2'	1:A:1494:G:C8	2.37	0.57
7:G:47:CYS:HB3	7:G:58:PRO:HG2	1.85	0.57
10:J:27:ALA:O	10:J:30:SER:OG	2.22	0.57
11:K:99:GLN:NE2	11:K:105:VAL:HG21	2.19	0.57
18:R:22:VAL:HG23	18:R:56:THR:HA	1.85	0.57
21:U:6:ARG:HG2	21:U:15:ARG:HE	1.69	0.57
1:A:258:G:H2'	1:A:259:G:C8	2.38	0.57
1:A:1223:C:H5''	1:A:1224:G:H5''	1.85	0.57
5:E:15:ARG:HG2	5:E:15:ARG:HH11	1.69	0.57
1:A:939:G:H5''	7:G:102:ARG:HH22	1.69	0.57
1:A:1121:U:H2'	1:A:1122:U:C6	2.40	0.57
2:B:112:VAL:O	2:B:115:LEU:N	2.37	0.57
16:P:53:VAL:O	16:P:55:ARG:N	2.38	0.57
19:S:22:LEU:HG	19:S:28:LYS:HD2	1.85	0.57
1:A:184:G:H2'	1:A:185:A:C8	2.39	0.57
1:A:1347:G:N2	1:A:1374:A:OP2	2.26	0.57
2:B:17:PHE:HD1	2:B:18:GLY:N	2.02	0.57
2:B:189:ASP:HB3	2:B:203:GLY:O	2.05	0.57
4:D:31:CYS:O	4:D:31:CYS:SG	2.62	0.57
1:A:1510:U:H2'	1:A:1511:G:H8	1.67	0.57
2:B:92:TYR:CD2	2:B:151:GLY:HA3	2.40	0.57
11:K:121:PRO:HD2	11:K:126:ARG:HD2	1.85	0.57
16:P:53:VAL:HG23	16:P:54:GLU:H	1.70	0.57
1:A:695:A:OP2	11:K:52:GLY:HA3	2.05	0.57
11:K:82:VAL:O	11:K:109:VAL:HG23	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:U:O2'	1:A:84:U:H5'	2.05	0.57
1:A:416:G:H2'	1:A:417:C:C6	2.40	0.57
1:A:1404:5MC:H1'	1:A:1499:A:H2	1.66	0.57
2:B:29:ALA:HA	2:B:32:ILE:HG13	1.87	0.57
5:E:130:ASN:N	5:E:130:ASN:OD1	2.35	0.57
9:I:15:ALA:HA	9:I:65:VAL:HB	1.85	0.57
1:A:254:G:OP1	17:Q:67:LYS:O	2.23	0.56
1:A:1329:A:P	13:M:28:ALA:HB3	2.45	0.56
7:G:5:ARG:NH1	7:G:8:GLU:H	2.03	0.56
17:Q:66:SER:O	17:Q:70:ARG:NH1	2.38	0.56
1:A:95:U:H2'	1:A:96:G:C8	2.39	0.56
1:A:401:C:H2'	1:A:402:G:H8	1.71	0.56
13:M:22:ILE:HG22	13:M:23:TYR:N	2.20	0.56
16:P:78:GLY:C	16:P:80:PHE:N	2.59	0.56
17:Q:29:HIS:CG	17:Q:30:PRO:HD2	2.40	0.56
1:A:1325:C:OP1	21:U:15:ARG:HD3	2.05	0.56
1:A:1427:U:H2'	1:A:1428:A:C8	2.41	0.56
5:E:31:LEU:HD21	5:E:43:LEU:HD21	1.88	0.56
9:I:32:ASP:OD1	9:I:33:PHE:N	2.38	0.56
13:M:8:GLU:CD	13:M:22:ILE:HA	2.31	0.56
17:Q:58:GLU:CB	17:Q:74:LEU:HB3	2.34	0.56
21:U:6:ARG:O	21:U:12:LYS:HE3	2.04	0.56
3:C:44:GLU:HA	3:C:52:LEU:HD21	1.87	0.56
1:A:17:U:H2'	1:A:18:C:C6	2.39	0.56
3:C:22:TRP:HB3	3:C:59:ARG:HB2	1.86	0.56
13:M:5:ALA:HB2	13:M:22:ILE:HD13	1.88	0.56
1:A:203:U:P	1:A:203:U:H3'	2.45	0.56
1:A:357:G:C2	1:A:358:U:C5	2.94	0.56
1:A:489:C:H2'	1:A:490:G:C8	2.41	0.56
1:A:837:G:C2	1:A:850:U:O2	2.59	0.56
1:A:1505:G:H3'	1:A:1505:G:H8	1.69	0.56
6:F:50:TYR:CE1	18:R:77:GLY:HA2	2.40	0.56
9:I:97:LYS:N	9:I:98:PRO:HD2	2.20	0.56
14:N:37:PHE:HD1	14:N:44:LEU:HD13	1.71	0.56
1:A:262:A:H5'	20:T:74:LYS:HG3	1.87	0.56
1:A:928:G:O2'	1:A:1533:C:OP1	2.21	0.56
1:A:1141:C:H2'	1:A:1142:G:C8	2.41	0.56
1:A:1234:C:H1'	1:A:1364:U:O2	2.05	0.56
2:B:240:GLN:OE1	2:B:240:GLN:N	2.39	0.56
6:F:11:ASN:HB2	6:F:86:ARG:CZ	2.36	0.56
16:P:57:ARG:HG3	16:P:79:VAL:HG12	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:C:H42	1:A:357:G:H1	1.54	0.56
1:A:939:G:H5''	7:G:102:ARG:NH2	2.20	0.56
5:E:146:ALA:O	5:E:149:GLU:HB2	2.05	0.56
10:J:78:ASN:O	10:J:82:ILE:HB	2.06	0.56
13:M:86:CYS:SG	13:M:87:TYR:N	2.78	0.56
19:S:16:LEU:O	19:S:20:LEU:HB2	2.05	0.56
1:A:976:G:H5''	1:A:1358:U:O2	2.06	0.56
1:A:1303:C:C2'	1:A:1304:G:H5'	2.36	0.56
6:F:77:ARG:O	6:F:81:ILE:HG13	2.05	0.56
12:L:60:LEU:N	12:L:64:TYR:O	2.38	0.56
16:P:78:GLY:C	16:P:80:PHE:H	2.12	0.56
19:S:19:VAL:HA	19:S:22:LEU:HB3	1.88	0.56
1:A:695:A:C2	1:A:787:A:H1'	2.41	0.56
1:A:1190:G:OP1	3:C:4:LYS:HA	2.06	0.56
1:A:1301:U:O2'	1:A:1302:U:H3'	2.07	0.56
5:E:80:ILE:HD12	5:E:80:ILE:N	2.20	0.56
18:R:43:PHE:CG	18:R:66:LEU:HD21	2.41	0.56
2:B:162:ILE:O	2:B:185:ILE:HG12	2.06	0.55
8:H:82:HIS:HE1	8:H:138:TRP:NE1	2.01	0.55
18:R:60:ALA:O	18:R:64:ARG:HG3	2.06	0.55
1:A:420:U:H3'	1:A:422:C:H41	1.71	0.55
1:A:572:A:H5'	1:A:573:A:OP2	2.06	0.55
1:A:1366:C:H2'	1:A:1367:C:C6	2.34	0.55
2:B:115:LEU:HD23	2:B:145:LEU:CB	2.36	0.55
1:A:1198:G:H2'	1:A:1199:U:C6	2.42	0.55
1:A:1531:A:O5'	1:A:1531:A:H8	1.89	0.55
2:B:54:THR:HG22	2:B:58:ILE:HD11	1.88	0.55
6:F:3:ARG:O	6:F:93:SER:HB2	2.06	0.55
12:L:62:SER:HB2	12:L:64:TYR:HB2	1.87	0.55
15:O:39:LEU:CD2	15:O:56:LEU:HB2	2.32	0.55
17:Q:81:ARG:NE	17:Q:84:LEU:HD11	2.22	0.55
1:A:481:G:O2'	1:A:482:A:H8	1.89	0.55
6:F:4:TYR:HD1	6:F:92:LYS:HA	1.72	0.55
7:G:60:LYS:HA	7:G:63:LYS:HB3	1.88	0.55
9:I:50:LEU:HD11	9:I:81:ILE:HD12	1.87	0.55
9:I:63:ILE:HG21	9:I:77:ILE:HG12	1.88	0.55
13:M:79:LYS:HA	13:M:82:MET:HE3	1.88	0.55
1:A:447:G:H2'	1:A:485:G:N2	2.22	0.55
1:A:665:A:C2	1:A:732:C:C2	2.94	0.55
2:B:162:ILE:CG2	2:B:164:VAL:HG23	2.37	0.55
1:A:1001:A:H2'	1:A:1002:G:H8	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:U:C2'	1:A:84:U:H5'	2.36	0.55
5:E:28:PHE:CD1	5:E:51:VAL:HG23	2.42	0.55
7:G:65:ALA:O	7:G:69:VAL:HG23	2.07	0.55
1:A:653:A:OP1	8:H:56:LYS:NZ	2.39	0.55
2:B:115:LEU:HD23	2:B:145:LEU:HB3	1.89	0.55
9:I:10:ARG:HD3	9:I:105:ASP:HB3	1.88	0.55
13:M:91:ARG:HB2	13:M:98:VAL:HG22	1.89	0.55
1:A:1255:G:H2'	1:A:1279:A:N6	2.21	0.55
1:A:280:C:H4'	1:A:281:G:OP2	2.07	0.54
1:A:1138:G:O2'	1:A:1140:C:H5'	2.06	0.54
4:D:127:THR:HG23	4:D:147:ALA:O	2.07	0.54
9:I:63:ILE:HD13	9:I:77:ILE:HG23	1.89	0.54
12:L:53:ARG:HG2	12:L:69:TYR:HE1	1.72	0.54
16:P:17:TYR:HE1	16:P:41:PRO:HG3	1.72	0.54
1:A:1011:G:H2'	1:A:1012:U:O4'	2.08	0.54
1:A:1127:G:H2'	1:A:1127:G:N3	2.22	0.54
10:J:82:ILE:HG22	10:J:83:GLU:OE1	2.06	0.54
1:A:80:G:H1	1:A:89:C:H42	1.56	0.54
1:A:390:C:O3'	16:P:28:ARG:NH2	2.40	0.54
1:A:457:C:H2'	1:A:458:C:C6	2.42	0.54
1:A:1163:C:C2'	1:A:1164:G:H5'	2.37	0.54
1:A:1351:U:H4'	7:G:33:ASP:CG	2.32	0.54
2:B:142:LEU:HD13	2:B:146:GLN:NE2	2.23	0.54
3:C:11:ARG:NH1	3:C:177:THR:O	2.40	0.54
15:O:15:PHE:CZ	15:O:85:LEU:HD21	2.43	0.54
20:T:29:LYS:O	20:T:32:ALA:HB3	2.06	0.54
1:A:525:C:H2'	1:A:526:C:C6	2.42	0.54
1:A:1303:C:H2'	1:A:1304:G:H5'	1.89	0.54
2:B:134:GLU:O	2:B:138:LEU:HG	2.07	0.54
1:A:1048:G:H2'	1:A:1050:G:C8	2.43	0.54
1:A:1054:C:OP1	1:A:1197:G:OP1	2.25	0.54
6:F:4:TYR:CD1	6:F:92:LYS:HA	2.42	0.54
1:A:858:G:O2'	1:A:859:A:H5''	2.08	0.54
1:A:946:A:H2'	1:A:947:G:C8	2.42	0.54
1:A:1243:C:H2'	1:A:1244:C:C6	2.43	0.54
1:A:1243:C:H2'	1:A:1244:C:H6	1.73	0.54
2:B:20:GLU:OE1	2:B:23:ARG:NH2	2.41	0.54
5:E:81:GLU:HG2	5:E:90:VAL:HG13	1.90	0.54
12:L:82:VAL:O	12:L:106:ASP:HB2	2.08	0.54
15:O:82:ILE:HD12	15:O:87:ILE:HB	1.90	0.54
19:S:28:LYS:HG2	19:S:29:ARG:H	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:39:THR:HG23	19:S:70:LYS:HE2	1.88	0.54
21:U:5:ASP:HB3	21:U:8:THR:OG1	2.08	0.54
1:A:92:C:O2'	1:A:93:G:H5'	2.07	0.54
1:A:139:G:C2'	1:A:140:A:H5'	2.37	0.54
1:A:269:C:H2'	1:A:270:A:H8	1.71	0.54
1:A:731:G:OP1	1:A:766:A:H1'	2.07	0.54
1:A:955:U:H2'	1:A:956:U:H6	1.73	0.54
2:B:21:ARG:HG3	2:B:22:LYS:H	1.72	0.54
13:M:40:ASN:ND2	13:M:42:ALA:HB3	2.22	0.54
15:O:21:ASP:OD1	15:O:24:SER:OG	2.25	0.54
1:A:413:G:N2	1:A:429:U:OP2	2.28	0.54
1:A:1000:U:H3	1:A:1041:A:H61	1.55	0.54
1:A:1179:A:H2'	1:A:1180:A:O4'	2.07	0.54
7:G:91:VAL:HG21	7:G:96:GLN:HG3	1.90	0.54
17:Q:97:SER:OG	17:Q:98:LEU:N	2.40	0.54
1:A:912:C:O2'	1:A:913:A:H5'	2.08	0.54
2:B:92:TYR:H	2:B:92:TYR:HD2	1.55	0.54
3:C:156:ARG:H	3:C:163:ALA:HA	1.72	0.54
6:F:60:PHE:CZ	18:R:78:LEU:HD21	2.42	0.54
18:R:59:SER:O	18:R:63:GLN:N	2.35	0.54
1:A:411:A:C5	1:A:413:G:H1'	2.43	0.54
1:A:551:U:H2'	1:A:552:U:C6	2.43	0.54
4:D:52:SER:O	4:D:56:VAL:HG23	2.07	0.54
5:E:11:ILE:CG2	5:E:31:LEU:HB3	2.34	0.54
5:E:86:ALA:HB3	5:E:125:SER:HB3	1.90	0.54
1:A:1357:A:H2'	1:A:1358:U:C5	2.43	0.53
2:B:163:PHE:CD1	2:B:185:ILE:HG13	2.43	0.53
18:R:59:SER:H	18:R:62:GLU:HB2	1.72	0.53
19:S:63:THR:HB	19:S:66:MET:HG3	1.90	0.53
1:A:686:U:O2'	1:A:687:A:C8	2.60	0.53
1:A:1185:G:C2'	1:A:1186:G:H5'	2.38	0.53
1:A:1191:A:H5''	3:C:4:LYS:HE3	1.90	0.53
1:A:1332:A:H5'	1:A:1332:A:H8	1.72	0.53
11:K:31:THR:C	11:K:32:ILE:HD13	2.33	0.53
4:D:111:ALA:HB2	4:D:120:LEU:HD12	1.90	0.53
10:J:79:ARG:HB2	10:J:80:LYS:HD2	1.89	0.53
14:N:15:LYS:HE3	14:N:16:PHE:CE1	2.43	0.53
16:P:66:PRO:HD2	16:P:71:ARG:HH12	1.73	0.53
1:A:673:G:H5''	6:F:87:ARG:NH1	2.22	0.53
1:A:1403:C:H2'	1:A:1404:5MC:C6	2.43	0.53
9:I:29:ASN:O	9:I:29:ASN:ND2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:6:ILE:HB	10:J:72:VAL:HB	1.90	0.53
1:A:335:C:O2'	1:A:1433:A:N3	2.36	0.53
1:A:1141:C:H2'	1:A:1142:G:H8	1.73	0.53
4:D:107:ARG:HH21	4:D:194:LEU:CD1	2.22	0.53
5:E:15:ARG:HG2	5:E:15:ARG:NH1	2.24	0.53
10:J:45:ARG:HD2	14:N:36:PHE:CE2	2.43	0.53
16:P:53:VAL:O	16:P:54:GLU:C	2.51	0.53
1:A:172:A:H2'	1:A:173:U:H5'	1.91	0.53
1:A:299:G:C6	1:A:300:A:C6	2.97	0.53
1:A:481:G:HO2'	1:A:482:A:H8	1.54	0.53
1:A:617:G:H1	1:A:623:C:N4	2.04	0.53
2:B:219:VAL:HA	2:B:222:ILE:HD12	1.91	0.53
7:G:151:TYR:O	7:G:154:TYR:HB2	2.09	0.53
12:L:25:PRO:HB3	12:L:27:LEU:HD13	1.91	0.53
12:L:58:VAL:O	12:L:65:GLU:HA	2.09	0.53
15:O:27:VAL:O	15:O:31:LEU:HB2	2.08	0.53
18:R:43:PHE:CD2	18:R:56:THR:HG22	2.43	0.53
1:A:476:G:H2'	1:A:477:G:C8	2.44	0.53
1:A:1145:C:O2'	1:A:1146:A:O5'	2.22	0.53
1:A:1212:U:O2'	1:A:1213:A:O5'	2.21	0.53
1:A:1270:C:OP2	21:U:24:ARG:NH2	2.42	0.53
3:C:43:LEU:HA	3:C:47:LEU:HD13	1.90	0.53
3:C:121:ALA:HB2	3:C:198:VAL:HG21	1.91	0.53
1:A:130:A:OP2	1:A:190(E):U:O2'	2.13	0.53
1:A:981:U:H5'	14:N:21:TYR:OH	2.09	0.53
4:D:92:VAL:O	4:D:96:LEU:HD13	2.09	0.53
12:L:93:LEU:O	12:L:96:VAL:HG23	2.09	0.53
12:L:113:ARG:HG3	12:L:113:ARG:NH1	2.23	0.53
1:A:328:C:O2'	1:A:329:A:OP2	2.13	0.53
1:A:1229:A:OP1	13:M:114:ARG:HD3	2.08	0.53
5:E:126:ARG:HH11	5:E:126:ARG:CG	2.18	0.53
9:I:126:SER:OG	9:I:127:LYS:HD2	2.09	0.53
14:N:39:LEU:HB3	14:N:43:CYS:CB	2.39	0.53
1:A:79:G:H1	1:A:90:U:H3	1.57	0.52
1:A:299:G:H2'	1:A:300:A:C8	2.44	0.52
1:A:434:U:H2'	1:A:435:C:C6	2.44	0.52
1:A:902:G:H2'	1:A:903:G:H8	1.74	0.52
1:A:922:G:C6	1:A:923:A:C6	2.97	0.52
1:A:1287:A:H2	1:A:1353:G:N3	2.06	0.52
3:C:26:LYS:NZ	10:J:45:ARG:HH22	2.06	0.52
4:D:35:ARG:O	4:D:36:ARG:HG3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:2:ALA:O	13:M:10:PRO:HD2	2.09	0.52
16:P:3:LYS:HD3	16:P:24:ALA:HB2	1.90	0.52
1:A:977:A:N6	25:A:2230:HOH:O	2.42	0.52
1:A:1066:C:H2'	1:A:1067:A:H5'	1.91	0.52
1:A:1250:A:H4'	9:I:68:GLY:N	2.24	0.52
1:A:1426:C:H42	1:A:1474:G:H1	1.56	0.52
6:F:67:MET:HB2	6:F:68:PRO:HD2	1.90	0.52
8:H:58:TYR:O	8:H:59:LEU:HD23	2.08	0.52
10:J:22:LYS:O	10:J:25:GLU:HB2	2.09	0.52
17:Q:90:ILE:O	17:Q:93:GLN:HB2	2.09	0.52
1:A:144:G:H1	1:A:178:C:H42	1.57	0.52
1:A:390:C:H4'	16:P:28:ARG:NH2	2.23	0.52
1:A:788:U:H5''	1:A:789:U:OP2	2.08	0.52
1:A:1228:C:OP1	13:M:115:LYS:HG3	2.09	0.52
4:D:36:ARG:HG2	4:D:38:TYR:OH	2.09	0.52
16:P:38:TYR:O	16:P:49:LEU:HD12	2.10	0.52
17:Q:27:PHE:O	17:Q:36:ILE:HD13	2.09	0.52
20:T:21:LYS:O	20:T:24:LEU:HB3	2.09	0.52
1:A:804:U:H5''	1:A:805:C:OP2	2.10	0.52
1:A:818:G:H3'	1:A:819:A:H5''	1.91	0.52
2:B:25:ASN:OD1	2:B:27:LYS:N	2.38	0.52
8:H:96:GLY:O	8:H:97:VAL:C	2.52	0.52
10:J:37:PRO:HA	10:J:72:VAL:H	1.74	0.52
1:A:527:7MG:OP2	22:A:1601:SRV:O32	2.25	0.52
1:A:765:G:H5''	1:A:766:A:OP1	2.08	0.52
1:A:794:A:C8	1:A:794:A:C3'	2.90	0.52
1:A:112:G:C2'	1:A:113:G:H5'	2.39	0.52
1:A:1128:C:O2'	1:A:1130:A:OP2	2.23	0.52
1:A:1358:U:H5''	14:N:35:ARG:CD	2.40	0.52
1:A:1502:A:H2	1:A:1505:G:H1	1.57	0.52
2:B:158:LEU:HD23	2:B:159:PRO:CD	2.40	0.52
6:F:2:ARG:O	6:F:66:GLU:HA	2.08	0.52
12:L:27:LEU:CG	12:L:28:LYS:H	2.21	0.52
12:L:28:LYS:HE2	12:L:33:ARG:NH1	2.25	0.52
15:O:87:ILE:HG22	15:O:88:ARG:N	2.23	0.52
1:A:788:U:H3'	1:A:789:U:O4'	2.09	0.52
1:A:835:U:OP1	18:R:64:ARG:NH2	2.43	0.52
1:A:1488:G:C2'	1:A:1489:G:H5'	2.39	0.52
4:D:20:TYR:CD1	4:D:27:TYR:HE2	2.28	0.52
12:L:28:LYS:HE2	12:L:33:ARG:HH12	1.74	0.52
1:A:115:G:O2'	1:A:116:A:OP2	2.19	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:552:U:H2'	1:A:553:A:H8	1.74	0.52
1:A:1070:U:H2'	1:A:1071:C:H6	1.73	0.52
5:E:143:ARG:NH1	8:H:77:GLU:OE1	2.37	0.52
7:G:57:GLU:O	7:G:59:LEU:N	2.43	0.52
19:S:15:LEU:O	19:S:18:LYS:HG3	2.09	0.52
1:A:909:A:H2'	1:A:910:C:O4'	2.10	0.52
7:G:26:PHE:CD1	7:G:101:LEU:HD22	2.43	0.52
1:A:539:A:H2'	1:A:540:G:C8	2.45	0.52
2:B:62:ALA:HB1	2:B:222:ILE:HG23	1.92	0.52
4:D:128:VAL:HG12	4:D:129:ASN:ND2	2.24	0.52
7:G:26:PHE:CE2	7:G:124:LEU:HD11	2.45	0.52
12:L:39:VAL:HG22	12:L:57:LYS:HB2	1.92	0.52
13:M:23:TYR:CE2	13:M:71:ARG:HB3	2.45	0.52
1:A:22:G:H2'	1:A:23:C:H6	1.75	0.51
1:A:448:A:H2'	1:A:449:C:C6	2.45	0.51
1:A:1095:U:H2'	1:A:1096:C:O4'	2.10	0.51
1:A:1112:C:O2	3:C:179:ARG:HG3	2.09	0.51
1:A:1202:G:C4	14:N:42:ILE:HD13	2.46	0.51
1:A:1225:A:H5'	1:A:1226:C:OP2	2.10	0.51
2:B:161:ALA:O	2:B:162:ILE:HD13	2.10	0.51
10:J:22:LYS:HA	10:J:25:GLU:HG3	1.91	0.51
19:S:5:LEU:O	19:S:6:LYS:HE3	2.10	0.51
1:A:1152:A:H5'	10:J:13:HIS:HB2	1.92	0.51
3:C:157:ILE:HD13	3:C:157:ILE:H	1.75	0.51
14:N:21:TYR:N	14:N:21:TYR:CD1	2.77	0.51
1:A:373:A:H1'	1:A:481:G:N3	2.25	0.51
1:A:559:A:O2'	1:A:560:U:OP2	2.24	0.51
1:A:1126:U:H4'	25:A:2105:HOH:O	2.09	0.51
1:A:1229:A:H2'	1:A:1230:C:C6	2.44	0.51
2:B:24:TRP:HA	2:B:191:ASP:HA	1.91	0.51
12:L:41:ARG:HH21	12:L:43:VAL:HG13	1.74	0.51
1:A:1314:C:O2'	1:A:1315:U:H5'	2.09	0.51
1:A:1342:C:O2'	9:I:124:GLN:HB2	2.11	0.51
4:D:68:TYR:HB3	4:D:70:ILE:HG12	1.90	0.51
7:G:108:ALA:HB2	7:G:123:GLU:HG2	1.91	0.51
8:H:53:VAL:HB	8:H:58:TYR:CD1	2.45	0.51
9:I:50:LEU:O	9:I:53:VAL:HG23	2.11	0.51
12:L:113:ARG:HH12	12:L:116:SER:H	1.59	0.51
16:P:10:GLY:HA3	16:P:14:ASN:O	2.09	0.51
18:R:70:ILE:O	18:R:73:ALA:N	2.44	0.51
1:A:262:A:H2'	1:A:263:A:C8	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1348:U:O2	1:A:1348:U:H2'	2.10	0.51
7:G:76:ARG:O	7:G:87:VAL:HG23	2.11	0.51
8:H:86:ILE:HG21	8:H:133:LEU:HD13	1.93	0.51
1:A:379:C:H42	1:A:384:G:H1	1.59	0.51
1:A:1278:U:H5'	1:A:1279:A:C8	2.45	0.51
3:C:25:GLY:O	3:C:29:TYR:HB2	2.10	0.51
4:D:110:PHE:HE2	4:D:146:ILE:HG22	1.76	0.51
9:I:53:VAL:HG11	9:I:92:TYR:CE1	2.46	0.51
21:U:10:ARG:HD3	21:U:13:ILE:CD1	2.41	0.51
1:A:502:G:H2'	1:A:503:C:O4'	2.09	0.51
1:A:921:U:O2'	5:E:18:ARG:HG3	2.11	0.51
2:B:24:TRP:CG	2:B:25:ASN:N	2.78	0.51
2:B:71:VAL:HG22	2:B:93:VAL:HB	1.92	0.51
1:A:157:G:H1	1:A:164:U:H3	1.58	0.51
1:A:1026:G:HO2'	1:A:1027:C:P	2.33	0.51
1:A:1337:G:H5''	1:A:1338:G:OP1	2.10	0.51
9:I:5:TYR:CD2	9:I:6:GLY:N	2.79	0.51
13:M:92:HIS:HA	13:M:110:ARG:HH22	1.75	0.51
16:P:53:VAL:O	16:P:56:ALA:N	2.44	0.51
1:A:253:U:OP1	17:Q:67:LYS:HD3	2.11	0.51
1:A:974:A:OP2	14:N:41:ARG:NH1	2.42	0.51
1:A:1145:C:HO2'	1:A:1146:A:P	2.34	0.51
1:A:1229:A:H2'	1:A:1230:C:H6	1.76	0.51
1:A:1241:G:H2'	1:A:1242:C:C6	2.46	0.51
1:A:1291:G:H2'	1:A:1292:U:C6	2.46	0.51
2:B:16:HIS:NE2	2:B:204:ASN:N	2.58	0.51
2:B:62:ALA:CB	2:B:222:ILE:HG23	2.41	0.51
4:D:76:ARG:HD2	4:D:207:TYR:CE2	2.46	0.51
4:D:187:ARG:CZ	4:D:188:LEU:H	2.24	0.51
9:I:25:LYS:HG2	9:I:60:ASP:OD1	2.11	0.51
15:O:30:ALA:HA	15:O:85:LEU:HD11	1.93	0.51
16:P:26:ARG:HD3	16:P:31:LYS:O	2.11	0.51
1:A:77:G:C2	1:A:93:G:C2	2.99	0.51
1:A:718:G:H5'	11:K:117:ASN:HB2	1.92	0.51
1:A:803:G:C6	1:A:804:U:C4	2.99	0.51
3:C:29:TYR:OH	14:N:54:PRO:HD2	2.10	0.51
5:E:46:GLY:H	5:E:58:ALA:HB2	1.76	0.51
12:L:6:THR:OG1	12:L:9:GLN:HG3	2.11	0.51
1:A:263:A:OP2	20:T:79:ARG:NH1	2.44	0.50
1:A:373:A:C2	1:A:374:A:C8	3.00	0.50
1:A:933:G:OP2	7:G:3:ARG:HB3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1179:A:OP2	9:I:93:ARG:NH2	2.44	0.50
1:A:1290:G:H2'	1:A:1291:G:C8	2.43	0.50
7:G:42:ILE:HG22	7:G:120:ILE:HD12	1.93	0.50
8:H:84:ARG:O	8:H:135:CYS:HB2	2.12	0.50
10:J:45:ARG:HD2	14:N:36:PHE:HE2	1.75	0.50
1:A:22:G:C5	1:A:23:C:C5	2.99	0.50
1:A:113:G:C1'	1:A:354:G:H5'	2.40	0.50
1:A:730:G:C5	1:A:731:G:H1'	2.46	0.50
1:A:1127:G:N2	1:A:1147:C:C4	2.79	0.50
6:F:14:LEU:HD21	6:F:84:ASN:ND2	2.26	0.50
8:H:70:GLN:OE1	8:H:70:GLN:HA	2.11	0.50
9:I:105:ASP:OD2	9:I:107:ARG:HG3	2.10	0.50
11:K:29:ILE:C	11:K:29:ILE:HD12	2.37	0.50
12:L:53:ARG:HG2	12:L:69:TYR:CE1	2.46	0.50
20:T:43:LEU:HD12	20:T:52:ALA:HA	1.94	0.50
1:A:1465:C:H2'	1:A:1466:C:O4'	2.10	0.50
1:A:1518:MA6:H102	1:A:1519:MA6:H103	1.92	0.50
16:P:3:LYS:CA	16:P:64:ALA:HB1	2.41	0.50
1:A:7:G:O6	5:E:92:LYS:NZ	2.35	0.50
1:A:18:C:H5''	5:E:127:ASN:ND2	2.25	0.50
1:A:580:U:H2'	1:A:581:G:O4'	2.12	0.50
1:A:858:G:O6	1:A:869:G:H3'	2.10	0.50
1:A:1521:G:H2'	1:A:1522:U:C6	2.47	0.50
5:E:147:ASP:HA	5:E:150:ARG:HG2	1.94	0.50
1:A:193:C:H4'	20:T:61:SER:HB2	1.93	0.50
1:A:953:G:H2'	1:A:954:G:O4'	2.11	0.50
6:F:4:TYR:HB2	6:F:65:VAL:CG2	2.42	0.50
10:J:69:ASN:O	10:J:70:ARG:HD3	2.12	0.50
1:A:236:G:H2'	1:A:237:C:O4'	2.11	0.50
1:A:243:A:H4'	1:A:244:U:O5'	2.12	0.50
1:A:692:U:H1'	1:A:695:A:N7	2.27	0.50
1:A:882:C:O2'	1:A:883:C:H5'	2.12	0.50
1:A:1281:U:H4'	1:A:1282:C:OP2	2.11	0.50
4:D:108:LEU:HD23	4:D:174:LEU:HD13	1.94	0.50
1:A:1063:C:OP2	1:A:1064:G:O2'	2.25	0.50
3:C:167:TRP:HE3	3:C:168:ALA:N	2.06	0.50
1:A:109:A:C6	1:A:327:A:C6	3.00	0.50
1:A:1249:C:HO2'	9:I:73:GLN:NE2	2.08	0.50
2:B:24:TRP:CG	2:B:25:ASN:H	2.28	0.50
3:C:166:GLU:HA	3:C:166:GLU:OE2	2.12	0.50
8:H:104:ARG:HG3	8:H:138:TRP:CD2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:30:ALA:O	15:O:33:THR:N	2.45	0.50
1:A:812:C:OP1	1:A:903:G:H1'	2.12	0.50
1:A:1218:C:H2'	1:A:1219:U:C6	2.47	0.50
4:D:173:TRP:HE3	4:D:173:TRP:H	1.58	0.50
4:D:173:TRP:NE1	4:D:189:PRO:HB3	2.27	0.50
5:E:118:ILE:HG12	5:E:119:LEU:H	1.77	0.50
12:L:47:LYS:HG3	12:L:48:PRO:CD	2.40	0.50
1:A:414:A:OP2	1:A:428:G:N2	2.38	0.49
1:A:657:G:C2'	1:A:658:G:H5'	2.42	0.49
1:A:1061:G:H1'	10:J:56:HIS:CE1	2.47	0.49
1:A:1403:C:H2'	1:A:1404:5MC:H6	1.77	0.49
5:E:11:ILE:HD11	5:E:105:VAL:HG13	1.93	0.49
7:G:87:VAL:HG12	7:G:88:PRO:HD2	1.93	0.49
8:H:4:ASP:OD1	8:H:85:ARG:NH1	2.44	0.49
8:H:112:LEU:HD23	8:H:133:LEU:HA	1.93	0.49
9:I:111:ARG:O	9:I:119:ALA:HB2	2.12	0.49
1:A:665:A:H3'	1:A:725:G:H21	1.76	0.49
1:A:1025:U:OP1	1:A:1025:U:H4'	2.11	0.49
10:J:16:LEU:HD13	10:J:70:ARG:HG2	1.93	0.49
18:R:36:ASN:O	18:R:40:LEU:HG	2.12	0.49
19:S:71:LEU:C	19:S:73:GLU:H	2.18	0.49
20:T:30:LYS:HG2	20:T:34:LYS:HE2	1.93	0.49
20:T:100:ILE:H	20:T:100:ILE:HD12	1.76	0.49
1:A:426:G:H4'	4:D:41:GLY:O	2.11	0.49
1:A:1317:C:OP2	14:N:17:LYS:NZ	2.23	0.49
2:B:108:ILE:HG22	2:B:152:PHE:CE2	2.47	0.49
10:J:64:GLU:HG2	14:N:59:ALA:HB2	1.94	0.49
17:Q:58:GLU:O	17:Q:59:ILE:HD13	2.12	0.49
1:A:66:G:N3	1:A:66:G:H2'	2.27	0.49
1:A:66:G:N7	1:A:104:G:N2	2.59	0.49
1:A:980:C:H3'	1:A:981:U:H6	1.76	0.49
1:A:980:C:H5'	1:A:981:U:OP2	2.12	0.49
1:A:1314:C:N4	19:S:4:SER:OG	2.43	0.49
7:G:77:SER:HA	7:G:86:GLN:HA	1.94	0.49
9:I:126:SER:CB	9:I:127:LYS:HD2	2.43	0.49
14:N:12:ARG:HB3	14:N:14:PRO:HD3	1.94	0.49
1:A:690:G:C6	1:A:691:G:C6	3.01	0.49
2:B:153:ARG:HH11	2:B:153:ARG:HB2	1.78	0.49
7:G:32:ARG:O	7:G:34:GLY:N	2.45	0.49
1:A:1029:C:N4	1:A:1032:G:H22	2.09	0.49
2:B:112:VAL:HG23	2:B:149:LEU:HD13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:212:GLN:O	2:B:216:SER:HB3	2.13	0.49
4:D:9:CYS:O	4:D:12:CYS:HB2	2.13	0.49
5:E:40:ARG:HG2	5:E:40:ARG:HH11	1.77	0.49
7:G:17:VAL:HB	7:G:44:TYR:OH	2.11	0.49
7:G:92:SER:HG	7:G:95:ARG:H	1.55	0.49
11:K:11:LYS:N	11:K:11:LYS:HE3	2.28	0.49
21:U:5:ASP:O	21:U:8:THR:OG1	2.30	0.49
1:A:1005:A:H5''	1:A:1006:C:C5	2.48	0.49
1:A:1067:A:HO2'	1:A:1094:G:H5'	1.77	0.49
4:D:173:TRP:CD1	4:D:189:PRO:HB3	2.46	0.49
1:A:177:C:OP2	20:T:65:LYS:NZ	2.46	0.49
1:A:748:C:H4'	1:A:749:C:O5'	2.13	0.49
1:A:1148:U:H2'	1:A:1149:C:O4'	2.13	0.49
1:A:1241:G:H2'	1:A:1242:C:H6	1.77	0.49
1:A:1280:A:H3'	1:A:1281:U:H5''	1.93	0.49
3:C:79:ARG:NH1	3:C:82:GLU:HB3	2.26	0.49
3:C:120:VAL:O	3:C:123:GLN:HB2	2.13	0.49
4:D:102:ASP:OD1	4:D:103:ASN:N	2.44	0.49
11:K:91:ARG:HH11	18:R:88:LYS:NZ	2.11	0.49
13:M:108:ARG:HD3	13:M:114:ARG:NH1	2.28	0.49
14:N:21:TYR:N	14:N:21:TYR:HD1	2.11	0.49
21:U:15:ARG:HH11	21:U:15:ARG:HG3	1.77	0.49
1:A:59:A:H3'	1:A:331:G:H22	1.77	0.49
1:A:448:A:H2'	1:A:449:C:H6	1.78	0.49
1:A:676:A:H1'	11:K:115:PRO:HB3	1.95	0.49
13:M:84:ILE:HB	19:S:74:PHE:HE2	1.77	0.49
15:O:34:LEU:O	15:O:38:ARG:HG2	2.12	0.49
1:A:273:A:N6	1:A:274:A:C6	2.81	0.49
1:A:328:C:HO2'	1:A:329:A:P	2.32	0.49
1:A:376:G:OP2	16:P:67:THR:HG21	2.13	0.49
1:A:420:U:H3'	1:A:422:C:N4	2.27	0.49
1:A:1370:G:C2	1:A:1371:G:N7	2.80	0.49
1:A:1474:G:H2'	1:A:1475:G:C8	2.46	0.49
2:B:185:ILE:HG22	2:B:199:TYR:HB2	1.95	0.49
5:E:118:ILE:HG12	5:E:119:LEU:N	2.28	0.49
8:H:86:ILE:HG22	8:H:87:SER:N	2.27	0.49
12:L:78:GLN:O	12:L:81:SER:HB2	2.13	0.49
20:T:39:LYS:HD3	20:T:55:ILE:HD12	1.95	0.49
1:A:44:G:H2'	1:A:45:U:O4'	2.14	0.48
1:A:1372:U:C2'	1:A:1373:G:H5'	2.43	0.48
1:A:1419:G:H1	1:A:1481:U:H3	1.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1505:G:C8	1:A:1505:G:C3'	2.93	0.48
7:G:9:VAL:HG12	7:G:10:ARG:O	2.13	0.48
7:G:17:VAL:HG12	7:G:18:TYR:CD1	2.37	0.48
9:I:33:PHE:CE2	9:I:43:ALA:HB1	2.48	0.48
10:J:65:LEU:HB2	14:N:56:VAL:HG22	1.95	0.48
13:M:54:VAL:HA	13:M:57:ARG:HD3	1.94	0.48
17:Q:100:LYS:HE2	17:Q:100:LYS:HA	1.95	0.48
18:R:43:PHE:C	18:R:44:LEU:HD23	2.38	0.48
1:A:107:G:N2	1:A:108:G:H1'	2.28	0.48
1:A:355:C:H5'	1:A:389:A:OP2	2.12	0.48
1:A:518:C:H5''	1:A:519:C:C6	2.49	0.48
1:A:1029:C:H2'	1:A:1030:C:H5'	1.95	0.48
1:A:1451:A:H5''	1:A:1452:C:H5	1.78	0.48
4:D:21:LEU:HD21	4:D:66:ARG:O	2.13	0.48
5:E:137:GLU:HG3	5:E:141:GLN:HE21	1.78	0.48
13:M:11:ARG:HD2	13:M:45:VAL:CG1	2.43	0.48
15:O:21:ASP:OD2	15:O:21:ASP:C	2.56	0.48
16:P:20:VAL:HG13	16:P:32:TYR:CD2	2.47	0.48
16:P:26:ARG:HG2	16:P:26:ARG:HH11	1.78	0.48
17:Q:63:ARG:HG2	17:Q:64:PRO:HD2	1.94	0.48
20:T:60:GLU:HA	20:T:63:ILE:HD12	1.95	0.48
1:A:216:G:C2	1:A:217:C:C4	3.01	0.48
1:A:1126:U:H3'	1:A:1127:G:C8	2.29	0.48
1:A:1326:C:OP1	21:U:12:LYS:HE2	2.13	0.48
1:A:1470:G:C2'	1:A:1471:G:H5'	2.43	0.48
1:A:1504:G:H5''	1:A:1504:G:H8	1.79	0.48
3:C:91:LEU:HD21	3:C:99:VAL:HG22	1.95	0.48
9:I:5:TYR:HD2	9:I:6:GLY:N	2.11	0.48
15:O:4:THR:OG1	15:O:5:LYS:N	2.46	0.48
1:A:184:G:H2'	1:A:185:A:H8	1.77	0.48
1:A:277:C:H5'	17:Q:68:ARG:NH1	2.28	0.48
1:A:491:G:C4	1:A:492:G:C8	3.01	0.48
1:A:778:G:H8	1:A:778:G:O5'	1.96	0.48
1:A:1065:U:C5	1:A:1190:G:H1'	2.49	0.48
1:A:1329:A:C5'	13:M:29:ARG:HD2	2.43	0.48
1:A:1426:C:H2'	1:A:1427:U:C6	2.48	0.48
2:B:32:ILE:CG2	2:B:40:HIS:HB3	2.44	0.48
2:B:92:TYR:CD2	2:B:92:TYR:N	2.81	0.48
3:C:112:SER:O	3:C:112:SER:OG	2.26	0.48
4:D:30:LYS:C	4:D:32:ALA:H	2.22	0.48
8:H:31:PHE:O	8:H:35:ILE:HG12	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:96:GLY:HA2	8:H:130:GLY:HA3	1.95	0.48
1:A:102:G:H2'	1:A:103:C:H6	1.79	0.48
1:A:935:A:H61	7:G:3:ARG:HG3	1.79	0.48
5:E:106:PRO:O	5:E:107:ARG:C	2.55	0.48
13:M:57:ARG:O	13:M:61:GLU:HB2	2.14	0.48
19:S:18:LYS:HD3	19:S:19:VAL:HB	1.95	0.48
1:A:1132:C:H2'	1:A:1133:G:H8	1.79	0.48
1:A:1196:U:H3'	1:A:1197:G:H5'	1.94	0.48
1:A:1285:A:H8	1:A:1285:A:O5'	1.97	0.48
4:D:60:GLU:OE1	4:D:60:GLU:HA	2.13	0.48
1:A:37:U:H2'	1:A:38:G:O4'	2.14	0.48
1:A:93:G:C2	1:A:95:U:C2	3.02	0.48
1:A:481:G:O2'	1:A:482:A:O5'	2.27	0.48
1:A:1026:G:O2'	1:A:1027:C:P	2.71	0.48
1:A:1029:C:H42	1:A:1032:G:H1	1.61	0.48
1:A:1496:C:HO2'	1:A:1497:G:P	2.31	0.48
2:B:60:ASP:O	2:B:64:ARG:HB2	2.13	0.48
4:D:15:GLU:HG3	4:D:63:LYS:HD3	1.95	0.48
4:D:38:TYR:CE1	4:D:45:GLN:HG2	2.48	0.48
11:K:40:ILE:HD13	11:K:40:ILE:HA	1.69	0.48
15:O:38:ARG:O	15:O:41:GLU:HB3	2.13	0.48
15:O:56:LEU:O	15:O:60:VAL:HG23	2.13	0.48
17:Q:29:HIS:ND1	17:Q:30:PRO:HD2	2.29	0.48
20:T:81:LYS:O	20:T:85:MET:HG3	2.13	0.48
1:A:438:G:H4'	4:D:123:HIS:ND1	2.28	0.48
1:A:597:G:H1'	1:A:644:G:N2	2.29	0.48
1:A:706:A:H1'	11:K:29:ILE:HD11	1.96	0.48
1:A:953:G:C6	1:A:954:G:C4	3.01	0.48
1:A:1068:G:OP2	1:A:1068:G:H8	1.97	0.48
1:A:1542:U:H2'	1:A:1543:C:C6	2.49	0.48
2:B:17:PHE:CD1	2:B:18:GLY:N	2.81	0.48
4:D:192:GLU:C	4:D:194:LEU:H	2.22	0.48
7:G:26:PHE:O	7:G:30:ILE:HD12	2.12	0.48
1:A:518:C:OP2	1:A:530:G:H1'	2.14	0.48
1:A:744:C:H4'	1:A:852:G:O2'	2.14	0.48
1:A:767:A:H2'	1:A:768:A:O4'	2.14	0.48
1:A:1361(A):C:O2	1:A:1362:C:H5	1.97	0.48
2:B:16:HIS:CD2	2:B:204:ASN:H	2.32	0.48
4:D:15:GLU:CG	4:D:63:LYS:HD3	2.43	0.48
4:D:32:ALA:O	4:D:36:ARG:N	2.47	0.48
6:F:97:PHE:C	6:F:97:PHE:CD2	2.92	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:77:LEU:HD21	12:L:107:ALA:HB2	1.96	0.48
17:Q:40:LYS:HD3	17:Q:42:TYR:OH	2.13	0.48
1:A:436:C:H2'	1:A:437:U:H6	1.78	0.48
1:A:1157:A:H4'	1:A:1158:C:O5'	2.14	0.48
1:A:1202:G:O2'	14:N:27:CYS:SG	2.66	0.48
1:A:1265:G:H2'	1:A:1266:G:O4'	2.14	0.48
4:D:200:GLU:HG2	4:D:201:GLN:H	1.78	0.48
5:E:107:ARG:O	5:E:111:GLU:HB2	2.14	0.48
10:J:54:PHE:O	10:J:55:LYS:HG3	2.14	0.48
11:K:19:ALA:HB2	11:K:80:VAL:HG11	1.96	0.48
1:A:34:C:H2'	1:A:35:G:C8	2.49	0.47
1:A:818:G:C3'	1:A:819:A:H5''	2.44	0.47
2:B:185:ILE:HG22	2:B:199:TYR:O	2.14	0.47
8:H:48:TYR:HA	8:H:60:ARG:O	2.14	0.47
17:Q:22:LEU:HD12	17:Q:22:LEU:HA	1.53	0.47
1:A:576:G:H3'	1:A:577:G:H5''	1.96	0.47
1:A:914:G:P	22:A:1601:SRY:HI33	2.53	0.47
1:A:943:U:H2'	1:A:944:G:H5'	1.97	0.47
2:B:196:LEU:HD22	2:B:196:LEU:HA	1.56	0.47
6:F:22:GLU:HA	6:F:25:ILE:HD12	1.96	0.47
6:F:99:ALA:HB1	18:R:62:GLU:OE2	2.14	0.47
9:I:19:LEU:HD12	9:I:84:ALA:HB3	1.97	0.47
9:I:111:ARG:O	9:I:113:LYS:HD2	2.14	0.47
12:L:11:VAL:HG12	12:L:12:ARG:N	2.29	0.47
12:L:84:LEU:HB3	12:L:101:VAL:HG23	1.96	0.47
20:T:92:LEU:O	20:T:96:GLY:HA2	2.13	0.47
1:A:106:C:C2'	1:A:107:G:H5'	2.43	0.47
1:A:1244:C:OP1	21:U:9:ARG:HB2	2.14	0.47
1:A:1304:G:C6	1:A:1305:G:N1	2.82	0.47
1:A:1505:G:H4'	1:A:1506:U:H5''	1.95	0.47
2:B:179:LYS:HA	8:H:72:PRO:HD3	1.96	0.47
4:D:194:LEU:HD12	4:D:195:ALA:H	1.77	0.47
7:G:5:ARG:NH1	7:G:8:GLU:HG3	2.20	0.47
9:I:17:VAL:HG13	9:I:63:ILE:HG12	1.95	0.47
11:K:18:ARG:HB2	11:K:33:THR:CG2	2.45	0.47
16:P:66:PRO:HD2	16:P:71:ARG:NH1	2.29	0.47
20:T:57:ARG:HD3	20:T:102:GLY:HA3	1.96	0.47
1:A:949:A:C2	1:A:1233:G:N3	2.82	0.47
2:B:32:ILE:HG21	2:B:40:HIS:HB3	1.95	0.47
7:G:140:ASP:O	7:G:144:MET:HG3	2.13	0.47
8:H:2:LEU:HD23	8:H:2:LEU:HA	1.68	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:32:ILE:HD13	11:K:32:ILE:N	2.29	0.47
20:T:53:LEU:HA	20:T:56:MET:HB3	1.96	0.47
1:A:49:U:O2'	1:A:50:A:H2'	2.15	0.47
1:A:234:C:H2'	1:A:235:C:C6	2.49	0.47
1:A:250:A:O5'	1:A:250:A:H8	1.96	0.47
1:A:405:U:O4	4:D:2:GLY:HA2	2.15	0.47
1:A:578:C:O2'	1:A:728:A:N3	2.47	0.47
1:A:781:A:C5	1:A:802:A:C2	3.02	0.47
1:A:1411:C:N4	1:A:1489:G:H1	2.10	0.47
2:B:97:TRP:CH2	2:B:101:MET:HB2	2.50	0.47
2:B:236:TYR:HD2	2:B:239:VAL:HG21	1.79	0.47
3:C:88:ARG:HG2	3:C:101:LEU:HB2	1.96	0.47
4:D:114:ARG:HH11	4:D:114:ARG:HG3	1.79	0.47
5:E:143:ARG:NH1	8:H:77:GLU:OE2	2.48	0.47
14:N:4:LYS:HB3	14:N:4:LYS:HE2	1.58	0.47
17:Q:53:LEU:HD12	17:Q:85:VAL:HG21	1.96	0.47
1:A:452:A:H2'	1:A:453:A:C8	2.50	0.47
1:A:500:G:H2'	1:A:501:C:C6	2.49	0.47
1:A:835:U:H3	1:A:851:G:H1	1.62	0.47
1:A:1004:A:H5''	1:A:1025:U:N3	2.28	0.47
1:A:1460:A:OP2	20:T:27:LYS:NZ	2.47	0.47
4:D:9:CYS:SG	4:D:31:CYS:O	2.73	0.47
5:E:82:VAL:O	5:E:88:LYS:HA	2.14	0.47
7:G:32:ARG:C	7:G:34:GLY:H	2.21	0.47
7:G:116:ALA:O	7:G:120:ILE:HG13	2.15	0.47
7:G:134:ALA:O	7:G:137:LYS:N	2.47	0.47
10:J:49:VAL:HG21	14:N:44:LEU:HD23	1.96	0.47
12:L:41:ARG:NH2	12:L:43:VAL:HG13	2.28	0.47
17:Q:31:LEU:HA	17:Q:31:LEU:HD12	1.49	0.47
17:Q:38:ARG:HD3	17:Q:38:ARG:HA	1.48	0.47
1:A:146:G:C2	1:A:147:G:C4	3.03	0.47
1:A:455:C:O5'	1:A:455:C:H6	1.98	0.47
1:A:765:G:H8	1:A:765:G:O5'	1.98	0.47
1:A:766:A:P	25:A:2188:HOH:O	2.72	0.47
1:A:935:A:N6	7:G:3:ARG:HG3	2.29	0.47
1:A:954:G:C6	1:A:955:U:N3	2.83	0.47
1:A:1228:C:N4	13:M:104:ARG:O	2.42	0.47
1:A:1237:C:C4	1:A:1336:C:O2	2.68	0.47
1:A:1293:G:H2'	1:A:1294:G:O4'	2.14	0.47
2:B:96:ARG:O	2:B:98:LEU:HD23	2.15	0.47
2:B:189:ASP:N	2:B:189:ASP:OD1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:88:ARG:HA	3:C:91:LEU:HD22	1.97	0.47
4:D:70:ILE:HG22	4:D:71:SER:O	2.14	0.47
8:H:104:ARG:HG2	8:H:104:ARG:HH11	1.79	0.47
18:R:26:LEU:HD12	18:R:42:ARG:HH11	1.79	0.47
18:R:37:VAL:CG2	18:R:78:LEU:HB3	2.45	0.47
1:A:19:C:P	5:E:127:ASN:HD22	2.37	0.47
1:A:286:G:H2'	1:A:287:U:H6	1.80	0.47
1:A:289:G:P	25:A:1908:HOH:O	2.73	0.47
1:A:509:A:H4'	1:A:510:A:OP1	2.15	0.47
1:A:751:U:H4'	15:O:24:SER:HB3	1.97	0.47
1:A:1147:C:H2'	1:A:1148:U:C6	2.49	0.47
1:A:1239:A:C4	1:A:1298:C:N4	2.82	0.47
3:C:33:LEU:HD21	14:N:53:LEU:HD22	1.96	0.47
4:D:10:ARG:O	4:D:13:ARG:HB2	2.15	0.47
9:I:89:ASN:O	9:I:92:TYR:HB2	2.15	0.47
12:L:19:ARG:H	12:L:19:ARG:HG2	1.21	0.47
1:A:177:C:P	20:T:65:LYS:HZ1	2.38	0.47
1:A:355:C:C4	1:A:356:A:N7	2.83	0.47
1:A:500:G:C6	1:A:501:C:C4	3.03	0.47
1:A:724:G:O2'	1:A:725:G:H5'	2.14	0.47
1:A:975:A:HO2'	1:A:976:G:P	2.37	0.47
1:A:1055:A:H1'	3:C:156:ARG:NH2	2.30	0.47
5:E:98:THR:HB	5:E:117:ASP:HB3	1.96	0.47
8:H:20:TYR:CE2	8:H:75:ARG:HD2	2.50	0.47
16:P:1:MET:HE2	16:P:1:MET:HB3	1.86	0.47
16:P:19:ILE:HD12	16:P:37:GLY:C	2.40	0.47
1:A:285:G:O2'	1:A:286:G:H5'	2.15	0.47
1:A:667:G:H4'	15:O:51:HIS:ND1	2.30	0.47
1:A:1298:C:OP2	7:G:114:ARG:NH2	2.48	0.47
1:A:1332:A:H2'	1:A:1333:A:H8	1.80	0.47
1:A:1347:G:O2'	1:A:1348:U:P	2.73	0.47
1:A:1518:MA6:C10	1:A:1519:MA6:H103	2.44	0.47
4:D:158:ILE:HA	4:D:158:ILE:HD13	1.76	0.47
4:D:176:LEU:HD21	4:D:178:VAL:HB	1.96	0.47
5:E:71:LEU:CD2	5:E:115:VAL:HG22	2.43	0.47
8:H:36:LEU:HD23	8:H:39:LEU:HD23	1.97	0.47
1:A:701:C:H4'	1:A:702:A:C5'	2.43	0.46
1:A:996:A:C8	1:A:997:U:C5	3.03	0.46
1:A:1225:A:H5''	1:A:1226:C:H5	1.80	0.46
1:A:1498:UR3:O5'	1:A:1498:UR3:H6	2.14	0.46
8:H:10:LEU:HD23	8:H:10:LEU:HA	1.57	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:96:LEU:HD23	13:M:96:LEU:HA	1.69	0.46
15:O:49:ASP:OD2	15:O:52:SER:OG	2.26	0.46
16:P:18:ARG:HD3	16:P:35:LYS:HD2	1.97	0.46
19:S:31:ILE:CG2	19:S:49:ILE:HD13	2.39	0.46
1:A:34:C:H2'	1:A:35:G:H8	1.80	0.46
1:A:102:G:H2'	1:A:103:C:C6	2.51	0.46
1:A:519:C:OP2	12:L:50:SER:OG	2.29	0.46
1:A:833:U:H2'	1:A:834:C:C6	2.51	0.46
1:A:954:G:H5''	1:A:955:U:OP2	2.15	0.46
3:C:39:ILE:CG2	3:C:91:LEU:HD12	2.45	0.46
3:C:155:GLY:HA2	3:C:164:ARG:H	1.80	0.46
5:E:123:LEU:HA	5:E:123:LEU:HD23	1.53	0.46
10:J:19:SER:HB2	10:J:91:PRO:HB3	1.97	0.46
11:K:19:ALA:HB3	11:K:82:VAL:HG22	1.96	0.46
1:A:6:G:O2'	1:A:7:G:H5''	2.16	0.46
1:A:622:A:H5''	1:A:623:C:OP2	2.15	0.46
1:A:1280:A:H5'	10:J:40:LEU:HD22	1.96	0.46
1:A:1293:G:C2	1:A:1294:G:C4	3.03	0.46
2:B:91:PRO:HG3	2:B:155:LEU:CD2	2.45	0.46
2:B:158:LEU:HD23	2:B:159:PRO:HD2	1.97	0.46
3:C:153:VAL:CG1	3:C:166:GLU:HB2	2.38	0.46
4:D:65:ARG:HG3	4:D:75:PHE:CG	2.50	0.46
7:G:75:VAL:HG11	7:G:86:GLN:HB3	1.97	0.46
10:J:31:GLY:HA3	10:J:81:THR:OG1	2.15	0.46
13:M:12:ASN:H	13:M:45:VAL:CG1	2.27	0.46
15:O:67:LEU:HD13	15:O:78:TYR:CE1	2.40	0.46
17:Q:56:VAL:O	17:Q:77:VAL:N	2.41	0.46
1:A:451:A:N7	1:A:481:G:C2	2.84	0.46
1:A:579:G:H2'	1:A:580:U:C6	2.50	0.46
1:A:668:G:O4'	15:O:49:ASP:HB2	2.16	0.46
1:A:1305:G:C8	1:A:1305:G:OP2	2.69	0.46
12:L:31:PRO:O	12:L:32:PHE:CG	2.68	0.46
12:L:126:LYS:HG2	12:L:128:ALA:HB2	1.97	0.46
20:T:33:ILE:O	20:T:34:LYS:C	2.58	0.46
1:A:392:G:C2	1:A:393:A:C4	3.03	0.46
1:A:838:G:C2'	1:A:839:U:H5''	2.45	0.46
1:A:976:G:OP1	14:N:32:SER:HA	2.15	0.46
1:A:1311:G:H5''	1:A:1312:G:OP2	2.16	0.46
1:A:1403:C:H3'	1:A:1404:5MC:HM53	1.97	0.46
1:A:1470:G:H2'	1:A:1471:G:H5'	1.98	0.46
4:D:131:ARG:HB2	4:D:131:ARG:NH1	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:186:LEU:N	4:D:186:LEU:HD23	2.31	0.46
11:K:82:VAL:HG11	11:K:95:ILE:HD11	1.97	0.46
20:T:63:ILE:O	20:T:66:ALA:HB3	2.15	0.46
1:A:89:C:C2'	1:A:90:U:H5'	2.46	0.46
1:A:448:A:C2	1:A:449:C:C4	3.04	0.46
1:A:463:A:H2'	1:A:474:G:C8	2.51	0.46
1:A:686:U:O2'	1:A:687:A:O5'	2.34	0.46
1:A:927:G:H4'	1:A:1503:A:N7	2.30	0.46
1:A:954:G:N2	1:A:1227:A:H62	2.13	0.46
1:A:1014:A:C2	19:S:34:TRP:CD1	3.04	0.46
1:A:1174:G:H2'	1:A:1175:G:C8	2.51	0.46
8:H:113:SER:HB2	8:H:134:ILE:HD11	1.97	0.46
19:S:6:LYS:HB3	19:S:7:LYS:H	1.33	0.46
1:A:1067:A:H8	1:A:1067:A:O5'	1.98	0.46
1:A:1495:U:O2'	1:A:1496:C:H5'	2.16	0.46
2:B:132:LYS:O	2:B:136:VAL:HG23	2.16	0.46
3:C:155:GLY:HA2	3:C:164:ARG:O	2.15	0.46
6:F:33:TYR:HE2	6:F:74:ASP:CB	2.29	0.46
12:L:120:TYR:O	12:L:122:THR:HG22	2.16	0.46
13:M:23:TYR:CZ	13:M:71:ARG:HB3	2.50	0.46
15:O:29:VAL:HG11	15:O:81:LEU:HD13	1.97	0.46
1:A:1152:A:H2'	1:A:1153:C:O4'	2.16	0.46
7:G:108:ALA:O	7:G:119:ARG:HB3	2.16	0.46
8:H:101:PRO:HG3	8:H:133:LEU:HD11	1.97	0.46
9:I:80:GLY:HA2	9:I:83:ARG:HG3	1.97	0.46
11:K:99:GLN:HE21	11:K:105:VAL:HG21	1.80	0.46
1:A:78:G:N1	1:A:92:C:C4	2.84	0.46
1:A:216:G:O2'	1:A:217:C:O5'	2.34	0.46
1:A:279:A:H5'	1:A:279:A:H8	1.81	0.46
1:A:689:C:OP1	11:K:44:SER:OG	2.30	0.46
1:A:1228:C:H6	1:A:1228:C:H5''	1.81	0.46
1:A:1447:G:C6	1:A:1460:A:C2	3.04	0.46
1:A:1542:U:H2'	1:A:1543:C:C5	2.50	0.46
2:B:24:TRP:HB3	2:B:40:HIS:CE1	2.51	0.46
8:H:20:TYR:HE2	8:H:75:ARG:HD2	1.80	0.46
10:J:62:HIS:HB2	14:N:59:ALA:HB3	1.97	0.46
11:K:18:ARG:HB2	11:K:33:THR:HG23	1.98	0.46
11:K:85:ARG:CD	11:K:111:ASP:HB3	2.46	0.46
13:M:67:GLU:O	13:M:71:ARG:HG2	2.16	0.46
13:M:67:GLU:HB3	13:M:68:GLY:H	1.55	0.46
13:M:82:MET:HA	13:M:89:GLY:HA3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:36:PHE:HD1	14:N:36:PHE:C	2.24	0.46
17:Q:81:ARG:HB2	17:Q:84:LEU:CD1	2.46	0.46
19:S:26:GLY:O	19:S:27:GLU:HG2	2.16	0.46
1:A:369:C:OP2	1:A:388:G:N2	2.45	0.46
1:A:616:G:H1'	1:A:625:G:N2	2.31	0.46
1:A:1097:C:C4	1:A:1098:C:N4	2.84	0.46
1:A:1392:G:N2	1:A:1502:A:H8	2.12	0.46
1:A:1399:C:O2	1:A:1401:G:C5	2.69	0.46
6:F:47:ARG:HA	6:F:57:GLN:HB3	1.98	0.46
6:F:79:LEU:HA	6:F:79:LEU:HD23	1.50	0.46
8:H:36:LEU:HD23	8:H:36:LEU:HA	1.63	0.46
10:J:6:ILE:HG22	10:J:7:LYS:N	2.31	0.46
11:K:65:ALA:HB1	11:K:98:LEU:CD1	2.38	0.46
1:A:324:G:OP1	20:T:22:ARG:HD2	2.15	0.45
1:A:344:A:H4'	1:A:345:C:OP2	2.15	0.45
1:A:475:G:C4	1:A:476:G:C8	3.04	0.45
1:A:657:G:H2'	1:A:658:G:H5'	1.99	0.45
1:A:661:G:H1	1:A:744:C:H42	1.63	0.45
1:A:1323:G:N7	19:S:3:ARG:HD2	2.31	0.45
3:C:21:ARG:NH2	3:C:56:ASP:HB3	2.31	0.45
3:C:22:TRP:CH2	3:C:32:LEU:HB2	2.51	0.45
3:C:202:ILE:CG2	3:C:204:LEU:HD23	2.45	0.45
8:H:28:ALA:HB3	8:H:57:PRO:HB2	1.98	0.45
17:Q:8:GLY:O	17:Q:56:VAL:HG13	2.16	0.45
1:A:446:G:H2'	1:A:447:G:H5'	1.98	0.45
1:A:1081:G:H5''	1:A:1081:G:H8	1.81	0.45
1:A:1221:G:H2'	1:A:1222:G:O4'	2.16	0.45
1:A:1277:C:O2'	1:A:1279:A:H1'	2.16	0.45
1:A:1374:A:OP1	7:G:36:LYS:NZ	2.49	0.45
2:B:223:ILE:O	2:B:227:GLY:N	2.50	0.45
4:D:110:PHE:HD1	4:D:162:LEU:HD21	1.80	0.45
5:E:151:LEU:HA	5:E:151:LEU:HD23	1.64	0.45
11:K:85:ARG:HD3	11:K:111:ASP:HB3	1.97	0.45
15:O:14:GLU:HB3	15:O:15:PHE:CD1	2.51	0.45
15:O:34:LEU:HD23	15:O:35:ARG:N	2.31	0.45
20:T:53:LEU:HB2	20:T:100:ILE:HD13	1.97	0.45
1:A:397:A:H5'	1:A:398:C:OP1	2.15	0.45
1:A:474:G:H4'	16:P:81:ARG:NH2	2.31	0.45
1:A:532:A:O2'	1:A:533:A:P	2.72	0.45
1:A:974:A:C8	14:N:31:ARG:HG2	2.50	0.45
1:A:1358:U:H5'	14:N:35:ARG:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:44:LEU:HA	2:B:44:LEU:HD23	1.64	0.45
3:C:87:LEU:O	3:C:91:LEU:HB3	2.17	0.45
7:G:45:ASP:O	7:G:49:ILE:HG13	2.15	0.45
8:H:124:ALA:O	8:H:128:GLY:N	2.49	0.45
9:I:63:ILE:CG2	9:I:77:ILE:HG12	2.46	0.45
16:P:60:LEU:HA	16:P:60:LEU:HD23	1.40	0.45
1:A:653:A:P	8:H:56:LYS:NZ	2.89	0.45
1:A:721:G:C6	1:A:733:A:C2	3.05	0.45
1:A:858:G:C5	25:A:2220:HOH:O	2.68	0.45
4:D:172:PRO:HD2	4:D:173:TRP:CZ3	2.52	0.45
7:G:3:ARG:HG2	7:G:3:ARG:HH11	1.81	0.45
7:G:40:ALA:CB	9:I:41:VAL:HG21	2.47	0.45
9:I:53:VAL:C	9:I:55:ALA:H	2.24	0.45
10:J:12:ASP:HB3	10:J:15:THR:CG2	2.46	0.45
11:K:115:PRO:C	11:K:117:ASN:H	2.24	0.45
15:O:18:PHE:CZ	15:O:21:ASP:HB2	2.51	0.45
16:P:40:ASP:HA	16:P:41:PRO:HD3	1.84	0.45
17:Q:43:LEU:HD23	17:Q:43:LEU:HA	1.51	0.45
21:U:18:TYR:CG	21:U:24:ARG:HG2	2.52	0.45
1:A:284:G:H2'	1:A:285:G:H8	1.81	0.45
1:A:350:G:C5'	1:A:350:G:H8	2.29	0.45
1:A:690:G:H2'	1:A:691:G:O4'	2.16	0.45
1:A:837:G:N2	1:A:850:U:O2	2.49	0.45
1:A:983:A:P	14:N:3:ARG:HH22	2.40	0.45
1:A:1174:G:C2	1:A:1175:G:C5	3.05	0.45
1:A:1372:U:O2'	1:A:1373:G:H5'	2.17	0.45
1:A:1442:G:N1	1:A:1446:A:N7	2.64	0.45
1:A:1527:C:O2'	1:A:1528:U:H5'	2.16	0.45
3:C:35:GLU:O	3:C:39:ILE:HG13	2.16	0.45
16:P:53:VAL:HG23	16:P:54:GLU:N	2.31	0.45
20:T:10:LEU:HD13	20:T:11:SER:N	2.30	0.45
1:A:82:U:O2'	1:A:83:U:H5'	2.16	0.45
1:A:192:U:H2'	1:A:193:C:H6	1.81	0.45
1:A:757:U:H5''	1:A:822:C:O2	2.17	0.45
1:A:991:U:O4	1:A:1212:U:H1'	2.16	0.45
1:A:1021:G:H2'	1:A:1021:G:N3	2.32	0.45
2:B:92:TYR:CD1	2:B:94:ASN:HB2	2.52	0.45
4:D:30:LYS:C	4:D:32:ALA:N	2.73	0.45
4:D:194:LEU:HA	4:D:194:LEU:HD13	1.47	0.45
6:F:14:LEU:HB3	6:F:18:GLN:HB2	1.97	0.45
6:F:40:VAL:HG23	6:F:63:TYR:CD1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:86:ILE:HD13	8:H:86:ILE:HA	1.59	0.45
14:N:53:LEU:O	14:N:56:VAL:HB	2.17	0.45
15:O:45:VAL:HB	15:O:46:HIS:ND1	2.32	0.45
15:O:70:LEU:HD12	15:O:78:TYR:HA	1.97	0.45
15:O:70:LEU:HD22	15:O:70:LEU:HA	1.58	0.45
1:A:74:C:H2'	1:A:75:G:C8	2.52	0.45
1:A:200:G:H1	1:A:217:C:N4	2.10	0.45
1:A:243:A:C2	1:A:246:A:C8	3.04	0.45
1:A:830:G:C6	1:A:831:U:C4	3.05	0.45
1:A:1300:G:O5'	1:A:1335:C:N4	2.50	0.45
1:A:1418:A:H2'	1:A:1419:G:O4'	2.17	0.45
3:C:150:LYS:HB2	3:C:169:ALA:HB2	1.99	0.45
17:Q:10:VAL:O	17:Q:53:LEU:HD13	2.17	0.45
1:A:35:G:C4	1:A:36:C:C5	3.05	0.45
1:A:451:A:N6	1:A:481:G:C5	2.85	0.45
1:A:778:G:H2'	1:A:779:C:O4'	2.16	0.45
1:A:792:A:N3	1:A:793:U:O2'	2.45	0.45
1:A:1036:G:N7	1:A:1037:C:C4	2.85	0.45
1:A:1070:U:H2'	1:A:1071:C:C6	2.52	0.45
1:A:1323:G:H2'	1:A:1324:A:C8	2.51	0.45
22:A:1601:SRV:HB11	22:A:1601:SRV:H11	1.55	0.45
2:B:15:VAL:HG22	2:B:209:ARG:NH1	2.32	0.45
2:B:217:ARG:HA	2:B:217:ARG:HD3	1.55	0.45
3:C:119:ARG:O	3:C:123:GLN:HG3	2.16	0.45
4:D:15:GLU:O	4:D:17:VAL:HG23	2.17	0.45
4:D:186:LEU:HD23	4:D:186:LEU:H	1.81	0.45
6:F:26:ILE:HG21	6:F:63:TYR:HE2	1.80	0.45
8:H:10:LEU:HD12	8:H:85:ARG:HB2	1.98	0.45
14:N:25:VAL:HG23	14:N:38:GLY:O	2.17	0.45
17:Q:36:ILE:HD13	17:Q:36:ILE:H	1.82	0.45
1:A:89:C:H2'	1:A:90:U:O4'	2.17	0.45
1:A:372:C:H4'	1:A:373:A:O5'	2.16	0.45
1:A:545:C:O2'	1:A:549:C:OP1	2.29	0.45
1:A:597:G:H5''	1:A:598:U:OP2	2.17	0.45
1:A:625:G:H4'	16:P:16:HIS:ND1	2.32	0.45
1:A:1091:U:H2'	1:A:1092:A:H5''	1.97	0.45
1:A:1112:C:C4	3:C:178:LEU:HD12	2.52	0.45
1:A:1342:C:H2'	1:A:1343:G:C8	2.52	0.45
2:B:68:ILE:HG12	2:B:161:ALA:HB3	1.99	0.45
3:C:88:ARG:HG3	3:C:101:LEU:HB2	1.97	0.45
3:C:152:ILE:HG22	3:C:153:VAL:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:125:HIS:O	4:D:126:ILE:HD13	2.17	0.45
6:F:9:VAL:HG13	6:F:60:PHE:CD2	2.52	0.45
10:J:24:VAL:HG21	10:J:37:PRO:HD3	1.98	0.45
1:A:139:G:H2'	1:A:140:A:H5'	1.99	0.45
1:A:1191:A:H2'	1:A:1192:C:C6	2.52	0.45
1:A:1320:C:OP1	19:S:70:LYS:NZ	2.49	0.45
2:B:219:VAL:O	2:B:223:ILE:HG12	2.17	0.45
3:C:117:ALA:HB2	3:C:200:ALA:HB2	1.99	0.45
9:I:111:ARG:HH12	9:I:113:LYS:HA	1.81	0.45
13:M:78:ILE:HG22	13:M:82:MET:HE2	1.98	0.45
1:A:38:G:N2	1:A:397:A:C4	2.85	0.44
1:A:350:G:O2'	1:A:351:G:H5'	2.17	0.44
1:A:353:A:H8	1:A:353:A:C5'	2.27	0.44
1:A:444:C:H2'	1:A:445:G:C8	2.52	0.44
4:D:20:TYR:CE1	4:D:27:TYR:HE2	2.34	0.44
14:N:24:CYS:HB2	14:N:39:LEU:HA	1.99	0.44
18:R:50:ILE:HG12	18:R:70:ILE:HD13	1.97	0.44
20:T:39:LYS:O	20:T:43:LEU:HG	2.17	0.44
1:A:89:C:C2	1:A:90:U:C6	3.05	0.44
1:A:344:A:H5'	1:A:345:C:H5	1.82	0.44
1:A:687:A:O2'	1:A:688:G:OP2	2.26	0.44
1:A:821:G:H2'	1:A:822:C:H6	1.81	0.44
1:A:836:G:OP1	18:R:61:LYS:NZ	2.48	0.44
1:A:1509:C:H42	1:A:1526:G:H1	1.66	0.44
2:B:147:LYS:HD2	2:B:148:TYR:CE2	2.52	0.44
3:C:134:ILE:O	3:C:138:VAL:HG23	2.17	0.44
5:E:11:ILE:HD11	5:E:105:VAL:HA	1.99	0.44
8:H:129:VAL:HG23	8:H:130:GLY:O	2.17	0.44
10:J:51:ARG:CZ	10:J:61:GLU:HB2	2.46	0.44
10:J:63:PHE:HE1	14:N:45:ARG:HA	1.82	0.44
11:K:30:VAL:HG21	11:K:65:ALA:HA	1.99	0.44
14:N:36:PHE:C	14:N:36:PHE:CD1	2.95	0.44
19:S:12:ASP:CG	19:S:38:SER:HB3	2.42	0.44
1:A:357:G:H2'	1:A:358:U:H6	1.82	0.44
1:A:475:G:H2'	1:A:476:G:H8	1.82	0.44
1:A:620:C:C1'	4:D:135:LEU:HD13	2.47	0.44
1:A:695:A:H2'	1:A:696:A:C8	2.52	0.44
1:A:1163:C:H2'	1:A:1164:G:C8	2.40	0.44
1:A:1275:A:H2'	1:A:1276:G:O4'	2.16	0.44
1:A:1314:C:H2'	1:A:1315:U:C6	2.52	0.44
1:A:1498:UR3:O2'	1:A:1499:A:OP2	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:57:PHE:CG	2:B:199:TYR:CE1	3.05	0.44
3:C:14:ILE:C	3:C:16:ARG:H	2.26	0.44
3:C:112:SER:O	3:C:116:VAL:HG23	2.18	0.44
3:C:188:LEU:HD13	3:C:189:ALA:N	2.32	0.44
5:E:89:ILE:HG13	5:E:90:VAL:N	2.33	0.44
5:E:92:LYS:HA	5:E:93:PRO:HD3	1.78	0.44
6:F:11:ASN:HB2	6:F:86:ARG:NH2	2.33	0.44
7:G:48:LYS:O	7:G:52:GLU:HB2	2.17	0.44
8:H:46:LYS:HG3	8:H:64:LYS:HB3	2.00	0.44
9:I:47:LEU:O	9:I:50:LEU:N	2.46	0.44
9:I:108:VAL:HG12	9:I:109:VAL:N	2.24	0.44
13:M:22:ILE:HG21	13:M:66:LEU:HD23	1.98	0.44
13:M:59:TYR:CE1	13:M:63:THR:HG21	2.52	0.44
1:A:279:A:H5'	1:A:279:A:C8	2.51	0.44
1:A:303:A:H2'	1:A:304:U:O4'	2.17	0.44
1:A:753:A:H2	8:H:1:MET:HE2	1.82	0.44
1:A:1000:U:H2'	1:A:1001:A:C8	2.52	0.44
1:A:1048:G:O3'	1:A:1049:U:H3'	2.17	0.44
1:A:1213:A:C6	1:A:1215:G:C4	3.05	0.44
1:A:1500:A:OP2	1:A:1505:G:OP1	2.35	0.44
1:A:1504:G:H5''	1:A:1504:G:C8	2.52	0.44
2:B:91:PRO:HG3	2:B:155:LEU:HD21	2.00	0.44
3:C:88:ARG:HE	3:C:100:ALA:CB	2.28	0.44
5:E:131:ILE:HA	5:E:131:ILE:HD13	1.50	0.44
9:I:65:VAL:HG11	9:I:77:ILE:HD11	1.99	0.44
12:L:46:LYS:N	12:L:92:OTD:O	2.48	0.44
12:L:60:LEU:HA	12:L:60:LEU:HD13	1.59	0.44
16:P:3:LYS:HA	16:P:64:ALA:HB1	2.00	0.44
17:Q:8:GLY:O	17:Q:56:VAL:HA	2.18	0.44
17:Q:51:TYR:CD1	17:Q:73:VAL:HG11	2.51	0.44
18:R:50:ILE:CG1	18:R:70:ILE:HD13	2.48	0.44
1:A:90:U:C4	1:A:91:C:N4	2.86	0.44
1:A:791:G:H2'	1:A:792:A:H5''	1.99	0.44
1:A:864:A:H2'	1:A:865:A:C8	2.52	0.44
1:A:1250:A:C6	1:A:1251:A:N1	2.86	0.44
3:C:26:LYS:HZ2	10:J:45:ARG:HH22	1.65	0.44
3:C:157:ILE:HD11	3:C:164:ARG:HB2	1.98	0.44
4:D:25:ARG:C	4:D:27:TYR:N	2.72	0.44
5:E:110:LEU:N	5:E:110:LEU:HD23	2.32	0.44
6:F:15:ASP:OD1	6:F:16:GLN:N	2.51	0.44
6:F:97:PHE:HE1	18:R:61:LYS:HE3	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:11:ARG:HD2	13:M:45:VAL:HG11	1.98	0.44
15:O:78:TYR:O	15:O:79:ARG:C	2.60	0.44
1:A:91:C:C5	1:A:92:C:H5	2.35	0.44
1:A:176:C:OP1	20:T:29:LYS:NZ	2.43	0.44
1:A:451:A:O5'	1:A:451:A:H8	2.00	0.44
1:A:1251:A:H4'	9:I:12:GLU:OE2	2.18	0.44
2:B:97:TRP:HZ3	2:B:176:GLU:OE2	2.00	0.44
5:E:80:ILE:CD1	5:E:91:LEU:HB2	2.48	0.44
8:H:111:ILE:O	8:H:134:ILE:HD12	2.18	0.44
8:H:113:SER:CB	8:H:134:ILE:HD11	2.48	0.44
10:J:48:THR:HG23	10:J:60:ARG:HB3	1.98	0.44
10:J:48:THR:OG1	10:J:62:HIS:CD2	2.71	0.44
14:N:3:ARG:HB3	14:N:6:LEU:HG	1.98	0.44
18:R:58:LEU:HD13	18:R:62:GLU:HB3	1.99	0.44
20:T:10:LEU:HD22	20:T:10:LEU:HA	1.66	0.44
20:T:30:LYS:O	20:T:34:LYS:HG2	2.17	0.44
1:A:1148:U:O3'	9:I:14:VAL:HG11	2.18	0.44
3:C:187:ALA:O	3:C:198:VAL:HG23	2.17	0.44
8:H:63:LEU:HD13	8:H:63:LEU:N	2.33	0.44
10:J:24:VAL:O	10:J:28:ARG:HB2	2.18	0.44
11:K:72:ALA:HB1	11:K:77:MET:CB	2.47	0.44
17:Q:60:ILE:C	17:Q:71:PHE:HD1	2.26	0.44
19:S:34:TRP:CH2	19:S:57:HIS:NE2	2.86	0.44
20:T:36:LEU:O	20:T:39:LYS:HB3	2.18	0.44
1:A:234:C:H2'	1:A:235:C:H6	1.81	0.44
1:A:671:G:H5'	6:F:77:ARG:HH21	1.83	0.44
1:A:679:C:H2'	1:A:680:C:C6	2.53	0.44
1:A:728:A:C8	15:O:54:ARG:NH1	2.86	0.44
1:A:766:A:OP2	25:A:2188:HOH:O	2.21	0.44
2:B:87:ARG:HH12	2:B:230:VAL:HG21	1.81	0.44
14:N:20:ALA:C	14:N:21:TYR:HD1	2.26	0.44
1:A:131:C:OP1	1:A:190(F):G:N2	2.44	0.44
1:A:179:A:H2'	1:A:180:U:H6	1.81	0.44
1:A:200:G:H3'	1:A:201:C:H5''	1.99	0.44
1:A:481:G:O2'	1:A:482:A:C8	2.69	0.44
1:A:695:A:N3	1:A:787:A:H1'	2.33	0.44
1:A:902:G:H2'	1:A:903:G:C8	2.53	0.44
1:A:1372:U:H2'	1:A:1373:G:O4'	2.18	0.44
2:B:101:MET:O	2:B:105:PHE:HD1	2.00	0.44
4:D:122:ARG:HA	4:D:134:ASP:O	2.17	0.44
4:D:187:ARG:NH2	4:D:188:LEU:HD12	2.29	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:110:LEU:CD1	5:E:118:ILE:HG21	2.48	0.44
7:G:71:PRO:O	7:G:91:VAL:HG21	2.18	0.44
16:P:54:GLU:C	16:P:54:GLU:CD	2.85	0.44
17:Q:50:LYS:HG3	17:Q:51:TYR:CE2	2.53	0.44
20:T:104:LEU:H	20:T:104:LEU:HG	1.51	0.44
1:A:442:C:H42	1:A:492:G:H1	1.65	0.43
1:A:1442:G:C6	1:A:1446:A:N7	2.86	0.43
6:F:100:ASN:O	18:R:28:GLU:HG3	2.18	0.43
8:H:112:LEU:CD2	8:H:133:LEU:HA	2.47	0.43
11:K:81:ASP:OD2	11:K:106:LYS:HE3	2.18	0.43
12:L:113:ARG:HH21	12:L:120:TYR:HE1	1.66	0.43
20:T:73:HIS:HB3	20:T:74:LYS:H	1.49	0.43
1:A:92:C:O2	1:A:93:G:C8	2.71	0.43
1:A:1279:A:H5''	1:A:1280:A:OP1	2.18	0.43
2:B:17:PHE:HD1	2:B:18:GLY:H	1.66	0.43
4:D:131:ARG:HB2	4:D:131:ARG:HH11	1.83	0.43
5:E:122:GLU:OE1	5:E:131:ILE:HG13	2.17	0.43
5:E:142:LEU:HA	5:E:142:LEU:HD23	1.68	0.43
6:F:74:ASP:OD1	6:F:74:ASP:N	2.51	0.43
13:M:5:ALA:CB	13:M:22:ILE:HD13	2.48	0.43
13:M:108:ARG:NH2	13:M:112:GLY:O	2.51	0.43
17:Q:85:VAL:O	17:Q:86:GLU:C	2.61	0.43
18:R:33:ASP:OD1	18:R:36:ASN:N	2.51	0.43
1:A:738:C:OP2	6:F:92:LYS:HE3	2.18	0.43
1:A:828:A:H4'	1:A:828:A:OP1	2.17	0.43
1:A:1022:G:C6	1:A:1024:G:C2	3.06	0.43
1:A:1054:C:H3'	1:A:1054:C:H6	1.83	0.43
1:A:1074:G:O3'	2:B:103:THR:HG21	2.18	0.43
1:A:1127:G:N2	1:A:1146:A:N6	2.67	0.43
1:A:1223:C:H5''	1:A:1224:G:C5'	2.47	0.43
1:A:1407:5MC:O2'	1:A:1408:A:H5'	2.18	0.43
1:A:1426:C:H2'	1:A:1427:U:H6	1.81	0.43
2:B:233:SER:HA	2:B:234:PRO:HD3	1.82	0.43
4:D:94:LEU:HD23	4:D:94:LEU:HA	1.83	0.43
6:F:15:ASP:H	6:F:18:GLN:CD	2.26	0.43
11:K:54:ARG:O	11:K:57:THR:HG22	2.19	0.43
12:L:25:PRO:HB3	12:L:27:LEU:HB2	1.99	0.43
13:M:49:THR:HG22	13:M:50:GLU:H	1.83	0.43
14:N:37:PHE:HB3	14:N:39:LEU:HD12	1.99	0.43
1:A:979:C:C5	1:A:980:C:C5	3.07	0.43
1:A:1003:G:N2	1:A:1039:C:C2	2.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1152:A:C5'	10:J:13:HIS:HB2	2.48	0.43
1:A:1181:G:C2	1:A:1182:G:N2	2.86	0.43
1:A:1253:G:C5	1:A:1254:C:C4	3.06	0.43
1:A:1360:A:OP2	14:N:35:ARG:NH2	2.51	0.43
2:B:92:TYR:HD2	2:B:92:TYR:N	2.14	0.43
2:B:157:ARG:HG2	2:B:158:LEU:N	2.32	0.43
2:B:187:LEU:HA	2:B:187:LEU:HD22	1.42	0.43
1:A:204:U:H4'	1:A:216:G:O5'	2.16	0.43
1:A:413:G:N2	1:A:428:G:H1'	2.33	0.43
1:A:491:G:C6	1:A:492:G:N7	2.86	0.43
1:A:659:U:OP2	15:O:8:LYS:NZ	2.38	0.43
1:A:939:G:H2'	1:A:940:C:C6	2.54	0.43
5:E:35:GLY:HA2	5:E:40:ARG:O	2.18	0.43
5:E:90:VAL:HG23	5:E:121:LYS:O	2.18	0.43
6:F:11:ASN:O	6:F:14:LEU:HD12	2.19	0.43
6:F:87:ARG:HG3	6:F:87:ARG:NH1	2.15	0.43
7:G:99:LEU:HA	7:G:99:LEU:HD23	1.54	0.43
9:I:89:ASN:HB3	9:I:92:TYR:CD1	2.54	0.43
10:J:4:ILE:HD13	10:J:4:ILE:HA	1.85	0.43
10:J:40:LEU:HG	10:J:71:LEU:HD21	2.00	0.43
13:M:11:ARG:HG3	13:M:12:ASN:HB2	1.99	0.43
1:A:456:C:C2	1:A:477:G:N2	2.87	0.43
1:A:475:G:H2'	1:A:476:G:C8	2.54	0.43
1:A:538:G:OP2	12:L:115:LYS:HB2	2.19	0.43
1:A:792:A:N7	1:A:794:A:C6	2.87	0.43
1:A:1008:C:O5'	1:A:1008:C:H6	2.01	0.43
1:A:1120:G:C6	1:A:1121:U:C4	3.06	0.43
1:A:1163:C:O2'	1:A:1164:G:H5'	2.18	0.43
1:A:1222:G:OP2	1:A:1322:C:N4	2.51	0.43
1:A:1358:U:H5''	14:N:35:ARG:CG	2.48	0.43
1:A:1494:G:C2	1:A:1495:U:C6	3.07	0.43
4:D:25:ARG:C	4:D:27:TYR:H	2.20	0.43
14:N:53:LEU:HA	14:N:54:PRO:HD3	1.64	0.43
15:O:6:GLU:HA	15:O:9:GLN:HB2	2.00	0.43
15:O:76:GLU:HA	15:O:76:GLU:OE2	2.18	0.43
16:P:71:ARG:O	16:P:74:LEU:HB2	2.18	0.43
17:Q:50:LYS:HG3	17:Q:51:TYR:CD2	2.54	0.43
18:R:39:VAL:HG13	18:R:40:LEU:CD2	2.47	0.43
1:A:106:C:H2'	1:A:107:G:O4'	2.19	0.43
1:A:117:G:O5'	1:A:117:G:H8	2.01	0.43
1:A:1064:G:H1'	1:A:1190:G:N2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1065:U:H5''	1:A:1190:G:N2	2.34	0.43
1:A:1202:G:C2	14:N:42:ILE:HG21	2.54	0.43
1:A:1427:U:H2'	1:A:1428:A:H8	1.83	0.43
3:C:6:HIS:HA	3:C:7:PRO:HD2	1.71	0.43
9:I:17:VAL:HG11	9:I:81:ILE:CA	2.45	0.43
19:S:71:LEU:C	19:S:73:GLU:N	2.77	0.43
1:A:451:A:N7	1:A:481:G:N1	2.67	0.43
1:A:518:C:H4'	1:A:519:C:O5'	2.19	0.43
1:A:877:C:O2'	8:H:3:THR:HG23	2.18	0.43
2:B:142:LEU:HD13	2:B:146:GLN:HE22	1.83	0.43
2:B:167:PRO:HG2	2:B:192:SER:CB	2.48	0.43
4:D:72:GLU:O	4:D:75:PHE:HB3	2.19	0.43
8:H:27:PRO:HA	8:H:58:TYR:CD2	2.54	0.43
19:S:49:ILE:O	19:S:60:VAL:HG23	2.18	0.43
19:S:50:ALA:HA	19:S:59:PRO:HA	2.00	0.43
1:A:279:A:C4	17:Q:98:LEU:HD23	2.53	0.43
1:A:1071:C:C2'	1:A:1072:G:H5'	2.49	0.43
1:A:1225:A:OP1	13:M:102:ARG:HA	2.18	0.43
4:D:192:GLU:C	4:D:194:LEU:N	2.73	0.43
4:D:200:GLU:HG2	4:D:201:GLN:N	2.33	0.43
4:D:203:VAL:O	4:D:204:ILE:C	2.62	0.43
8:H:112:LEU:HD23	8:H:112:LEU:HA	1.30	0.43
8:H:118:VAL:C	8:H:119:LEU:HD23	2.43	0.43
12:L:27:LEU:O	12:L:29:GLY:N	2.52	0.43
18:R:50:ILE:HD11	18:R:70:ILE:HG21	2.01	0.43
20:T:16:HIS:CE1	20:T:20:LEU:HD23	2.54	0.43
1:A:384:G:C4	1:A:385:C:C5	3.07	0.43
1:A:457:C:C2	1:A:476:G:C2	3.07	0.43
1:A:500:G:C5	1:A:501:C:C4	3.07	0.43
1:A:923:A:OP1	5:E:21:ALA:HB2	2.18	0.43
1:A:1067:A:O2'	1:A:1094:G:H5'	2.18	0.43
1:A:1219:U:C4	1:A:1220:G:N7	2.87	0.43
1:A:1505:G:H5''	25:A:1919:HOH:O	2.18	0.43
3:C:157:ILE:HD13	3:C:157:ILE:N	2.33	0.43
9:I:7:THR:HG22	9:I:8:GLY:N	2.33	0.43
11:K:107:SER:O	11:K:108:ILE:HD13	2.19	0.43
13:M:19:LEU:HD11	13:M:56:LEU:HD11	2.01	0.43
17:Q:9:VAL:HG23	17:Q:56:VAL:HG22	2.00	0.43
1:A:109:A:C4	1:A:327:A:C2	3.07	0.42
1:A:295:C:H2'	1:A:296:U:O4'	2.19	0.42
1:A:392:G:C6	1:A:393:A:C6	3.07	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:852:G:C3'	1:A:853:G:H5''	2.49	0.42
1:A:858:G:O6	1:A:869:G:C8	2.72	0.42
1:A:1332:A:H2'	1:A:1333:A:C8	2.54	0.42
1:A:1506:U:O2'	1:A:1507:A:H5'	2.18	0.42
2:B:73:THR:O	2:B:73:THR:HG22	2.19	0.42
2:B:115:LEU:HD23	2:B:145:LEU:HB2	2.00	0.42
4:D:22:LYS:HA	4:D:22:LYS:HD2	1.59	0.42
6:F:1:MET:HA	6:F:67:MET:O	2.18	0.42
7:G:60:LYS:NZ	7:G:63:LYS:HD2	2.34	0.42
9:I:63:ILE:HD11	9:I:81:ILE:HD11	2.01	0.42
10:J:78:ASN:ND2	10:J:79:ARG:HE	2.17	0.42
11:K:92:GLU:O	11:K:96:ARG:HD3	2.19	0.42
11:K:95:ILE:HD13	11:K:95:ILE:HA	1.85	0.42
12:L:42:THR:CG2	12:L:52:LEU:HB3	2.49	0.42
19:S:43:GLU:OE1	19:S:43:GLU:N	2.51	0.42
1:A:109:A:C6	1:A:326:G:C6	3.07	0.42
1:A:946:A:H2'	1:A:947:G:H8	1.83	0.42
1:A:1056:U:O2'	1:A:1057:G:H5'	2.19	0.42
1:A:1313:U:O4	19:S:4:SER:OG	2.28	0.42
1:A:1374:A:H2'	1:A:1375:A:H8	1.84	0.42
4:D:200:GLU:H	4:D:200:GLU:CD	2.27	0.42
8:H:95:VAL:HG11	8:H:133:LEU:HG	2.01	0.42
9:I:113:LYS:H	9:I:119:ALA:HA	1.83	0.42
17:Q:61:GLU:HA	17:Q:71:PHE:CD1	2.53	0.42
18:R:48:GLY:HA3	18:R:82:THR:HA	2.01	0.42
21:U:10:ARG:O	21:U:13:ILE:HB	2.19	0.42
1:A:267:C:OP2	17:Q:67:LYS:HE3	2.19	0.42
1:A:861:G:C5	1:A:862:C:C5	3.07	0.42
1:A:1125:U:O2'	1:A:1126:U:H5'	2.20	0.42
1:A:1308:U:OP2	13:M:99:ARG:HG2	2.19	0.42
1:A:1342:C:H2'	1:A:1343:G:H8	1.83	0.42
1:A:1352:C:H2'	1:A:1353:G:C8	2.54	0.42
3:C:92:ALA:HB2	3:C:99:VAL:O	2.20	0.42
4:D:15:GLU:CD	4:D:59:ARG:HH21	2.27	0.42
4:D:101:LEU:O	4:D:105:VAL:HG23	2.19	0.42
6:F:25:ILE:HA	6:F:28:ARG:HD3	2.00	0.42
9:I:4:TYR:CG	9:I:88:TYR:HB2	2.53	0.42
9:I:45:ALA:HB1	9:I:78:LYS:NZ	2.34	0.42
1:A:512:U:P	4:D:46:LYS:HZ3	2.41	0.42
1:A:913:A:OP1	12:L:91:LYS:HE2	2.19	0.42
1:A:1064:G:H1'	1:A:1190:G:H21	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1366:C:C2	1:A:1367:C:C5	3.07	0.42
1:A:1374:A:N3	1:A:1375:A:C8	2.87	0.42
2:B:74:LYS:NZ	2:B:206:ASP:HB2	2.34	0.42
2:B:131:PRO:O	2:B:134:GLU:HG2	2.20	0.42
4:D:11:LEU:HD23	4:D:11:LEU:HA	1.68	0.42
5:E:64:ARG:O	5:E:65:ASN:HB3	2.19	0.42
7:G:17:VAL:HB	7:G:44:TYR:CZ	2.54	0.42
7:G:85:TYR:O	7:G:87:VAL:HG22	2.19	0.42
18:R:36:ASN:OD1	18:R:39:VAL:HG12	2.19	0.42
1:A:47:C:C6	1:A:365:U:H2'	2.55	0.42
1:A:243:A:C2	1:A:245:C:C2	3.07	0.42
1:A:336:C:O2'	1:A:337:C:H5'	2.19	0.42
1:A:429:U:H1'	1:A:430:A:H5''	2.00	0.42
1:A:1185:G:H2'	1:A:1186:G:H5'	2.00	0.42
1:A:1274:G:H2'	1:A:1275:A:C8	2.54	0.42
1:A:1525:G:OP1	11:K:120:ARG:NH2	2.53	0.42
4:D:110:PHE:HA	4:D:162:LEU:HD21	2.01	0.42
6:F:39:LYS:NZ	6:F:64:GLN:OE1	2.51	0.42
12:L:67:THR:O	12:L:67:THR:OG1	2.34	0.42
21:U:18:TYR:CD1	21:U:24:ARG:HG2	2.53	0.42
1:A:59:A:C2	1:A:354:G:C4	3.07	0.42
1:A:397:A:H3'	1:A:397:A:N3	2.34	0.42
1:A:721:G:H4'	1:A:722:A:O4'	2.20	0.42
1:A:727:G:N2	1:A:730:G:OP2	2.47	0.42
1:A:829:G:C6	1:A:858:G:N2	2.87	0.42
1:A:836:G:C6	1:A:851:G:C6	3.08	0.42
1:A:1113:C:H4'	3:C:14:ILE:HD11	2.00	0.42
1:A:1309:G:C6	1:A:1310:G:C5	3.07	0.42
2:B:21:ARG:HA	2:B:39:ILE:HA	2.01	0.42
2:B:172:ILE:H	2:B:172:ILE:HG12	1.46	0.42
3:C:188:LEU:HA	3:C:188:LEU:HD22	1.65	0.42
7:G:120:ILE:O	7:G:121:ALA:C	2.63	0.42
10:J:15:THR:HG23	10:J:94:VAL:HG22	2.01	0.42
11:K:91:ARG:NH1	18:R:88:LYS:HZ1	2.18	0.42
12:L:44:THR:HA	12:L:45:PRO:HD3	1.82	0.42
17:Q:34:LYS:HG3	17:Q:35:VAL:N	2.35	0.42
1:A:123:C:O2'	1:A:290:C:O2	2.33	0.42
1:A:454:C:N4	1:A:479:C:N3	2.67	0.42
1:A:1123:A:H61	1:A:1149:C:H42	1.66	0.42
1:A:1544:U:O5'	1:A:1544:U:H6	2.02	0.42
3:C:180:ALA:O	3:C:181:ASN:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:41:VAL:HG13	5:E:113:ALA:HB2	2.01	0.42
8:H:97:VAL:HG12	8:H:98:LYS:N	2.35	0.42
10:J:62:HIS:CB	14:N:59:ALA:HB3	2.50	0.42
16:P:67:THR:HG22	16:P:68:ASP:N	2.35	0.42
18:R:33:ASP:O	18:R:40:LEU:HD11	2.20	0.42
19:S:55:LYS:HD3	19:S:56:GLN:HG2	2.02	0.42
20:T:22:ARG:O	20:T:23:ARG:C	2.63	0.42
1:A:45:U:H2'	1:A:46:G:C8	2.55	0.42
1:A:448:A:C4	1:A:487:A:C2	3.07	0.42
1:A:1071:C:O2'	1:A:1072:G:H5'	2.19	0.42
1:A:1193:G:O2'	1:A:1194:U:H5'	2.20	0.42
3:C:32:LEU:O	3:C:35:GLU:HB3	2.20	0.42
3:C:39:ILE:HD12	3:C:57:ILE:HD11	2.02	0.42
8:H:57:PRO:HG2	8:H:57:PRO:O	2.19	0.42
8:H:127:LEU:HD22	8:H:127:LEU:HA	1.74	0.42
8:H:137:VAL:HG12	8:H:138:TRP:N	2.33	0.42
9:I:111:ARG:NH1	9:I:113:LYS:HA	2.35	0.42
12:L:26:ALA:O	12:L:33:ARG:HD2	2.19	0.42
13:M:117:VAL:HG12	13:M:118:ALA:N	2.34	0.42
14:N:39:LEU:HD22	14:N:43:CYS:HB3	2.01	0.42
15:O:36:ILE:HG22	15:O:37:ASN:N	2.32	0.42
19:S:31:ILE:HD12	19:S:32:LYS:H	1.85	0.42
1:A:22:G:C5	1:A:914:G:C6	3.08	0.42
1:A:511:C:H42	1:A:540:G:H1	1.68	0.42
1:A:945:G:N1	1:A:1337:G:C2	2.88	0.42
1:A:1284:C:OP2	1:A:1285:A:O2'	2.34	0.42
1:A:1347:G:C2'	1:A:1348:U:OP2	2.67	0.42
2:B:127:ILE:H	2:B:127:ILE:HG13	1.59	0.42
2:B:224:GLN:HG3	2:B:229:VAL:HG22	2.02	0.42
3:C:54:ARG:HB3	3:C:69:HIS:HB2	2.02	0.42
8:H:104:ARG:HG3	8:H:138:TRP:CG	2.55	0.42
11:K:40:ILE:HG22	11:K:41:THR:N	2.35	0.42
11:K:59:TYR:O	11:K:63:LEU:HG	2.20	0.42
12:L:35:GLY:O	12:L:83:VAL:HG12	2.20	0.42
13:M:23:TYR:CE2	13:M:70:LEU:HD13	2.55	0.42
19:S:20:LEU:HD12	19:S:20:LEU:HA	1.87	0.42
19:S:40:ILE:HD11	19:S:62:ILE:HD12	2.01	0.42
20:T:33:ILE:CD1	20:T:63:ILE:HA	2.50	0.42
20:T:87:LYS:O	20:T:91:LEU:HG	2.20	0.42
1:A:358:U:H2'	1:A:359:U:H6	1.84	0.42
1:A:474:G:H2'	1:A:475:G:O4'	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:484:G:O2'	1:A:485:G:OP2	2.26	0.42
1:A:509:A:C8	1:A:509:A:C3'	3.03	0.42
1:A:585:G:C6	1:A:586:C:C4	3.08	0.42
1:A:693:G:C6	1:A:694:A:C5	3.07	0.42
1:A:1120:G:O6	1:A:1153:C:N4	2.53	0.42
1:A:1250:A:N1	1:A:1251:A:C2	2.88	0.42
1:A:1320:C:O2'	19:S:73:GLU:OE1	2.35	0.42
1:A:1504:G:H4'	1:A:1505:G:H5'	2.02	0.42
3:C:6:HIS:HD2	3:C:8:ILE:H	1.67	0.42
4:D:187:ARG:HD2	4:D:187:ARG:HA	1.15	0.42
6:F:30:LEU:HD23	6:F:75:LEU:HD21	2.01	0.42
6:F:98:LEU:HB2	6:F:101:ALA:HB2	2.02	0.42
7:G:104:LEU:N	7:G:104:LEU:HD23	2.34	0.42
7:G:124:LEU:HD23	7:G:124:LEU:HA	1.60	0.42
17:Q:4:LYS:HG2	17:Q:6:LEU:CD2	2.49	0.42
1:A:284:G:H2'	1:A:285:G:C8	2.54	0.41
1:A:527:7MG:O2'	1:A:535:A:N1	2.37	0.41
1:A:578:C:H2'	1:A:579:G:O4'	2.20	0.41
1:A:1112:C:H1'	3:C:179:ARG:NH1	2.35	0.41
1:A:1134:G:C6	1:A:1141:C:C4	3.07	0.41
1:A:1197:G:H5''	1:A:1198:G:OP2	2.20	0.41
4:D:187:ARG:NH1	4:D:188:LEU:H	2.18	0.41
5:E:53:LEU:HD23	5:E:53:LEU:HA	1.66	0.41
5:E:80:ILE:HD12	5:E:91:LEU:HB2	2.00	0.41
6:F:23:LYS:O	6:F:27:GLN:HG2	2.20	0.41
6:F:41:GLU:OE1	18:R:35:ARG:NH2	2.53	0.41
8:H:4:ASP:OD2	8:H:85:ARG:NH1	2.53	0.41
18:R:53:ARG:HA	18:R:56:THR:OG1	2.19	0.41
1:A:134:A:H2'	1:A:135:C:O4'	2.19	0.41
1:A:940:C:H2'	1:A:941:G:O4'	2.20	0.41
1:A:1144:G:N2	1:A:1146:A:H62	2.17	0.41
1:A:1243:C:H5''	21:U:8:THR:HG22	2.02	0.41
1:A:1250:A:H4'	9:I:68:GLY:CA	2.50	0.41
1:A:1399:C:H4'	1:A:1400:5MC:H5''	2.02	0.41
1:A:1435:G:H2'	1:A:1436:U:H6	1.79	0.41
2:B:124:SER:HB2	2:B:126:GLU:OE1	2.20	0.41
11:K:44:SER:H	11:K:47:VAL:HB	1.85	0.41
12:L:55:VAL:HG12	12:L:69:TYR:HA	2.02	0.41
18:R:22:VAL:HG23	18:R:55:ARG:O	2.20	0.41
1:A:27:G:H1	1:A:556:C:N4	2.18	0.41
1:A:109:A:H2'	1:A:326:G:N2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:669:U:OP1	15:O:48:LYS:NZ	2.41	0.41
1:A:831:U:O2'	1:A:832:C:H5'	2.21	0.41
1:A:1070:U:O2	1:A:1106:G:C2	2.73	0.41
1:A:1171:G:C6	1:A:1172:C:N4	2.88	0.41
1:A:1296:C:H4'	1:A:1302:U:C5	2.54	0.41
1:A:1541:PSU:H3'	1:A:1541:PSU:C6	2.53	0.41
2:B:28:PHE:O	2:B:28:PHE:CD2	2.74	0.41
2:B:102:LEU:HB3	2:B:180:LEU:HD11	2.02	0.41
4:D:38:TYR:CD1	4:D:45:GLN:HG2	2.55	0.41
4:D:57:ARG:HG3	4:D:202:LEU:HD13	2.03	0.41
8:H:6:ILE:HG23	8:H:6:ILE:HD12	1.66	0.41
9:I:126:SER:O	9:I:128:ARG:N	2.53	0.41
10:J:78:ASN:CG	10:J:79:ARG:HE	2.28	0.41
17:Q:58:GLU:C	17:Q:59:ILE:HD13	2.44	0.41
20:T:41:ILE:O	20:T:44:ALA:HB3	2.21	0.41
1:A:141:A:H1'	1:A:182:U:O2	2.20	0.41
1:A:431:A:H2'	1:A:432:A:O4'	2.20	0.41
1:A:922:G:N2	1:A:1396:A:C5	2.89	0.41
1:A:1118:C:H1'	1:A:1179:A:C5	2.54	0.41
1:A:1118:C:H5'	9:I:104:ARG:HG3	2.02	0.41
1:A:1226:C:C5	13:M:104:ARG:HA	2.54	0.41
2:B:158:LEU:HD23	2:B:158:LEU:HA	1.70	0.41
4:D:120:LEU:HD23	4:D:120:LEU:HA	1.72	0.41
7:G:58:PRO:HA	7:G:61:VAL:HB	2.03	0.41
11:K:18:ARG:O	11:K:33:THR:HG22	2.21	0.41
13:M:23:TYR:HB3	13:M:67:GLU:CA	2.48	0.41
16:P:22:THR:HA	16:P:33:ILE:HG13	2.02	0.41
17:Q:10:VAL:HG23	17:Q:54:GLY:H	1.85	0.41
1:A:88:A:H2'	1:A:89:C:H6	1.85	0.41
1:A:1053:G:O2'	1:A:1199:U:H5	2.01	0.41
1:A:1172:C:O2'	1:A:1173:G:H5'	2.20	0.41
1:A:1250:A:C2	1:A:1287:A:C2	3.09	0.41
1:A:1255:G:C2'	1:A:1279:A:H61	2.31	0.41
2:B:79:ASP:O	2:B:82:ARG:N	2.54	0.41
2:B:182:ILE:HA	2:B:183:PRO:HD3	1.78	0.41
4:D:27:TYR:HE1	4:D:168:ARG:HH22	1.68	0.41
5:E:112:LEU:C	5:E:114:GLY:H	2.28	0.41
8:H:104:ARG:CZ	8:H:138:TRP:CZ2	3.04	0.41
12:L:30:ALA:HA	12:L:31:PRO:HD3	1.68	0.41
14:N:12:ARG:HB2	14:N:13:THR:H	1.61	0.41
21:U:3:LYS:HB2	21:U:3:LYS:HE3	1.75	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:C:N4	1:A:384:G:H1	2.18	0.41
1:A:491:G:C2	1:A:492:G:C8	3.07	0.41
1:A:824:C:H2'	1:A:825:G:C8	2.56	0.41
1:A:1130:A:OP1	1:A:1131:G:N7	2.53	0.41
2:B:76:GLN:O	2:B:208:ILE:HD12	2.20	0.41
3:C:32:LEU:H	3:C:32:LEU:HG	1.58	0.41
4:D:62:GLN:NE2	4:D:66:ARG:HD2	2.35	0.41
5:E:148:VAL:O	5:E:152:ARG:HG3	2.20	0.41
6:F:36:ARG:HB3	6:F:36:ARG:NH1	2.21	0.41
7:G:32:ARG:C	7:G:34:GLY:N	2.79	0.41
9:I:49:PRO:HB2	9:I:81:ILE:HG22	2.02	0.41
13:M:18:ALA:O	13:M:21:TYR:HB2	2.19	0.41
16:P:8:ARG:HB3	16:P:28:ARG:NH1	2.35	0.41
19:S:21:GLU:O	19:S:25:LYS:HB2	2.21	0.41
20:T:49:ALA:O	20:T:52:ALA:HB3	2.20	0.41
1:A:147:G:H1	1:A:175:C:H42	1.69	0.41
1:A:1073:U:O2	2:B:104:ASN:ND2	2.54	0.41
1:A:1119:C:OP1	9:I:83:ARG:NH1	2.53	0.41
1:A:1249:C:H5'	1:A:1250:A:OP2	2.21	0.41
1:A:1351:U:H4'	7:G:33:ASP:OD2	2.20	0.41
4:D:120:LEU:HD23	4:D:125:HIS:CD2	2.56	0.41
9:I:94:ALA:O	9:I:98:PRO:HG3	2.21	0.41
12:L:33:ARG:HG3	12:L:61:THR:OG1	2.20	0.41
12:L:85:ILE:CG2	12:L:98:TYR:HB3	2.49	0.41
13:M:22:ILE:HG22	13:M:23:TYR:H	1.86	0.41
13:M:40:ASN:HD21	13:M:42:ALA:HB3	1.86	0.41
17:Q:65:ILE:HB	17:Q:69:LYS:HB3	2.03	0.41
1:A:268:C:H2'	1:A:269:C:H6	1.85	0.41
1:A:372:C:H1'	1:A:373:A:OP2	2.21	0.41
1:A:854:G:C2	1:A:855:G:C8	3.08	0.41
1:A:1226:C:N4	13:M:104:ARG:HG3	2.36	0.41
2:B:211:ILE:O	2:B:215:LEU:HB2	2.20	0.41
3:C:25:GLY:HA3	3:C:29:TYR:HB2	2.03	0.41
4:D:22:LYS:CB	4:D:26:CYS:HB2	2.51	0.41
4:D:203:VAL:O	4:D:206:PHE:HB3	2.21	0.41
5:E:91:LEU:HD23	5:E:91:LEU:N	2.35	0.41
7:G:58:PRO:HA	7:G:61:VAL:CG2	2.51	0.41
8:H:9:MET:O	8:H:10:LEU:C	2.62	0.41
12:L:84:LEU:HD12	12:L:84:LEU:HA	1.91	0.41
16:P:19:ILE:HD12	16:P:38:TYR:N	2.36	0.41
17:Q:12:SER:HB3	17:Q:20:THR:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:20:THR:CG2	17:Q:41:LYS:HG2	2.51	0.41
17:Q:24:GLU:HG3	17:Q:39:SER:HB3	2.03	0.41
18:R:37:VAL:O	18:R:40:LEU:N	2.54	0.41
20:T:58:LYS:O	20:T:58:LYS:HG3	2.19	0.41
1:A:8:A:H5'	5:E:101:ILE:HG23	2.02	0.41
1:A:458:C:H2'	1:A:459:G:O4'	2.21	0.41
1:A:519:C:H2'	1:A:520:A:C8	2.55	0.41
1:A:738:C:OP1	6:F:92:LYS:HD3	2.21	0.41
1:A:861:G:C6	1:A:862:C:C4	3.08	0.41
1:A:922:G:C2	1:A:1396:A:C6	3.09	0.41
1:A:965:A:OP1	1:A:1198:G:H5''	2.20	0.41
1:A:976:G:C8	1:A:1358:U:O2	2.74	0.41
1:A:1133:G:C2	1:A:1134:G:C8	3.08	0.41
1:A:1164:G:C2	1:A:1165:C:C2	3.09	0.41
1:A:1285:A:H5'	1:A:1286:A:C5	2.56	0.41
1:A:1295:G:C6	1:A:1296:C:C4	3.08	0.41
1:A:1375:A:N1	1:A:1376:U:C2	2.89	0.41
2:B:46:LYS:HA	2:B:49:GLU:OE2	2.20	0.41
2:B:155:LEU:HD23	2:B:155:LEU:HA	1.64	0.41
3:C:113:ALA:HB3	3:C:114:PRO:HD3	2.03	0.41
3:C:182:ILE:HA	3:C:202:ILE:O	2.20	0.41
4:D:20:TYR:CD2	4:D:20:TYR:N	2.88	0.41
4:D:192:GLU:O	4:D:194:LEU:N	2.54	0.41
5:E:143:ARG:NH1	8:H:77:GLU:CD	2.74	0.41
6:F:91:VAL:HG12	6:F:92:LYS:O	2.21	0.41
7:G:42:ILE:HD13	7:G:42:ILE:HG21	1.88	0.41
8:H:86:ILE:HG21	8:H:133:LEU:HB3	2.02	0.41
10:J:24:VAL:O	10:J:24:VAL:HG12	2.21	0.41
12:L:7:ILE:HG23	17:Q:34:LYS:HE2	2.02	0.41
12:L:98:TYR:CD1	12:L:98:TYR:N	2.89	0.41
13:M:54:VAL:HA	13:M:57:ARG:CD	2.50	0.41
14:N:14:PRO:C	14:N:16:PHE:H	2.29	0.41
15:O:21:ASP:OD2	15:O:23:GLY:N	2.54	0.41
16:P:4:ILE:O	16:P:66:PRO:HA	2.21	0.41
1:A:24:U:H2'	1:A:25:C:C6	2.56	0.41
1:A:70:G:C6	1:A:73:C:C4	3.09	0.41
1:A:95:U:H2'	1:A:96:G:H8	1.85	0.41
1:A:966:M2G:C8	1:A:967:5MC:HM53	2.56	0.41
1:A:974:A:H4'	1:A:975:A:H3'	2.03	0.41
1:A:976:G:OP2	1:A:1358:U:H1'	2.21	0.41
2:B:236:TYR:HD2	2:B:236:TYR:HA	1.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:137:ALA:HA	3:C:140:ARG:CZ	2.51	0.41
4:D:196:LEU:HA	4:D:197:PRO:HD3	1.65	0.41
9:I:5:TYR:CE1	9:I:18:PHE:HE2	2.39	0.41
9:I:10:ARG:O	9:I:11:LYS:C	2.64	0.41
11:K:25:TYR:CZ	11:K:88:GLY:HA2	2.56	0.41
15:O:45:VAL:O	15:O:46:HIS:C	2.64	0.41
17:Q:67:LYS:O	17:Q:68:ARG:HB3	2.21	0.41
1:A:349:A:H2'	1:A:350:G:C5'	2.50	0.40
1:A:1150:U:H2'	1:A:1151:A:H5'	2.03	0.40
1:A:1172:C:H2'	1:A:1173:G:C8	2.55	0.40
1:A:1182:G:H4'	1:A:1183:A:C5'	2.49	0.40
1:A:1368:G:OP2	9:I:112:LYS:HD3	2.21	0.40
2:B:9:GLU:C	2:B:10:LEU:HD23	2.47	0.40
2:B:59:GLU:O	2:B:60:ASP:C	2.64	0.40
2:B:188:ALA:O	2:B:202:PRO:HA	2.21	0.40
4:D:199:ASN:HD22	4:D:202:LEU:HG	1.86	0.40
5:E:55:VAL:HG12	5:E:56:GLN:N	2.35	0.40
7:G:37:ASN:HB3	7:G:38:LEU:HD12	2.03	0.40
11:K:58:PRO:HB2	11:K:93:GLN:HG3	2.02	0.40
11:K:120:ARG:HA	11:K:121:PRO:HD3	1.86	0.40
19:S:18:LYS:HD2	19:S:31:ILE:HG12	2.03	0.40
19:S:43:GLU:CD	19:S:43:GLU:H	2.29	0.40
1:A:245:C:O2	1:A:283:C:N3	2.55	0.40
1:A:266:G:P	25:A:2234:HOH:O	2.79	0.40
1:A:393:A:O2'	1:A:394:G:H5'	2.21	0.40
1:A:575:G:O2'	1:A:821:G:H5'	2.21	0.40
1:A:782:A:H2'	1:A:783:C:O4'	2.21	0.40
1:A:830:G:C5	1:A:831:U:C5	3.10	0.40
1:A:981:U:O4	1:A:1222:G:O6	2.40	0.40
1:A:1112:C:O2'	3:C:179:ARG:NH1	2.54	0.40
1:A:1126:U:C5'	1:A:1126:U:H6	2.35	0.40
1:A:1213:A:N1	1:A:1215:G:H1'	2.36	0.40
1:A:1513:A:H2'	1:A:1514:C:C6	2.55	0.40
1:A:1528:U:H6	1:A:1528:U:H2'	1.65	0.40
2:B:97:TRP:CZ2	2:B:101:MET:HB2	2.57	0.40
3:C:114:PRO:HG3	3:C:185:GLY:HA3	2.04	0.40
5:E:86:ALA:CB	5:E:125:SER:HB3	2.50	0.40
5:E:105:VAL:HG11	5:E:131:ILE:HG22	2.03	0.40
6:F:97:PHE:C	6:F:97:PHE:HD2	2.29	0.40
7:G:151:TYR:CD1	7:G:151:TYR:N	2.89	0.40
8:H:103:VAL:HG12	8:H:108:GLY:HA3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:51:ARG:HB2	9:I:51:ARG:HH11	1.86	0.40
13:M:36:LYS:HD2	13:M:59:TYR:OH	2.21	0.40
16:P:3:LYS:HG3	16:P:65:GLN:O	2.21	0.40
20:T:16:HIS:ND1	20:T:16:HIS:C	2.80	0.40
20:T:74:LYS:HA	20:T:74:LYS:HD3	1.72	0.40
1:A:88:A:C4	1:A:89:C:C6	3.09	0.40
1:A:287:U:C2'	1:A:288:A:H5'	2.52	0.40
1:A:325:A:N6	1:A:326:G:C2	2.90	0.40
1:A:631:G:H2'	1:A:632:A:C8	2.57	0.40
1:A:779:C:H5''	11:K:122:LYS:HB3	2.02	0.40
1:A:943:U:H1'	9:I:124:GLN:HE22	1.86	0.40
1:A:1003:G:C2	1:A:1003(A):G:C5	3.09	0.40
1:A:1066:C:C2'	1:A:1067:A:H5'	2.50	0.40
1:A:1402:4OC:O2	1:A:1500:A:N1	2.55	0.40
1:A:1476:G:H2'	1:A:1477:C:C6	2.57	0.40
1:A:1527:C:C2'	1:A:1528:U:H5'	2.52	0.40
2:B:23:ARG:O	2:B:24:TRP:HD1	2.05	0.40
3:C:61:ALA:C	3:C:63:ASN:H	2.30	0.40
8:H:6:ILE:HG13	8:H:31:PHE:HE2	1.86	0.40
14:N:23:ARG:HD3	14:N:28:GLY:O	2.20	0.40
15:O:39:LEU:HD12	15:O:39:LEU:HA	1.77	0.40
16:P:9:PHE:HD1	16:P:9:PHE:HA	1.64	0.40
17:Q:22:LEU:HD12	17:Q:40:LYS:O	2.21	0.40
1:A:428:G:C6	1:A:430:A:C6	3.09	0.40
1:A:820:U:H4'	1:A:821:G:OP2	2.22	0.40
1:A:1081:G:H5''	1:A:1081:G:C8	2.57	0.40
1:A:1422:G:C2	1:A:1423:G:C8	3.10	0.40
1:A:1540:PSU:C6	1:A:1540:PSU:H3'	2.57	0.40
3:C:6:HIS:CD2	3:C:8:ILE:HB	2.56	0.40
4:D:152:SER:HA	4:D:155:LEU:HD21	2.03	0.40
10:J:22:LYS:NZ	10:J:90:LEU:HD12	2.37	0.40
12:L:46:LYS:C	12:L:48:PRO:HD2	2.46	0.40
13:M:54:VAL:HG23	13:M:57:ARG:HH11	1.87	0.40
19:S:50:ALA:HA	19:S:58:VAL:O	2.20	0.40
20:T:62:LEU:O	20:T:62:LEU:HD22	2.21	0.40
20:T:71:THR:C	20:T:72:LEU:HD23	2.46	0.40
20:T:80:ARG:HG3	20:T:80:ARG:NH1	2.37	0.40
1:A:20:U:C6	1:A:20:U:H3'	2.56	0.40
1:A:227:G:H21	16:P:62:VAL:HG12	1.86	0.40
1:A:418:C:H1'	1:A:540:G:O2'	2.22	0.40
1:A:943:U:C2'	1:A:944:G:H5'	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:987:G:N2	1:A:1219:U:O2	2.54	0.40
1:A:990:C:H42	1:A:1215:G:H1	1.68	0.40
1:A:1164:G:C8	1:A:1164:G:OP2	2.74	0.40
1:A:1321:C:C5	1:A:1322:C:C2	3.08	0.40
1:A:1539:C:C4	1:A:1540:PSU:C2	3.09	0.40
2:B:161:ALA:C	2:B:162:ILE:HD13	2.46	0.40
3:C:51:GLY:O	3:C:115:LEU:HG	2.21	0.40
12:L:10:LEU:HD22	12:L:10:LEU:HA	1.75	0.40
19:S:64:GLU:O	19:S:67:VAL:HG23	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	232/256 (91%)	199 (86%)	30 (13%)	3 (1%)	9	38
3	C	204/239 (85%)	172 (84%)	30 (15%)	2 (1%)	12	43
4	D	206/209 (99%)	186 (90%)	17 (8%)	3 (2%)	8	35
5	E	148/162 (91%)	137 (93%)	9 (6%)	2 (1%)	9	36
6	F	99/101 (98%)	96 (97%)	3 (3%)	0	100	100
7	G	153/156 (98%)	137 (90%)	15 (10%)	1 (1%)	18	50
8	H	136/138 (99%)	129 (95%)	7 (5%)	0	100	100
9	I	125/128 (98%)	112 (90%)	12 (10%)	1 (1%)	16	47
10	J	96/105 (91%)	74 (77%)	20 (21%)	2 (2%)	5	30
11	K	114/129 (88%)	98 (86%)	16 (14%)	0	100	100
12	L	121/135 (90%)	105 (87%)	14 (12%)	2 (2%)	7	33
13	M	116/126 (92%)	103 (89%)	10 (9%)	3 (3%)	4	26
14	N	58/61 (95%)	48 (83%)	10 (17%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	O	85/89 (96%)	75 (88%)	10 (12%)	0	100	100
16	P	81/88 (92%)	74 (91%)	6 (7%)	1 (1%)	10	39
17	Q	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
18	R	68/88 (77%)	60 (88%)	8 (12%)	0	100	100
19	S	78/93 (84%)	70 (90%)	5 (6%)	3 (4%)	2	20
20	T	97/106 (92%)	81 (84%)	16 (16%)	0	100	100
21	U	22/27 (82%)	20 (91%)	2 (9%)	0	100	100
All	All	2336/2541 (92%)	2066 (88%)	247 (11%)	23 (1%)	12	43

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
19	S	31	ILE
19	S	70	LYS
2	B	21	ARG
2	B	24	TRP
3	C	15	THR
12	L	28	LYS
19	S	30	LEU
4	D	35	ARG
7	G	59	LEU
9	I	117	HIS
2	B	229	VAL
4	D	160	GLN
13	M	59	TYR
13	M	61	GLU
5	E	129	ILE
10	J	34	VAL
3	C	66	VAL
4	D	5	ILE
13	M	7	VAL
16	P	53	VAL
5	E	70	PRO
10	J	72	VAL
12	L	25	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	202/220 (92%)	141 (70%)	61 (30%)	0	2
3	C	160/188 (85%)	106 (66%)	54 (34%)	0	1
4	D	180/181 (99%)	136 (76%)	44 (24%)	1	5
5	E	115/123 (94%)	74 (64%)	41 (36%)	0	0
6	F	90/90 (100%)	65 (72%)	25 (28%)	0	3
7	G	126/127 (99%)	84 (67%)	42 (33%)	0	1
8	H	119/119 (100%)	87 (73%)	32 (27%)	0	4
9	I	98/99 (99%)	74 (76%)	24 (24%)	1	5
10	J	87/92 (95%)	65 (75%)	22 (25%)	0	4
11	K	88/99 (89%)	70 (80%)	18 (20%)	1	8
12	L	103/110 (94%)	75 (73%)	28 (27%)	0	3
13	M	94/101 (93%)	68 (72%)	26 (28%)	0	3
14	N	49/50 (98%)	42 (86%)	7 (14%)	3	17
15	O	79/80 (99%)	57 (72%)	22 (28%)	0	3
16	P	72/74 (97%)	59 (82%)	13 (18%)	2	11
17	Q	94/97 (97%)	71 (76%)	23 (24%)	1	5
18	R	61/77 (79%)	44 (72%)	17 (28%)	0	3
19	S	71/80 (89%)	52 (73%)	19 (27%)	0	4
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%)	1436 (72%)	547 (28%)	0	3

All (547) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	7	VAL
2	B	8	LYS
2	B	10	LEU

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Mol	Chain	Res	Type
2	B	12	GLU
2	B	16	HIS
2	B	19	HIS
2	B	23	ARG
2	B	26	PRO
2	B	30	ARG
2	B	32	ILE
2	B	39	ILE
2	B	46	LYS
2	B	47	THR
2	B	48	MET
2	B	49	GLU
2	B	51	LEU
2	B	53	ARG
2	B	59	GLU
2	B	69	LEU
2	B	84	GLU
2	B	87	ARG
2	B	92	TYR
2	B	96	ARG
2	B	97	TRP
2	B	98	LEU
2	B	102	LEU
2	B	106	LYS
2	B	112	VAL
2	B	121	LEU
2	B	127	ILE
2	B	129	GLU
2	B	142	LEU
2	B	144	ARG
2	B	147	LYS
2	B	150	SER
2	B	153	ARG
2	B	154	LEU
2	B	157	ARG
2	B	162	ILE
2	B	164	VAL
2	B	165	VAL
2	B	169	LYS
2	B	178	ARG
2	B	180	LEU
2	B	184	VAL

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Mol	Chain	Res	Type
2	B	185	ILE
2	B	187	LEU
2	B	193	ASP
2	B	196	LEU
2	B	197	VAL
2	B	200	ILE
2	B	201	ILE
2	B	208	ILE
2	B	215	LEU
2	B	216	SER
2	B	217	ARG
2	B	221	LEU
2	B	223	ILE
2	B	231	GLU
2	B	232	PRO
2	B	236	TYR
3	C	3	ASN
3	C	4	LYS
3	C	14	ILE
3	C	15	THR
3	C	20	SER
3	C	21	ARG
3	C	26	LYS
3	C	28	GLN
3	C	30	ARG
3	C	32	LEU
3	C	33	LEU
3	C	34	LEU
3	C	39	ILE
3	C	42	LEU
3	C	49	SER
3	C	57	ILE
3	C	62	ASP
3	C	63	ASN
3	C	64	VAL
3	C	72	LYS
3	C	75	VAL
3	C	76	VAL
3	C	79	ARG
3	C	86	VAL
3	C	91	LEU
3	C	94	LEU

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Mol	Chain	Res	Type
3	C	98	ASN
3	C	99	VAL
3	C	101	LEU
3	C	102	ASN
3	C	107	GLN
3	C	108	ASN
3	C	112	SER
3	C	115	LEU
3	C	118	GLN
3	C	130	VAL
3	C	131	ARG
3	C	134	ILE
3	C	139	GLN
3	C	147	LYS
3	C	156	ARG
3	C	157	ILE
3	C	162	GLN
3	C	165	THR
3	C	167	TRP
3	C	172	ARG
3	C	175	LEU
3	C	178	LEU
3	C	188	LEU
3	C	195	VAL
3	C	196	LEU
3	C	198	VAL
3	C	204	LEU
3	C	207	VAL
4	D	3	ARG
4	D	5	ILE
4	D	9	CYS
4	D	12	CYS
4	D	15	GLU
4	D	18	LYS
4	D	19	LEU
4	D	20	TYR
4	D	22	LYS
4	D	25	ARG
4	D	26	CYS
4	D	30	LYS
4	D	52	SER
4	D	58	LEU

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Mol	Chain	Res	Type
4	D	61	LYS
4	D	64	LEU
4	D	71	SER
4	D	83	SER
4	D	86	LYS
4	D	88	VAL
4	D	91	SER
4	D	108	LEU
4	D	112	VAL
4	D	115	ARG
4	D	119	GLN
4	D	120	LEU
4	D	121	VAL
4	D	122	ARG
4	D	127	THR
4	D	129	ASN
4	D	135	LEU
4	D	137	SER
4	D	140	VAL
4	D	141	ARG
4	D	148	VAL
4	D	157	LEU
4	D	165	MET
4	D	174	LEU
4	D	186	LEU
4	D	187	ARG
4	D	192	GLU
4	D	194	LEU
4	D	198	VAL
4	D	202	LEU
5	E	9	LYS
5	E	12	LEU
5	E	16	THR
5	E	18	ARG
5	E	19	MET
5	E	20	GLN
5	E	26	PHE
5	E	31	LEU
5	E	34	VAL
5	E	41	VAL
5	E	51	VAL
5	E	53	LEU

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Mol	Chain	Res	Type
5	E	56	GLN
5	E	61	TYR
5	E	67	VAL
5	E	68	GLU
5	E	69	VAL
5	E	75	THR
5	E	76	ILE
5	E	79	GLU
5	E	80	ILE
5	E	82	VAL
5	E	87	SER
5	E	88	LYS
5	E	90	VAL
5	E	92	LYS
5	E	100	VAL
5	E	112	LEU
5	E	116	THR
5	E	118	ILE
5	E	119	LEU
5	E	121	LYS
5	E	125	SER
5	E	126	ARG
5	E	130	ASN
5	E	131	ILE
5	E	144	THR
5	E	147	ASP
5	E	148	VAL
5	E	151	LEU
5	E	152	ARG
6	F	5	GLU
6	F	9	VAL
6	F	15	ASP
6	F	19	LEU
6	F	23	LYS
6	F	36	ARG
6	F	37	VAL
6	F	39	LYS
6	F	43	LEU
6	F	47	ARG
6	F	51	PRO
6	F	54	LYS
6	F	55	ASP

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Mol	Chain	Res	Type
6	F	61	LEU
6	F	69	GLU
6	F	75	LEU
6	F	82	ARG
6	F	83	ASP
6	F	87	ARG
6	F	88	VAL
6	F	92	LYS
6	F	93	SER
6	F	97	PHE
6	F	98	LEU
6	F	100	ASN
7	G	3	ARG
7	G	5	ARG
7	G	6	ARG
7	G	8	GLU
7	G	12	LEU
7	G	15	ASP
7	G	17	VAL
7	G	22	LEU
7	G	24	THR
7	G	27	ILE
7	G	30	ILE
7	G	32	ARG
7	G	49	ILE
7	G	50	ILE
7	G	52	GLU
7	G	53	LYS
7	G	54	THR
7	G	57	GLU
7	G	67	GLU
7	G	72	ARG
7	G	75	VAL
7	G	77	SER
7	G	80	VAL
7	G	84	ASN
7	G	86	GLN
7	G	87	VAL
7	G	89	MET
7	G	91	VAL
7	G	95	ARG
7	G	97	GLN

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Mol	Chain	Res	Type
7	G	106	GLN
7	G	110	GLN
7	G	111	ARG
7	G	113	GLU
7	G	115	ARG
7	G	120	ILE
7	G	125	MET
7	G	126	ASP
7	G	129	GLU
7	G	138	LYS
7	G	146	GLU
7	G	155	ARG
8	H	3	THR
8	H	5	PRO
8	H	6	ILE
8	H	8	ASP
8	H	11	THR
8	H	19	VAL
8	H	26	VAL
8	H	29	SER
8	H	35	ILE
8	H	39	LEU
8	H	50	ARG
8	H	51	VAL
8	H	63	LEU
8	H	79	VAL
8	H	81	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	95	VAL
8	H	97	VAL
8	H	98	LYS
8	H	104	ARG
8	H	105	ARG
8	H	115	SER
8	H	118	VAL
8	H	120	THR
8	H	127	LEU

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Mol	Chain	Res	Type
8	H	129	VAL
8	H	133	LEU
9	I	4	TYR
9	I	20	ARG
9	I	26	VAL
9	I	27	THR
9	I	53	VAL
9	I	65	VAL
9	I	70	LYS
9	I	78	LYS
9	I	79	LEU
9	I	81	ILE
9	I	83	ARG
9	I	86	VAL
9	I	93	ARG
9	I	99	LEU
9	I	102	LEU
9	I	103	THR
9	I	107	ARG
9	I	108	VAL
9	I	109	VAL
9	I	112	LYS
9	I	113	LYS
9	I	114	TYR
9	I	127	LYS
9	I	128	ARG
10	J	3	LYS
10	J	4	ILE
10	J	7	LYS
10	J	8	LEU
10	J	17	ASP
10	J	21	GLN
10	J	23	ILE
10	J	30	SER
10	J	38	ILE
10	J	43	ARG
10	J	48	THR
10	J	49	VAL
10	J	57	LYS
10	J	59	SER
10	J	65	LEU
10	J	68	HIS

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Mol	Chain	Res	Type
10	J	69	ASN
10	J	79	ARG
10	J	82	ILE
10	J	87	THR
10	J	96	ILE
10	J	98	ILE
11	K	11	LYS
11	K	13	GLN
11	K	14	VAL
11	K	18	ARG
11	K	29	ILE
11	K	30	VAL
11	K	32	ILE
11	K	40	ILE
11	K	48	ILE
11	K	75	TYR
11	K	85	ARG
11	K	87	THR
11	K	98	LEU
11	K	101	SER
11	K	104	GLN
11	K	105	VAL
11	K	109	VAL
11	K	119	CYS
12	L	6	THR
12	L	10	LEU
12	L	11	VAL
12	L	12	ARG
12	L	18	VAL
12	L	19	ARG
12	L	20	LYS
12	L	33	ARG
12	L	36	VAL
12	L	41	ARG
12	L	43	VAL
12	L	47	LYS
12	L	53	ARG
12	L	55	VAL
12	L	59	ARG
12	L	60	LEU
12	L	61	THR
12	L	62	SER

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Mol	Chain	Res	Type
12	L	64	TYR
12	L	66	VAL
12	L	80	HIS
12	L	81	SER
12	L	97	ARG
12	L	101	VAL
12	L	115	LYS
12	L	119	LYS
12	L	122	THR
12	L	126	LYS
13	M	3	ARG
13	M	12	ASN
13	M	14	ARG
13	M	16	ASP
13	M	19	LEU
13	M	27	LYS
13	M	31	LYS
13	M	34	LEU
13	M	35	GLU
13	M	39	ILE
13	M	45	VAL
13	M	48	LEU
13	M	49	THR
13	M	54	VAL
13	M	56	LEU
13	M	60	VAL
13	M	66	LEU
13	M	67	GLU
13	M	70	LEU
13	M	71	ARG
13	M	74	VAL
13	M	80	ARG
13	M	103	THR
13	M	109	THR
13	M	113	PRO
13	M	115	LYS
14	N	9	LYS
14	N	21	TYR
14	N	25	VAL
14	N	31	ARG
14	N	41	ARG
14	N	45	ARG

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Mol	Chain	Res	Type
14	N	58	LYS
15	O	4	THR
15	O	9	GLN
15	O	10	LYS
15	O	17	ARG
15	O	21	ASP
15	O	29	VAL
15	O	32	LEU
15	O	33	THR
15	O	34	LEU
15	O	38	ARG
15	O	42	HIS
15	O	44	LYS
15	O	45	VAL
15	O	48	LYS
15	O	52	SER
15	O	56	LEU
15	O	63	ARG
15	O	67	LEU
15	O	70	LEU
15	O	75	PRO
15	O	77	ARG
15	O	85	LEU
16	P	2	VAL
16	P	3	LYS
16	P	8	ARG
16	P	31	LYS
16	P	43	LYS
16	P	44	THR
16	P	55	ARG
16	P	62	VAL
16	P	68	ASP
16	P	71	ARG
16	P	74	LEU
16	P	75	ARG
16	P	79	VAL
17	Q	6	LEU
17	Q	7	THR
17	Q	9	VAL
17	Q	10	VAL
17	Q	14	LYS
17	Q	21	VAL

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Mol	Chain	Res	Type
17	Q	24	GLU
17	Q	34	LYS
17	Q	35	VAL
17	Q	36	ILE
17	Q	37	LYS
17	Q	50	LYS
17	Q	53	LEU
17	Q	57	VAL
17	Q	59	ILE
17	Q	60	ILE
17	Q	76	LEU
17	Q	81	ARG
17	Q	86	GLU
17	Q	87	LYS
17	Q	96	GLN
17	Q	97	SER
17	Q	99	SER
18	R	19	LYS
18	R	21	LYS
18	R	22	VAL
18	R	26	LEU
18	R	30	ASP
18	R	47	THR
18	R	50	ILE
18	R	51	LEU
18	R	55	ARG
18	R	56	THR
18	R	58	LEU
18	R	65	ILE
18	R	69	THR
18	R	71	LYS
18	R	84	LYS
18	R	87	ARG
18	R	88	LYS
19	S	3	ARG
19	S	5	LEU
19	S	7	LYS
19	S	15	LEU
19	S	18	LYS
19	S	20	LEU
19	S	22	LEU
19	S	31	ILE

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Mol	Chain	Res	Type
19	S	33	THR
19	S	35	SER
19	S	39	THR
19	S	41	VAL
19	S	43	GLU
19	S	49	ILE
19	S	51	VAL
19	S	55	LYS
19	S	60	VAL
19	S	64	GLU
19	S	71	LEU
20	T	10	LEU
20	T	18	GLN
20	T	19	SER
20	T	20	LEU
20	T	22	ARG
20	T	25	ARG
20	T	30	LYS
20	T	33	ILE
20	T	35	THR
20	T	42	GLN
20	T	45	GLN
20	T	53	LEU
20	T	56	MET
20	T	62	LEU
20	T	65	LYS
20	T	72	LEU
20	T	75	ASN
20	T	79	ARG
20	T	84	LEU
20	T	86	ARG
20	T	90	GLN
20	T	91	LEU
20	T	92	LEU
20	T	99	LEU
20	T	100	ILE
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 (23) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	135	GLN
2	B	204	ASN
3	C	98	ASN
3	C	118	GLN
3	C	181	ASN
4	D	43	HIS
4	D	119	GLN
4	D	123	HIS
4	D	129	ASN
5	E	56	GLN
7	G	86	GLN
8	H	82	HIS
9	I	31	GLN
9	I	124	GLN
10	J	33	GLN
10	J	56	HIS
10	J	62	HIS
11	K	38	ASN
11	K	99	GLN
13	M	77	ASN
16	P	82	GLN
17	Q	16	GLN
17	Q	45	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1511/1522 (99%)	430 (28%)	62 (4%)

All (430) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	G
1	A	7	G
1	A	8	A
1	A	9	G
1	A	21	G
1	A	22	G
1	A	31	G
1	A	32	A
1	A	39	G
1	A	41	G

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Mol	Chain	Res	Type
1	A	44	G
1	A	47	C
1	A	48	C
1	A	49	U
1	A	50	A
1	A	51	A
1	A	66	G
1	A	70	G
1	A	73	C
1	A	81	U
1	A	82	U
1	A	88	A
1	A	92	C
1	A	96	G
1	A	99	C
1	A	101	A
1	A	108	G
1	A	115	G
1	A	116	A
1	A	121	C
1	A	129(A)	G
1	A	130	A
1	A	131	C
1	A	134	A
1	A	144	G
1	A	149	A
1	A	151	A
1	A	156	G
1	A	159	G
1	A	163	C
1	A	167	G
1	A	173	U
1	A	181	G
1	A	182	U
1	A	183	G
1	A	187	C
1	A	190(E)	U
1	A	190(G)	G
1	A	195	A
1	A	197	A
1	A	201	C
1	A	202	U

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Mol	Chain	Res	Type
1	A	203	U
1	A	204	U
1	A	216	G
1	A	220	G
1	A	231	G
1	A	243	A
1	A	244	U
1	A	246	A
1	A	247	G
1	A	251	G
1	A	252	U
1	A	253	U
1	A	254	G
1	A	266	G
1	A	267	C
1	A	274	A
1	A	287	U
1	A	289	G
1	A	291	C
1	A	296	U
1	A	297	G
1	A	298	A
1	A	301	G
1	A	321	A
1	A	326	G
1	A	328	C
1	A	329	A
1	A	332	G
1	A	344	A
1	A	345	C
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	371	G
1	A	373	A
1	A	374	A
1	A	384	G
1	A	390	C

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Mol	Chain	Res	Type
1	A	392	G
1	A	397	A
1	A	398	C
1	A	406	G
1	A	409	G
1	A	411	A
1	A	412	A
1	A	413	G
1	A	417	C
1	A	420	U
1	A	421	U
1	A	422	C
1	A	423	G
1	A	424	G
1	A	429	U
1	A	430	A
1	A	439	A
1	A	450	G
1	A	453	A
1	A	455	C
1	A	459	G
1	A	460	A
1	A	461	C
1	A	475	G
1	A	476	G
1	A	478	A
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	504	C
1	A	509	A
1	A	510	A
1	A	511	C
1	A	517	G
1	A	518	C
1	A	519	C
1	A	522	C
1	A	527	7MG

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Mol	Chain	Res	Type
1	A	530	G
1	A	531	U
1	A	532	A
1	A	533	A
1	A	547	A
1	A	548	G
1	A	559	A
1	A	560	U
1	A	562	C
1	A	563	A
1	A	566	G
1	A	568	G
1	A	572	A
1	A	573	A
1	A	576	G
1	A	577	G
1	A	579	G
1	A	588	G
1	A	597	G
1	A	608	A
1	A	616	G
1	A	622	A
1	A	631	G
1	A	634	C
1	A	641	U
1	A	651	C
1	A	652	U
1	A	653	A
1	A	658	G
1	A	665	A
1	A	670	G
1	A	684	A
1	A	686	U
1	A	687	A
1	A	688	G
1	A	693	G
1	A	695	A
1	A	701	C
1	A	702	A
1	A	703	G
1	A	714	G
1	A	722	A

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Mol	Chain	Res	Type
1	A	723	U
1	A	724	G
1	A	731	G
1	A	733	A
1	A	734	G
1	A	741	G
1	A	749	C
1	A	755	G
1	A	759	A
1	A	761	G
1	A	773	G
1	A	774	G
1	A	777	A
1	A	781	A
1	A	787	A
1	A	788	U
1	A	789	U
1	A	791	G
1	A	792	A
1	A	793	U
1	A	794	A
1	A	795	C
1	A	812	C
1	A	813	U
1	A	815	A
1	A	817	C
1	A	819	A
1	A	821	G
1	A	827	U
1	A	828	A
1	A	839	U
1	A	840	C
1	A	841	U
1	A	848	C
1	A	852	G
1	A	853	G
1	A	855	G
1	A	859	A
1	A	869	G
1	A	870	U
1	A	871	U
1	A	872	A

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Mol	Chain	Res	Type
1	A	873	A
1	A	876	G
1	A	885	G
1	A	895	G
1	A	902	G
1	A	907	A
1	A	910	C
1	A	914	G
1	A	917	G
1	A	922	G
1	A	926	G
1	A	927	G
1	A	932	C
1	A	934	C
1	A	935	A
1	A	938	A
1	A	940	C
1	A	950	U
1	A	954	G
1	A	960	U
1	A	966	M2G
1	A	969	A
1	A	971	G
1	A	974	A
1	A	975	A
1	A	976	G
1	A	977	A
1	A	982	U
1	A	984	C
1	A	986	A
1	A	987	G
1	A	989	C
1	A	990	C
1	A	991	U
1	A	992	U
1	A	993	G
1	A	996	A
1	A	1004	A
1	A	1005	A
1	A	1007	C
1	A	1008	C
1	A	1010	G

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Mol	Chain	Res	Type
1	A	1023	G
1	A	1024	G
1	A	1026	G
1	A	1027	C
1	A	1030(B)	C
1	A	1031	G
1	A	1037	C
1	A	1045	C
1	A	1046	A
1	A	1049	U
1	A	1050	G
1	A	1051	C
1	A	1054	C
1	A	1060	C
1	A	1064	G
1	A	1065	U
1	A	1066	C
1	A	1068	G
1	A	1072	G
1	A	1085	U
1	A	1092	A
1	A	1093	A
1	A	1094	G
1	A	1095	U
1	A	1101	A
1	A	1104	G
1	A	1126	U
1	A	1127	G
1	A	1128	C
1	A	1129	C
1	A	1130	A
1	A	1131	G
1	A	1137	C
1	A	1139	G
1	A	1140	C
1	A	1141	C
1	A	1142	G
1	A	1145	C
1	A	1146	A
1	A	1149	C
1	A	1152	A
1	A	1159	U

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Mol	Chain	Res	Type
1	A	1160	G
1	A	1161	C
1	A	1162	C
1	A	1164	G
1	A	1165	C
1	A	1168	A
1	A	1171	G
1	A	1172	C
1	A	1176	A
1	A	1182	G
1	A	1183	A
1	A	1184	G
1	A	1190	G
1	A	1191	A
1	A	1194	U
1	A	1196	U
1	A	1197	G
1	A	1198	G
1	A	1200	C
1	A	1201	A
1	A	1202	G
1	A	1206	G
1	A	1210	C
1	A	1211	U
1	A	1212	U
1	A	1214	C
1	A	1223	C
1	A	1224	G
1	A	1225	A
1	A	1226	C
1	A	1228	C
1	A	1229	A
1	A	1233	G
1	A	1238	A
1	A	1241	G
1	A	1242	C
1	A	1243	C
1	A	1245	A
1	A	1249	C
1	A	1253	G
1	A	1257	U
1	A	1258	G

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Mol	Chain	Res	Type
1	A	1260	C
1	A	1261	A
1	A	1270	C
1	A	1273	G
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	1285	A
1	A	1286	A
1	A	1287	A
1	A	1289	A
1	A	1297	C
1	A	1300	G
1	A	1301	U
1	A	1302	U
1	A	1304	G
1	A	1305	G
1	A	1306	A
1	A	1311	G
1	A	1312	G
1	A	1315	U
1	A	1319	A
1	A	1320	C
1	A	1322	C
1	A	1332	A
1	A	1335	C
1	A	1336	C
1	A	1338	G
1	A	1340	A
1	A	1346	A
1	A	1347	G
1	A	1348	U
1	A	1353	G
1	A	1358	U
1	A	1359	C
1	A	1364	U
1	A	1370	G
1	A	1376	U
1	A	1378	C

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Mol	Chain	Res	Type
1	A	1379	G
1	A	1380	U
1	A	1381	U
1	A	1394	A
1	A	1398	A
1	A	1399	C
1	A	1402	4OC
1	A	1403	C
1	A	1411	C
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	1454	G
1	A	1463	C
1	A	1464	G
1	A	1476	G
1	A	1483	A
1	A	1487	G
1	A	1489	G
1	A	1493	A
1	A	1494	G
1	A	1497	G
1	A	1498	UR3
1	A	1499	A
1	A	1502	A
1	A	1503	A
1	A	1504	G
1	A	1505	G
1	A	1506	U
1	A	1518	MA6
1	A	1520	G
1	A	1522	U
1	A	1529	G
1	A	1530	G
1	A	1531	A
1	A	1533	C
1	A	1540	PSU
1	A	1541	PSU
1	A	1542	U

All (62) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	5	U
1	A	20	U
1	A	21	G
1	A	49	U
1	A	108	G
1	A	115	G
1	A	129(A)	G
1	A	181	G
1	A	204	U
1	A	243	A
1	A	246	A
1	A	250	A
1	A	251	G
1	A	328	C
1	A	344	A
1	A	350	G
1	A	353	A
1	A	372	C
1	A	412	A
1	A	413	G
1	A	428	G
1	A	429	U
1	A	452	A
1	A	460	A
1	A	484	G
1	A	509	A
1	A	532	A
1	A	559	A
1	A	687	A
1	A	701	C
1	A	748	C
1	A	793	U
1	A	812	C
1	A	870	U
1	A	913	A
1	A	975	A
1	A	992	U
1	A	1004	A
1	A	1026	G
1	A	1049	U
1	A	1065	U
1	A	1067	A

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Mol	Chain	Res	Type
1	A	1139	G
1	A	1145	C
1	A	1182	G
1	A	1183	A
1	A	1190	G
1	A	1201	A
1	A	1224	G
1	A	1257	U
1	A	1281	U
1	A	1285	A
1	A	1300	G
1	A	1301	U
1	A	1335	C
1	A	1346	A
1	A	1347	G
1	A	1380	U
1	A	1442	G
1	A	1504	G
1	A	1505	G
1	A	1541	PSU

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

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	1519	1	23,26,27	1.86	5 (21%)	33,38,41	0.99	3 (9%)
12	0TD	L	92	12	8,9,10	1.67	3 (37%)	6,11,13	3.95	4 (66%)
1	MA6	A	1518	1	23,26,27	1.37	4 (17%)	33,38,41	1.03	2 (6%)
1	PSU	A	516	1,23	18,21,22	1.70	2 (11%)	21,30,33	1.31	4 (19%)
1	7MG	A	527	1	23,26,27	4.20	4 (17%)	27,39,42	2.38	9 (33%)
1	4OC	A	1402	1	20,23,24	1.42	5 (25%)	25,32,35	0.85	2 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	5MC	A	1404	1	19,22,23	1.47	4 (21%)	26,32,35	1.18	4 (15%)
1	PSU	A	1540	1	18,21,22	1.27	1 (5%)	21,30,33	1.99	4 (19%)
1	PSU	A	1541	1	18,21,22	1.53	2 (11%)	21,30,33	2.20	6 (28%)
1	5MC	A	1400	1	19,22,23	1.55	3 (15%)	26,32,35	1.17	1 (3%)
1	M2G	A	966	1	24,27,28	0.86	1 (4%)	33,40,43	1.12	3 (9%)
1	5MC	A	967	1	19,22,23	1.38	2 (10%)	26,32,35	0.68	0
1	5MC	A	1407	1	19,22,23	1.33	2 (10%)	26,32,35	1.40	4 (15%)
1	2MG	A	1207	1	23,26,27	1.84	4 (17%)	33,38,41	0.99	2 (6%)
1	UR3	A	1498	1,23	19,22,23	1.29	4 (21%)	26,32,35	1.14	2 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MA6	A	1519	1	-	4/11/29/30	0/3/3/3
12	0TD	L	92	12	-	2/7/12/14	-
1	MA6	A	1518	1	-	2/11/29/30	0/3/3/3
1	PSU	A	516	1,23	-	0/7/25/26	0/2/2/2
1	7MG	A	527	1	-	2/7/37/38	0/3/3/3
1	4OC	A	1402	1	-	2/9/29/30	0/2/2/2
1	5MC	A	1404	1	-	0/7/25/26	0/2/2/2
1	PSU	A	1540	1	-	3/7/25/26	0/2/2/2
1	PSU	A	1541	1	-	3/7/25/26	0/2/2/2
1	5MC	A	1400	1	-	2/7/25/26	0/2/2/2
1	M2G	A	966	1	-	0/11/29/30	0/3/3/3
1	5MC	A	967	1	-	0/7/25/26	0/2/2/2
1	5MC	A	1407	1	-	0/7/25/26	0/2/2/2
1	2MG	A	1207	1	-	0/9/27/28	0/3/3/3
1	UR3	A	1498	1,23	-	0/7/25/26	0/2/2/2

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	527	7MG	C8-N9	-18.09	1.34	1.45
1	A	516	PSU	C6-C5	5.58	1.41	1.35
1	A	1207	2MG	C2-N1	5.45	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	527	7MG	C5-N7	5.44	1.42	1.35
1	A	1541	PSU	C6-C5	4.99	1.40	1.35
1	A	1519	MA6	C9-N6	4.68	1.56	1.45
1	A	1540	PSU	C6-C5	4.54	1.40	1.35
1	A	1207	2MG	C2-N2	4.42	1.42	1.33
1	A	1400	5MC	C5-C4	-4.31	1.40	1.44
1	A	967	5MC	C5-C4	-4.29	1.40	1.44
1	A	527	7MG	C2-N2	4.28	1.44	1.34
1	A	1519	MA6	C5-C4	3.92	1.46	1.39
1	A	1519	MA6	C2-N1	3.84	1.40	1.33
1	A	1407	5MC	O2-C2	-3.72	1.16	1.23
1	A	1402	4OC	CM4-N4	3.46	1.51	1.45
1	A	1518	MA6	C8-N9	3.41	1.43	1.37
1	A	1404	5MC	C1'-N1	-3.19	1.38	1.47
1	A	1400	5MC	C2-N1	3.14	1.46	1.40
1	A	1404	5MC	C2-N3	3.10	1.42	1.36
1	A	967	5MC	C2-N3	2.99	1.42	1.36
1	A	1519	MA6	C8-N9	2.96	1.42	1.37
1	A	1404	5MC	C6-N1	-2.89	1.33	1.38
1	A	1402	4OC	O2-C2	-2.89	1.18	1.23
1	A	1518	MA6	C5-C4	2.85	1.44	1.39
1	A	1404	5MC	C5-C4	-2.79	1.42	1.44
1	A	1407	5MC	C2-N1	2.79	1.45	1.40
1	A	1541	PSU	C1'-C5	2.73	1.56	1.50
1	A	1207	2MG	C6-N1	2.73	1.44	1.38
1	A	1498	UR3	C4-N3	-2.69	1.35	1.40
1	A	1207	2MG	C8-N9	2.67	1.43	1.37
1	A	1518	MA6	C2-N1	2.64	1.38	1.33
1	A	1498	UR3	C6-N1	-2.62	1.31	1.38
1	A	966	M2G	C8-N9	2.60	1.43	1.37
12	L	92	0TD	CB-CG	2.51	1.56	1.52
1	A	516	PSU	C2-N1	2.46	1.39	1.36
1	A	1402	4OC	C6-N1	-2.45	1.32	1.38
1	A	1518	MA6	C4-N9	-2.45	1.32	1.37
1	A	1402	4OC	C4-N3	-2.42	1.28	1.32
1	A	1498	UR3	C2-N1	2.37	1.41	1.38
1	A	1400	5MC	C2-N3	2.28	1.40	1.36
1	A	1519	MA6	C4-N3	2.26	1.38	1.34
1	A	1498	UR3	O3'-C3'	2.26	1.48	1.43
12	L	92	0TD	CB-CA	-2.20	1.54	1.54
12	L	92	0TD	O-C	2.15	1.28	1.20
1	A	527	7MG	C8-N7	-2.10	1.32	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1402	4OC	C2-N3	2.01	1.40	1.36

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	L	92	0TD	CSB-SB-CB	-6.96	89.85	102.36
1	A	1541	PSU	C6-C5-C4	-6.84	113.56	118.17
12	L	92	0TD	CB-CA-N	-6.03	96.88	109.10
1	A	527	7MG	C5-C6-N1	5.37	120.39	110.94
1	A	1540	PSU	O2-C2-N1	-4.98	117.65	122.79
1	A	527	7MG	C2-N3-C4	4.93	120.80	112.30
1	A	527	7MG	N9-C4-N3	4.12	131.50	125.46
1	A	527	7MG	C5-C4-N3	-4.10	120.44	128.13
1	A	527	7MG	C6-C5-N7	3.99	138.11	131.93
1	A	1540	PSU	N1-C2-N3	3.97	119.35	115.17
1	A	1407	5MC	C4-N3-C2	-3.78	115.57	120.81
1	A	1540	PSU	C4-N3-C2	-3.77	121.18	126.37
1	A	527	7MG	N9-C8-N7	3.66	108.56	103.37
1	A	1541	PSU	O2-C2-N1	-3.61	119.06	122.79
1	A	527	7MG	C6-C5-C4	-3.40	116.42	122.40
1	A	1540	PSU	C6-N1-C2	-3.36	119.58	122.69
1	A	527	7MG	C2-N1-C6	-3.29	119.14	125.11
1	A	516	PSU	C4-N3-C2	-3.09	122.11	126.37
1	A	966	M2G	C5-C4-N3	-3.04	123.55	128.39
1	A	966	M2G	O6-C6-N1	-2.78	114.88	120.11
1	A	1400	5MC	C5-C4-N3	2.73	124.56	121.75
1	A	1541	PSU	C3'-C2'-C1'	-2.70	98.51	101.69
1	A	1407	5MC	C5-C6-N1	-2.64	120.44	123.31
1	A	1404	5MC	C5-C4-N3	2.64	124.47	121.75
1	A	1404	5MC	C4-N3-C2	-2.61	117.19	120.81
1	A	1407	5MC	C5-C4-N3	2.60	124.42	121.75
1	A	1541	PSU	C5-C6-N1	2.54	125.67	122.14
1	A	966	M2G	O6-C6-C5	2.51	133.17	126.53
1	A	1407	5MC	O2-C2-N3	-2.39	118.56	122.33
1	A	1519	MA6	C4-C5-C6	2.37	118.36	115.91
1	A	1518	MA6	N1-C6-N6	-2.35	113.99	116.86
1	A	1519	MA6	C2-N1-C6	2.29	117.41	111.83
1	A	527	7MG	O6-C6-N1	-2.20	115.97	120.11
1	A	1541	PSU	O4'-C4'-C3'	-2.19	100.80	105.15
1	A	1207	2MG	N2-C2-N3	-2.17	117.75	120.51
1	A	516	PSU	O4-C4-C5	-2.15	118.66	124.01
1	A	1519	MA6	N1-C6-N6	2.11	119.43	116.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1498	UR3	C6-N1-C2	-2.11	120.07	121.80
12	L	92	0TD	OD1-CG-CB	-2.09	118.06	122.44
1	A	1518	MA6	C4-N9-C1'	-2.08	121.76	126.63
1	A	1402	4OC	C4-N3-C2	-2.08	117.36	120.11
1	A	516	PSU	N1-C2-N3	2.06	117.34	115.17
1	A	1498	UR3	C2'-C3'-C4'	2.06	106.59	102.61
1	A	1402	4OC	C5-C4-N4	-2.05	117.89	122.40
1	A	1541	PSU	O2-C2-N3	2.04	125.49	121.86
1	A	1404	5MC	C6-N1-C2	2.03	123.66	120.95
1	A	1207	2MG	O6-C6-C5	2.02	131.86	126.53
1	A	1404	5MC	C5-C6-N1	-2.01	121.13	123.31
12	L	92	0TD	OD2-CG-CB	2.01	117.50	113.15
1	A	516	PSU	C6-N1-C2	-2.00	120.83	122.69

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1402	4OC	O4'-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	1541	PSU	O4'-C4'-C5'-O5'
1	A	527	7MG	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	1540	PSU	O4'-C4'-C5'-O5'
1	A	1402	4OC	C3'-C4'-C5'-O5'
1	A	1541	PSU	C3'-C4'-C5'-O5'
1	A	1400	5MC	C3'-C4'-C5'-O5'
1	A	1518	MA6	C3'-C4'-C5'-O5'
1	A	1519	MA6	N1-C6-N6-C10
1	A	1540	PSU	C3'-C4'-C5'-O5'
12	L	92	0TD	CG-CB-SB-CSB
12	L	92	0TD	SB-CB-CG-OD1
1	A	1540	PSU	O4'-C1'-C5-C6
1	A	1541	PSU	O4'-C1'-C5-C6

There are no ring outliers.

13 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1519	MA6	3	0
12	L	92	0TD	2	0
1	A	1518	MA6	3	0
1	A	527	7MG	2	0
1	A	1402	4OC	1	0
1	A	1404	5MC	5	0
1	A	1540	PSU	2	0
1	A	1541	PSU	2	0
1	A	1400	5MC	1	0
1	A	966	M2G	1	0
1	A	967	5MC	1	0
1	A	1407	5MC	1	0
1	A	1498	UR3	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 276 ligands modelled in this entry, 275 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	2.44	10 (25%)	49,63,63	2.78	22 (44%)

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	-	-	2/20/87/87	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	1601	SRY	CD1-N31	9.88	1.50	1.33
22	A	1601	SRY	CA1-N11	6.03	1.43	1.33
22	A	1601	SRY	O53-C53	-4.20	1.34	1.44
22	A	1601	SRY	CA1-NB1	3.36	1.46	1.34
22	A	1601	SRY	C11-N11	-3.34	1.40	1.45
22	A	1601	SRY	CD1-NE1	3.07	1.45	1.34
22	A	1601	SRY	C21-C31	-2.57	1.48	1.53
22	A	1601	SRY	O51-C51	-2.46	1.36	1.43
22	A	1601	SRY	C23-N23	-2.33	1.43	1.47
22	A	1601	SRY	O32-C32	-2.19	1.40	1.44

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1601	SRY	O13-C13-C23	7.13	119.64	108.07
22	A	1601	SRY	C13-O13-C22	-6.53	105.15	116.26
22	A	1601	SRY	C11-N11-CA1	-6.09	111.33	123.39
22	A	1601	SRY	C12-O42-C42	-5.59	99.45	108.48
22	A	1601	SRY	CI3-N23-C23	-5.12	107.62	114.23
22	A	1601	SRY	C41-C31-N31	4.69	118.39	110.91
22	A	1601	SRY	O41-C12-O42	-4.47	106.80	111.37
22	A	1601	SRY	C31-N31-CD1	-3.86	115.75	123.39
22	A	1601	SRY	O51-C51-C61	-3.70	101.65	110.38
22	A	1601	SRY	O61-C61-C11	3.66	116.86	109.58
22	A	1601	SRY	O13-C22-C32	3.25	118.98	111.79
22	A	1601	SRY	C13-O53-C53	-3.08	107.70	113.72
22	A	1601	SRY	O21-C21-C11	3.06	115.67	109.58
22	A	1601	SRY	C13-C23-N23	3.05	116.23	110.92
22	A	1601	SRY	C12-O41-C41	-2.60	111.82	117.98
22	A	1601	SRY	O51-C51-C41	2.47	116.26	109.94
22	A	1601	SRY	C43-C33-C23	-2.37	106.95	110.40
22	A	1601	SRY	O41-C41-C51	2.31	113.11	107.23
22	A	1601	SRY	C61-C11-N11	-2.30	106.38	110.62
22	A	1601	SRY	O61-C61-C51	-2.21	105.17	110.38
22	A	1601	SRY	C51-C61-C11	-2.16	107.25	110.40
22	A	1601	SRY	O13-C13-O53	-2.05	105.29	110.69

There are no chirality outliers.

All (2) torsion outliers are listed below:

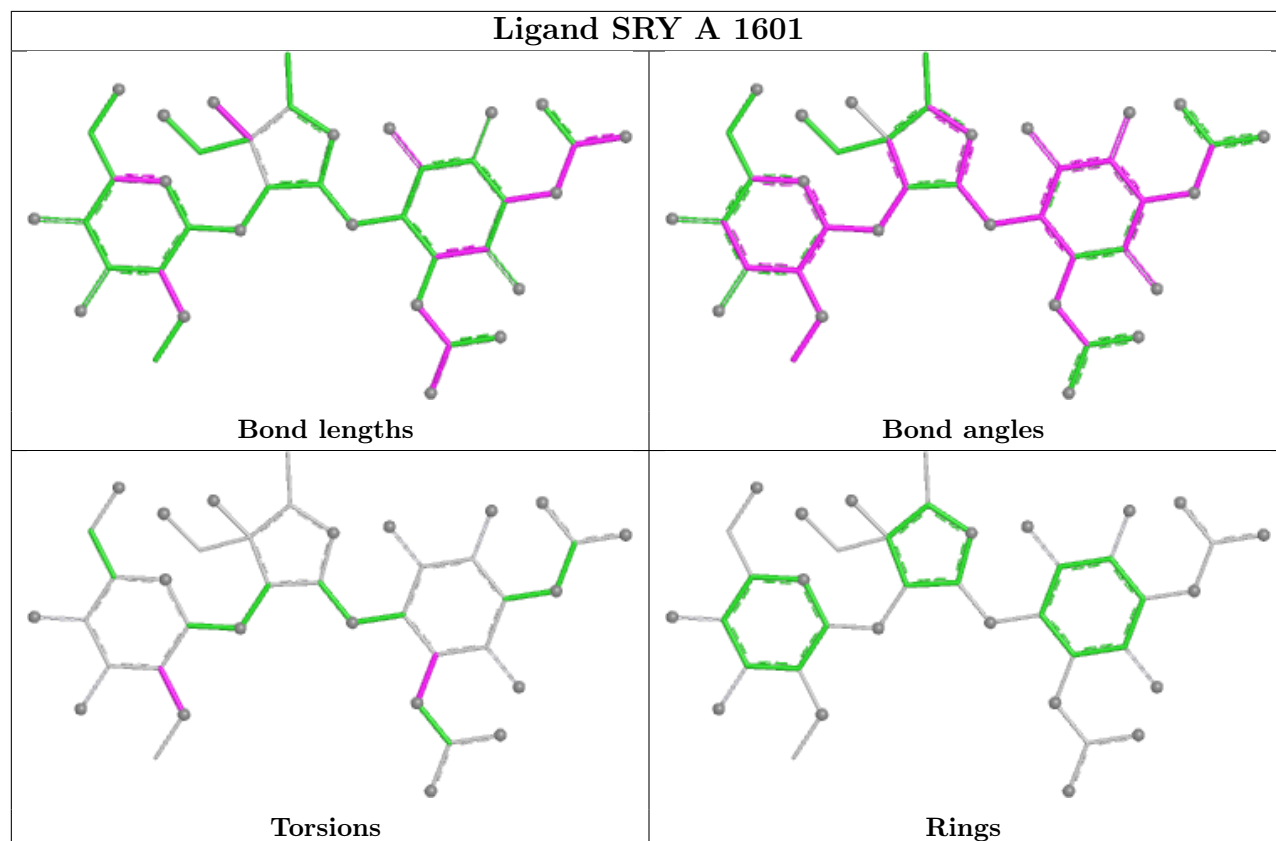
Mol	Chain	Res	Type	Atoms
22	A	1601	SRY	C13-C23-N23-CI3
22	A	1601	SRY	C21-C31-N31-CD1

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A	1601	SRY	7	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1498/1522 (98%)	-0.45	17 (1%) 78 53	74, 131, 262, 364	0
2	B	234/256 (91%)	-0.48	1 (0%) 88 72	82, 143, 231, 264	0
3	C	206/239 (86%)	-0.24	4 (1%) 66 41	123, 191, 239, 272	0
4	D	208/209 (99%)	-0.16	9 (4%) 40 25	85, 134, 177, 200	0
5	E	150/162 (92%)	-0.71	0 100 100	73, 106, 144, 182	0
6	F	101/101 (100%)	-0.62	0 100 100	106, 153, 181, 203	0
7	G	155/156 (99%)	-0.31	2 (1%) 75 49	128, 180, 226, 251	0
8	H	138/138 (100%)	-0.71	0 100 100	68, 96, 145, 159	0
9	I	127/128 (99%)	-0.14	5 (3%) 43 27	126, 199, 236, 258	0
10	J	98/105 (93%)	0.03	1 (1%) 79 55	165, 229, 278, 305	0
11	K	116/129 (89%)	-0.36	1 (0%) 81 57	94, 131, 177, 219	0
12	L	123/135 (91%)	-0.32	2 (1%) 70 44	71, 124, 172, 206	0
13	M	118/126 (93%)	-0.23	2 (1%) 69 43	122, 164, 204, 231	0
14	N	60/61 (98%)	-0.04	0 100 100	133, 189, 234, 267	0
15	O	87/89 (97%)	-0.62	0 100 100	74, 122, 165, 180	0
16	P	83/88 (94%)	-0.43	0 100 100	92, 125, 166, 203	0
17	Q	99/105 (94%)	-0.55	0 100 100	84, 107, 140, 168	0
18	R	70/88 (79%)	-0.67	0 100 100	92, 129, 180, 220	0
19	S	80/93 (86%)	0.29	9 (11%) 10 10	174, 217, 268, 283	0
20	T	99/106 (93%)	-0.38	2 (2%) 65 40	95, 130, 179, 210	0
21	U	24/27 (88%)	0.65	3 (12%) 8 9	151, 187, 219, 221	0
All	All	3874/4063 (95%)	-0.39	58 (1%) 72 46	68, 141, 239, 364	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1129	C	6.3
10	J	37	PRO	6.1
20	T	106	ALA	5.2
12	L	73	GLU	5.0
19	S	2	PRO	4.4
1	A	793	U	4.3
19	S	77	THR	3.9
13	M	8	GLU	3.8
21	U	16	GLY	3.6
1	A	81	U	3.5
4	D	5	ILE	3.5
19	S	44	MET	3.4
1	A	532	A	3.3
4	D	2	GLY	3.2
19	S	3	ARG	3.1
19	S	35	SER	3.1
4	D	4	TYR	3.1
4	D	26	CYS	3.0
9	I	8	GLY	3.0
12	L	47	LYS	3.0
3	C	2	GLY	3.0
4	D	6	GLY	2.9
1	A	1201	A	2.9
7	G	33	ASP	2.9
2	B	203	GLY	2.9
1	A	1052	U	2.8
1	A	993	G	2.8
1	A	221	C	2.7
1	A	1539	C	2.7
4	D	22	LYS	2.6
9	I	9	ARG	2.6
9	I	109	VAL	2.6
1	A	1147	C	2.6
19	S	40	ILE	2.5
19	S	78	ARG	2.5
4	D	31	CYS	2.5
4	D	9	CYS	2.4
3	C	178	LEU	2.4
1	A	6	G	2.3
19	S	37	ARG	2.3
1	A	792	A	2.3
1	A	1261	A	2.2
1	A	220	G	2.2

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Mol	Chain	Res	Type	RSRZ
3	C	103	VAL	2.2
9	I	128	ARG	2.2
1	A	1200	C	2.2
4	D	23	GLY	2.1
11	K	19	ALA	2.1
19	S	79	THR	2.1
13	M	117	VAL	2.1
21	U	5	ASP	2.1
7	G	5	ARG	2.1
21	U	6	ARG	2.1
9	I	127	LYS	2.0
20	T	9	ASN	2.0
1	A	1148	U	2.0
3	C	84	ILE	2.0
1	A	985	C	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	PSU	A	1541	20/21	0.78	0.18	159,231,317,318	0
1	PSU	A	1540	20/21	0.80	0.21	207,241,323,324	0
1	MA6	A	1519	24/25	0.95	0.09	105,122,132,134	0
1	UR3	A	1498	21/22	0.96	0.10	112,123,141,146	0
1	PSU	A	516	20/21	0.96	0.08	110,141,152,153	0
1	2MG	A	1207	24/25	0.96	0.15	175,210,229,233	0
1	5MC	A	1404	21/22	0.96	0.13	114,124,129,132	0
1	MA6	A	1518	24/25	0.97	0.08	121,127,148,148	0
1	M2G	A	966	25/26	0.97	0.08	123,141,169,173	0
1	5MC	A	1407	21/22	0.97	0.07	136,148,157,159	0
1	7MG	A	527	24/25	0.97	0.07	103,112,124,131	0
1	5MC	A	1400	21/22	0.98	0.06	95,124,131,135	0
1	4OC	A	1402	22/23	0.98	0.07	108,117,120,127	0
1	5MC	A	967	21/22	0.98	0.07	129,133,145,149	0
12	0TD	L	92	10/11	0.99	0.07	87,120,138,251	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	MG	A	1853	1/1	-0.22	0.13	338,338,338,338	0
23	MG	A	1731	1/1	0.62	0.18	95,95,95,95	0
23	MG	A	1837	1/1	0.64	0.27	103,103,103,103	0
23	MG	A	1783	1/1	0.70	0.27	133,133,133,133	0
23	MG	A	1800	1/1	0.70	0.14	108,108,108,108	0
23	MG	A	1661	1/1	0.72	0.28	89,89,89,89	0
23	MG	A	1761	1/1	0.73	0.24	97,97,97,97	0
23	MG	A	1788	1/1	0.75	0.28	99,99,99,99	0
23	MG	A	1765	1/1	0.75	0.26	124,124,124,124	0
23	MG	A	1715	1/1	0.76	0.33	120,120,120,120	0
23	MG	A	1748	1/1	0.77	0.08	143,143,143,143	0
23	MG	A	1755	1/1	0.77	0.10	159,159,159,159	0
23	MG	A	1737	1/1	0.77	0.18	128,128,128,128	0
23	MG	A	1702	1/1	0.78	0.21	106,106,106,106	0
23	MG	A	1796	1/1	0.79	0.56	107,107,107,107	0
23	MG	A	1821	1/1	0.79	0.15	338,338,338,338	0
23	MG	H	204	1/1	0.79	0.32	105,105,105,105	0
23	MG	Q	201	1/1	0.80	0.11	115,115,115,115	0
23	MG	A	1713	1/1	0.81	0.44	96,96,96,96	0
23	MG	A	1767	1/1	0.81	0.12	93,93,93,93	0
23	MG	A	1782	1/1	0.81	0.11	108,108,108,108	0
23	MG	A	1801	1/1	0.82	0.20	111,111,111,111	0
23	MG	A	1698	1/1	0.82	0.19	170,170,170,170	0
23	MG	A	1696	1/1	0.82	0.17	141,141,141,141	0
23	MG	A	1794	1/1	0.82	0.20	127,127,127,127	0
23	MG	A	1718	1/1	0.82	0.14	95,95,95,95	0
23	MG	A	1720	1/1	0.82	0.16	112,112,112,112	0
23	MG	A	1832	1/1	0.83	0.37	109,109,109,109	0
23	MG	A	1797	1/1	0.83	0.23	127,127,127,127	0
23	MG	A	1624	1/1	0.83	0.19	97,97,97,97	0
23	MG	A	1741	1/1	0.83	0.41	113,113,113,113	0
23	MG	A	1699	1/1	0.83	0.11	221,221,221,221	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	MG	A	1671	1/1	0.84	0.46	125,125,125,125	0
23	MG	A	1730	1/1	0.84	0.23	91,91,91,91	0
23	MG	A	1685	1/1	0.85	0.07	269,269,269,269	0
23	MG	P	102	1/1	0.85	0.12	100,100,100,100	0
23	MG	A	1798	1/1	0.85	0.16	122,122,122,122	0
23	MG	A	1727	1/1	0.86	0.18	95,95,95,95	0
23	MG	A	1706	1/1	0.86	0.21	97,97,97,97	0
23	MG	D	302	1/1	0.86	0.16	123,123,123,123	0
23	MG	A	1795	1/1	0.86	0.11	107,107,107,107	0
23	MG	A	1709	1/1	0.86	0.76	117,117,117,117	0
23	MG	A	1682	1/1	0.86	0.08	171,171,171,171	0
23	MG	A	1774	1/1	0.87	0.12	272,272,272,272	0
23	MG	A	1667	1/1	0.87	0.16	100,100,100,100	0
23	MG	A	1739	1/1	0.87	0.68	92,92,92,92	0
23	MG	A	1772	1/1	0.87	0.21	117,117,117,117	0
23	MG	A	1792	1/1	0.87	0.11	111,111,111,111	0
23	MG	S	101	1/1	0.87	0.21	93,93,93,93	0
23	MG	A	1623	1/1	0.88	0.16	146,146,146,146	0
23	MG	A	1847	1/1	0.88	0.19	296,296,296,296	0
23	MG	A	1760	1/1	0.88	0.40	105,105,105,105	0
23	MG	B	301	1/1	0.88	0.12	110,110,110,110	0
23	MG	A	1665	1/1	0.88	0.11	176,176,176,176	0
23	MG	A	1804	1/1	0.88	0.22	77,77,77,77	0
23	MG	A	1726	1/1	0.88	0.23	91,91,91,91	0
23	MG	A	1732	1/1	0.88	0.20	114,114,114,114	0
23	MG	A	1836	1/1	0.88	0.10	175,175,175,175	0
23	MG	A	1781	1/1	0.89	0.23	101,101,101,101	0
23	MG	A	1841	1/1	0.89	0.17	392,392,392,392	0
23	MG	A	1768	1/1	0.89	0.16	112,112,112,112	0
23	MG	A	1627	1/1	0.89	0.31	97,97,97,97	0
23	MG	A	1659	1/1	0.89	0.26	108,108,108,108	0
23	MG	A	1719	1/1	0.90	0.31	113,113,113,113	0
23	MG	A	1849	1/1	0.90	0.08	296,296,296,296	0
23	MG	A	1852	1/1	0.90	0.08	404,404,404,404	0
23	MG	A	1604	1/1	0.90	0.17	92,92,92,92	0
23	MG	A	1793	1/1	0.90	0.23	105,105,105,105	0
23	MG	A	1778	1/1	0.90	0.17	129,129,129,129	0
23	MG	A	1779	1/1	0.90	0.31	91,91,91,91	0
23	MG	J	201	1/1	0.90	0.18	107,107,107,107	0
23	MG	N	102	1/1	0.90	0.07	112,112,112,112	0
23	MG	A	1684	1/1	0.90	0.07	133,133,133,133	0
23	MG	P	103	1/1	0.90	0.08	102,102,102,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	MG	A	1753	1/1	0.90	0.08	168,168,168,168	0
23	MG	A	1626	1/1	0.90	0.40	146,146,146,146	0
23	MG	A	1712	1/1	0.91	0.13	91,91,91,91	0
23	MG	A	1664	1/1	0.91	0.17	133,133,133,133	0
23	MG	A	1738	1/1	0.91	0.29	89,89,89,89	0
23	MG	A	1695	1/1	0.91	0.30	121,121,121,121	0
23	MG	A	1740	1/1	0.91	0.09	123,123,123,123	0
23	MG	A	1660	1/1	0.91	0.09	173,173,173,173	0
23	MG	A	1787	1/1	0.91	0.20	81,81,81,81	0
23	MG	A	1656	1/1	0.91	0.08	152,152,152,152	0
23	MG	A	1750	1/1	0.91	0.38	115,115,115,115	0
23	MG	A	1834	1/1	0.92	0.37	130,130,130,130	0
23	MG	A	1835	1/1	0.92	0.28	128,128,128,128	0
23	MG	A	1725	1/1	0.92	0.13	91,91,91,91	0
23	MG	A	1663	1/1	0.92	0.10	109,109,109,109	0
23	MG	A	1645	1/1	0.92	0.14	138,138,138,138	0
23	MG	A	1745	1/1	0.92	0.28	85,85,85,85	0
23	MG	A	1769	1/1	0.92	0.12	112,112,112,112	0
23	MG	A	1747	1/1	0.92	0.35	111,111,111,111	0
23	MG	A	1650	1/1	0.92	0.22	127,127,127,127	0
23	MG	A	1775	1/1	0.92	0.06	235,235,235,235	0
23	MG	A	1632	1/1	0.92	0.34	105,105,105,105	0
23	MG	A	1799	1/1	0.92	0.35	109,109,109,109	0
23	MG	A	1693	1/1	0.92	0.10	104,104,104,104	0
23	MG	A	1754	1/1	0.92	0.16	177,177,177,177	0
23	MG	A	1668	1/1	0.92	0.23	149,149,149,149	0
23	MG	A	1723	1/1	0.92	0.23	92,92,92,92	0
23	MG	A	1784	1/1	0.92	0.33	93,93,93,93	0
23	MG	A	1833	1/1	0.92	0.34	98,98,98,98	0
23	MG	A	1721	1/1	0.93	0.24	115,115,115,115	0
23	MG	A	1848	1/1	0.93	0.13	336,336,336,336	0
23	MG	A	1744	1/1	0.93	0.18	99,99,99,99	0
23	MG	A	1802	1/1	0.93	0.24	86,86,86,86	0
23	MG	A	1789	1/1	0.93	0.09	118,118,118,118	0
23	MG	A	1758	1/1	0.93	0.16	98,98,98,98	0
23	MG	A	1823	1/1	0.93	0.21	317,317,317,317	0
23	MG	A	1603	1/1	0.93	0.13	126,126,126,126	0
23	MG	A	1746	1/1	0.93	0.18	123,123,123,123	0
23	MG	M	201	1/1	0.93	0.16	101,101,101,101	0
23	MG	A	1654	1/1	0.93	0.50	143,143,143,143	0
23	MG	A	1634	1/1	0.93	0.09	82,82,82,82	0
23	MG	A	1657	1/1	0.93	0.16	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	1608	1/1	0.93	0.12	80,80,80,80	0
23	MG	A	1785	1/1	0.93	0.07	74,74,74,74	0
23	MG	T	201	1/1	0.93	0.12	92,92,92,92	0
23	MG	A	1616	1/1	0.94	0.44	90,90,90,90	0
23	MG	A	1651	1/1	0.94	0.31	108,108,108,108	0
23	MG	A	1617	1/1	0.94	0.07	75,75,75,75	0
23	MG	E	201	1/1	0.94	0.05	228,228,228,228	0
23	MG	H	202	1/1	0.94	0.09	83,83,83,83	0
23	MG	A	1735	1/1	0.94	0.18	95,95,95,95	0
23	MG	A	1638	1/1	0.94	0.19	96,96,96,96	0
23	MG	A	1673	1/1	0.94	0.18	73,73,73,73	0
23	MG	A	1790	1/1	0.94	0.54	129,129,129,129	0
23	MG	A	1780	1/1	0.94	0.11	107,107,107,107	0
23	MG	A	1678	1/1	0.94	0.20	149,149,149,149	0
23	MG	A	1810	1/1	0.94	0.21	85,85,85,85	0
23	MG	A	1815	1/1	0.94	0.17	355,355,355,355	0
23	MG	A	1629	1/1	0.94	0.12	138,138,138,138	0
23	MG	A	1751	1/1	0.95	0.07	108,108,108,108	0
23	MG	A	1703	1/1	0.95	0.09	109,109,109,109	0
23	MG	A	1644	1/1	0.95	0.08	117,117,117,117	0
23	MG	A	1708	1/1	0.95	0.20	135,135,135,135	0
23	MG	A	1680	1/1	0.95	0.34	104,104,104,104	0
23	MG	A	1710	1/1	0.95	0.22	73,73,73,73	0
23	MG	A	1602	1/1	0.95	0.07	144,144,144,144	0
23	MG	A	1846	1/1	0.95	0.12	399,399,399,399	0
23	MG	A	1762	1/1	0.95	0.17	122,122,122,122	0
23	MG	A	1764	1/1	0.95	0.17	118,118,118,118	0
23	MG	A	1633	1/1	0.95	0.12	88,88,88,88	0
23	MG	A	1766	1/1	0.95	0.11	146,146,146,146	0
23	MG	A	1618	1/1	0.95	0.08	108,108,108,108	0
23	MG	A	1716	1/1	0.95	0.15	86,86,86,86	0
23	MG	A	1686	1/1	0.95	0.12	130,130,130,130	0
23	MG	A	1742	1/1	0.95	0.09	77,77,77,77	0
23	MG	A	1743	1/1	0.95	0.21	113,113,113,113	0
23	MG	H	203	1/1	0.95	0.07	124,124,124,124	0
23	MG	A	1652	1/1	0.95	0.08	114,114,114,114	0
23	MG	A	1777	1/1	0.95	0.06	485,485,485,485	0
23	MG	A	1637	1/1	0.95	0.15	127,127,127,127	0
23	MG	M	202	1/1	0.95	0.18	111,111,111,111	0
23	MG	A	1655	1/1	0.95	0.26	137,137,137,137	0
23	MG	A	1813	1/1	0.95	0.08	228,228,228,228	0
23	MG	A	1814	1/1	0.95	0.16	360,360,360,360	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	MG	A	1625	1/1	0.95	0.11	179,179,179,179	0
23	MG	A	1643	1/1	0.95	0.08	90,90,90,90	0
23	MG	A	1658	1/1	0.95	0.09	120,120,120,120	0
23	MG	A	1828	1/1	0.96	0.22	289,289,289,289	0
23	MG	A	1639	1/1	0.96	0.14	116,116,116,116	0
23	MG	A	1691	1/1	0.96	0.39	163,163,163,163	0
23	MG	A	1653	1/1	0.96	0.10	145,145,145,145	0
23	MG	A	1763	1/1	0.96	0.14	93,93,93,93	0
23	MG	A	1666	1/1	0.96	0.19	136,136,136,136	0
23	MG	A	1791	1/1	0.96	0.10	74,74,74,74	0
23	MG	A	1838	1/1	0.96	0.08	126,126,126,126	0
23	MG	A	1839	1/1	0.96	0.08	137,137,137,137	0
23	MG	A	1840	1/1	0.96	0.35	386,386,386,386	0
23	MG	A	1641	1/1	0.96	0.07	87,87,87,87	0
23	MG	A	1607	1/1	0.96	0.08	156,156,156,156	0
23	MG	A	1606	1/1	0.96	0.37	96,96,96,96	0
23	MG	A	1609	1/1	0.96	0.16	108,108,108,108	0
23	MG	A	1677	1/1	0.96	0.19	97,97,97,97	0
23	MG	A	1770	1/1	0.96	0.15	108,108,108,108	0
23	MG	A	1704	1/1	0.96	0.04	105,105,105,105	0
23	MG	A	1854	1/1	0.96	0.24	103,103,103,103	0
23	MG	A	1773	1/1	0.96	0.06	135,135,135,135	0
23	MG	B	302	1/1	0.96	0.05	89,89,89,89	0
23	MG	A	1646	1/1	0.96	0.08	99,99,99,99	0
23	MG	A	1729	1/1	0.96	0.23	102,102,102,102	0
23	MG	A	1749	1/1	0.96	0.23	99,99,99,99	0
23	MG	A	1803	1/1	0.96	0.07	123,123,123,123	0
23	MG	A	1647	1/1	0.96	0.07	115,115,115,115	0
23	MG	A	1807	1/1	0.96	0.22	111,111,111,111	0
23	MG	A	1809	1/1	0.96	0.03	96,96,96,96	0
23	MG	A	1648	1/1	0.96	0.07	227,227,227,227	0
23	MG	A	1619	1/1	0.96	0.08	141,141,141,141	0
23	MG	P	101	1/1	0.96	0.16	77,77,77,77	0
23	MG	A	1733	1/1	0.96	0.11	111,111,111,111	0
23	MG	A	1614	1/1	0.96	0.15	83,83,83,83	0
23	MG	A	1757	1/1	0.96	0.07	106,106,106,106	0
23	MG	A	1736	1/1	0.96	0.09	84,84,84,84	0
23	MG	A	1826	1/1	0.96	0.18	304,304,304,304	0
23	MG	A	1805	1/1	0.97	0.03	93,93,93,93	0
23	MG	A	1786	1/1	0.97	0.14	78,78,78,78	0
23	MG	A	1808	1/1	0.97	0.09	107,107,107,107	0
23	MG	A	1683	1/1	0.97	0.10	159,159,159,159	0

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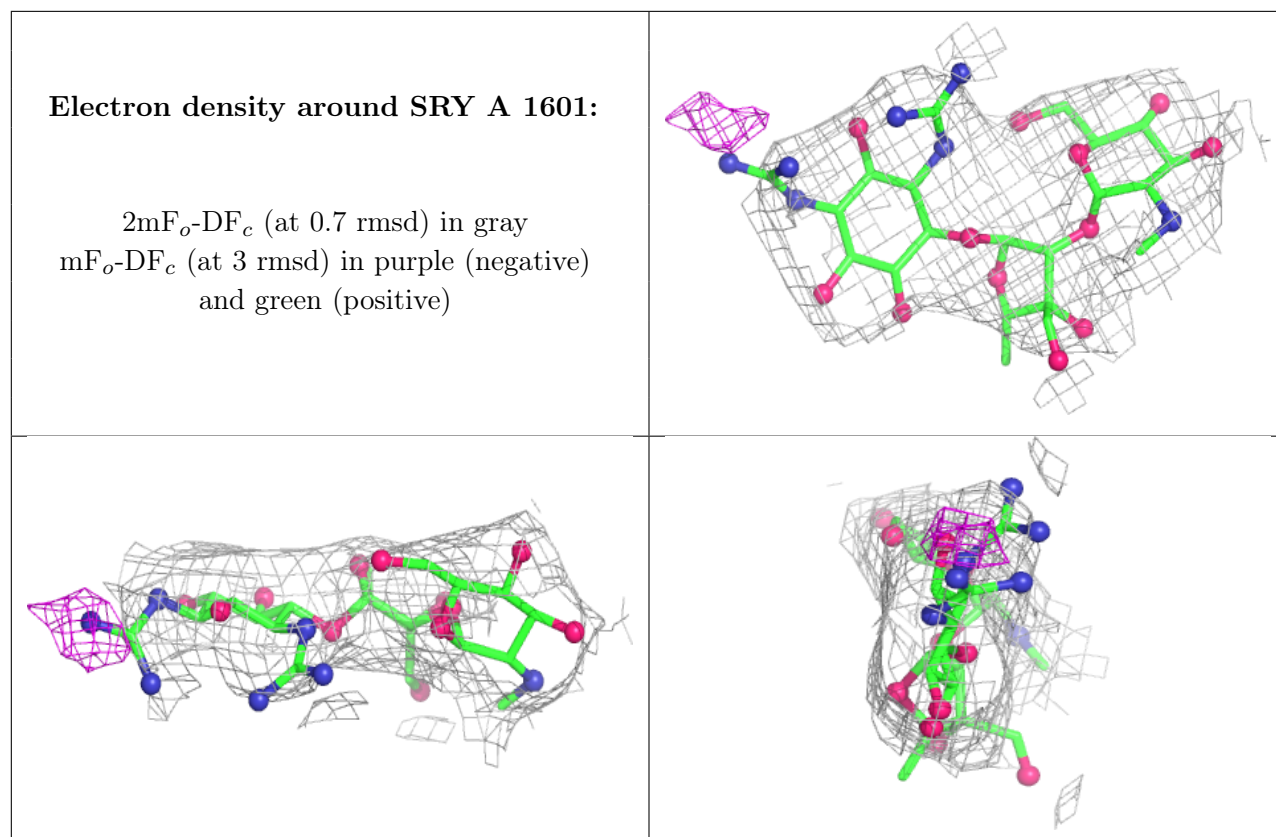
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	MG	A	1670	1/1	0.97	0.10	113,113,113,113	0
23	MG	A	1851	1/1	0.97	0.05	208,208,208,208	0
23	MG	A	1811	1/1	0.97	0.07	87,87,87,87	0
23	MG	A	1812	1/1	0.97	0.10	183,183,183,183	0
23	MG	A	1615	1/1	0.97	0.09	94,94,94,94	0
23	MG	A	1752	1/1	0.97	0.06	110,110,110,110	0
23	MG	A	1771	1/1	0.97	0.05	77,77,77,77	0
23	MG	A	1816	1/1	0.97	0.07	282,282,282,282	0
23	MG	A	1611	1/1	0.97	0.05	127,127,127,127	0
23	MG	H	201	1/1	0.97	0.09	83,83,83,83	0
23	MG	A	1687	1/1	0.97	0.08	210,210,210,210	0
23	MG	A	1824	1/1	0.97	0.09	168,168,168,168	0
23	MG	A	1705	1/1	0.97	0.06	97,97,97,97	0
23	MG	A	1620	1/1	0.97	0.10	128,128,128,128	0
23	MG	A	1724	1/1	0.97	0.10	71,71,71,71	0
23	MG	A	1759	1/1	0.97	0.15	96,96,96,96	0
23	MG	A	1707	1/1	0.97	0.14	113,113,113,113	0
23	MG	A	1621	1/1	0.97	0.15	87,87,87,87	0
23	MG	A	1694	1/1	0.97	0.05	95,95,95,95	0
23	MG	A	1622	1/1	0.97	0.06	86,86,86,86	0
22	SRY	A	1601	40/40	0.97	0.08	85,115,145,148	0
23	MG	A	1697	1/1	0.97	0.17	145,145,145,145	0
23	MG	A	1714	1/1	0.97	0.11	130,130,130,130	0
24	ZN	D	301	1/1	0.97	0.18	127,127,127,127	0
23	MG	A	1679	1/1	0.98	0.07	116,116,116,116	0
23	MG	A	1844	1/1	0.98	0.20	383,383,383,383	0
23	MG	A	1717	1/1	0.98	0.04	106,106,106,106	0
23	MG	A	1613	1/1	0.98	0.13	98,98,98,98	0
23	MG	A	1681	1/1	0.98	0.09	208,208,208,208	0
23	MG	A	1700	1/1	0.98	0.15	107,107,107,107	0
23	MG	A	1649	1/1	0.98	0.09	162,162,162,162	0
23	MG	A	1669	1/1	0.98	0.07	102,102,102,102	0
23	MG	A	1662	1/1	0.98	0.14	141,141,141,141	0
23	MG	A	1628	1/1	0.98	0.14	171,171,171,171	0
23	MG	A	1672	1/1	0.98	0.10	123,123,123,123	0
23	MG	A	1817	1/1	0.98	0.18	312,312,312,312	0
23	MG	A	1818	1/1	0.98	0.07	266,266,266,266	0
23	MG	A	1610	1/1	0.98	0.17	129,129,129,129	0
23	MG	A	1822	1/1	0.98	0.05	157,157,157,157	0
23	MG	A	1728	1/1	0.98	0.10	82,82,82,82	0
23	MG	A	1689	1/1	0.98	0.05	75,75,75,75	0
23	MG	A	1674	1/1	0.98	0.15	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	MG	A	1827	1/1	0.98	0.09	200,200,200,200	0
23	MG	J	202	1/1	0.98	0.07	105,105,105,105	0
23	MG	A	1692	1/1	0.98	0.12	170,170,170,170	0
23	MG	A	1711	1/1	0.98	0.11	93,93,93,93	0
23	MG	A	1776	1/1	0.98	0.08	299,299,299,299	0
23	MG	A	1675	1/1	0.98	0.09	79,79,79,79	0
23	MG	A	1734	1/1	0.98	0.30	108,108,108,108	0
23	MG	A	1756	1/1	0.98	0.08	203,203,203,203	0
23	MG	A	1676	1/1	0.98	0.11	81,81,81,81	0
23	MG	A	1640	1/1	0.98	0.06	96,96,96,96	0
23	MG	A	1636	1/1	0.98	0.12	176,176,176,176	0
23	MG	T	202	1/1	0.98	0.17	267,267,267,267	0
23	MG	A	1806	1/1	0.98	0.05	88,88,88,88	0
23	MG	A	1825	1/1	0.99	0.10	272,272,272,272	0
23	MG	A	1631	1/1	0.99	0.09	71,71,71,71	0
23	MG	A	1612	1/1	0.99	0.04	75,75,75,75	0
23	MG	A	1845	1/1	0.99	0.06	159,159,159,159	0
23	MG	A	1701	1/1	0.99	0.30	87,87,87,87	0
23	MG	A	1829	1/1	0.99	0.03	93,93,93,93	0
23	MG	A	1830	1/1	0.99	0.12	322,322,322,322	0
23	MG	A	1831	1/1	0.99	0.09	168,168,168,168	0
23	MG	A	1850	1/1	0.99	0.11	270,270,270,270	0
23	MG	A	1642	1/1	0.99	0.16	105,105,105,105	0
23	MG	A	1688	1/1	0.99	0.04	99,99,99,99	0
23	MG	A	1819	1/1	0.99	0.06	286,286,286,286	0
23	MG	A	1820	1/1	0.99	0.20	313,313,313,313	0
23	MG	A	1605	1/1	0.99	0.04	123,123,123,123	0
23	MG	A	1690	1/1	0.99	0.13	324,324,324,324	0
23	MG	A	1722	1/1	0.99	0.07	71,71,71,71	0
23	MG	A	1630	1/1	0.99	0.07	145,145,145,145	0
23	MG	A	1843	1/1	1.00	0.06	55,55,55,55	0
23	MG	A	1635	1/1	1.00	0.02	62,62,62,62	0
23	MG	A	1842	1/1	1.00	0.04	73,73,73,73	0
24	ZN	N	101	1/1	1.00	0.03	168,168,168,168	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.