Full wwPDB X-ray Structure Validation Report ⓘ

Jan 4, 2024 – 06:38 pm GMT

PDB ID	:	5JVG
Title	:	The large ribosomal subunit from Deinococcus radiodurans in complex with avilamycin
Authors	:	Krupkin, M.; Wekselman, I.; Matzov, D.; Eyal, Z.; Diskin Posner, Y.; Rozenberg, H.; Zimmerman, E.; Bashan, A.; Yonath, A.
Deposited on	:	2016-05-11
Resolution	:	3.43 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:

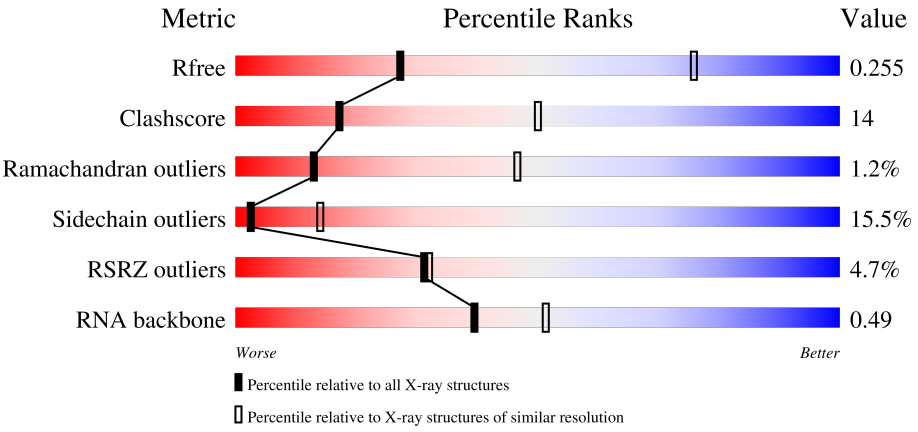
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.43 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}	130704	1486 (3.50-3.34)
Clashscore	141614	1572 (3.50-3.34)
Ramachandran outliers	138981	1534 (3.50-3.34)
Sidechain outliers	138945	1535 (3.50-3.34)
RSRZ outliers	127900	1395 (3.50-3.34)
RNA backbone	3102	1012 (3.88-2.96)

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 <=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	X	2877	46% 37% 11% • 6%
2	Y	124	% 48% 36% 11% • •
3	A	275	6% 51% 39% 8% ••

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Mol	Chain	Length	Quality of chain
4	B	211	2% 59% 29% 9%
5	C	205	5% 43% 44% 8% 5%
6	D	180	13% 55% 37% 6%
7	E	185	3% 68% 23% 8%
8	F	144	15% 34% 9% 56%
9	G	174	6% 42% 31% 9% 18%
10	H	134	63% 30% 7%
11	I	156	11% 49% 28% 10% 14%
12	J	141	6% 53% 35% 8%
13	K	116	% 59% 34% 6%
14	L	114	18% 37% 35% 18% 9%
15	M	166	3% 42% 25% 28%
16	N	118	% 51% 44%
17	O	100	4% 49% 41% 7%
18	P	134	2% 49% 41% 5%
19	Q	95	5% 59% 33% 6%
20	R	115	10% 47% 40% 9%
21	S	237	9% 44% 28% 24%
22	T	91	13% 48% 30% 19%
23	U	81	26% 37% 38% 16% 9%
24	V	67	10% 76% 18%
25	W	55	22% 51% 42% 7%
26	Z	60	48% 40% 7% 5%
27	1	55	24% 33% 44% 20%
28	2	47	13% 51% 34% 13%

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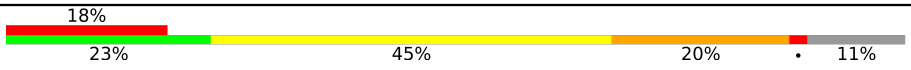
Mol	Chain	Length	Quality of chain
29	3	66	

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
31	MG	3	101	-	-	-	X
31	MG	X	2904	-	-	-	X
31	MG	X	2958	-	-	-	X
31	MG	X	3000	-	-	-	X
31	MG	X	3010	-	-	-	X
31	MG	X	3033	-	-	-	X
31	MG	X	3039	-	-	-	X
31	MG	X	3054	-	-	-	X
31	MG	X	3064	-	-	-	X
31	MG	X	3072	-	-	-	X
31	MG	X	3073	-	-	-	X
31	MG	X	3089	-	-	-	X
31	MG	X	3102	-	-	-	X
31	MG	X	3103	-	-	-	X
31	MG	X	3104	-	-	-	X
31	MG	X	3160	-	-	-	X
31	MG	X	3170	-	-	-	X
31	MG	X	3189	-	-	-	X
31	MG	X	3215	-	-	-	X
31	MG	X	3219	-	-	-	X
31	MG	X	3225	-	-	-	X
31	MG	X	3231	-	-	-	X
31	MG	X	3234	-	-	-	X
31	MG	X	3239	-	-	-	X
31	MG	X	3248	-	-	-	X
31	MG	X	3250	-	-	-	X
31	MG	X	3252	-	-	-	X
31	MG	X	3261	-	-	-	X
31	MG	X	3266	-	-	-	X
31	MG	X	3300	-	-	-	X
31	MG	X	3301	-	-	-	X
31	MG	X	3314	-	-	-	X
31	MG	Y	209	-	-	-	X
32	MPD	X	3316	-	-	X	-

2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 85766 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 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	X	2710	58191	25957	10742	18782	2710	0	1	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	1526	U	C	conflict	GB 1026245073
X	1890	A	G	conflict	GB 1026245073

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	Y	120	2561	1143	471	827	120	0	0	0

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	A	272	2085	1299	416	366	4	0	0	0

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	B	205	1539	965	295	271	8	0	0	0

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	C	195	1489	925	285	276	3	0	0	0

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	D	177	Total	C	N	O	S	0	0	0
			1367	869	241	250	7			

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	E	171	Total	C	N	O	S	0	0	0
			1286	812	237	236	1			

- Molecule 8 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	F	63	Total	C	N	O	S	0	0	0
			451	280	82	86	3			

- Molecule 9 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	G	142	Total	C	N	O	S	0	0	0
			1114	704	209	198	3			

- Molecule 10 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	H	134	Total	C	N	O	S	0	0	0
			997	614	198	180	5			

- Molecule 11 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	I	134	Total	C	N	O	0	0	0
			982	601	195	186			

- Molecule 12 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	J	136	Total	C	N	O	S	0	0	0
			1060	680	192	181	7			

- Molecule 13 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	K	115	Total	C	N	O	S	0	0	0
			897	552	183	159	3			

- Molecule 14 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	L	104	Total	C	N	O	0	0	0
			779	476	161	142			

- Molecule 15 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	M	119	Total	C	N	O	0	0	0
			939	586	185	168			

- Molecule 16 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	N	117	Total	C	N	O	S	0	0	0
			978	608	210	159	1			

- Molecule 17 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	O	97	Total	C	N	O	0	0	0
			759	477	142	140			

- Molecule 18 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	P	128	Total	C	N	O	S	0	0	0
			1015	640	200	173	2			

- Molecule 19 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Q	93	Total	C	N	O	S	0	0	0
			726	458	136	130	2			

- Molecule 20 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	R	110	Total	C	N	O	S	0	0	0
			809	504	153	151	1			

- Molecule 21 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	S	180	Total	C	N	O	S	0	0	0
			1370	864	241	259	6			

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	T	74	Total	C	N	O	S	0	0	0
			556	351	107	97	1			

- Molecule 23 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
23	U	74	Total	C	N	O	0	0	0
			549	341	111	97			

- Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	V	65	Total	C	N	O	S	0	0	0
			525	322	106	95	2			

- Molecule 25 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	W	55	Total	C	N	O	S	0	0	0
			424	264	82	76	2			

- Molecule 26 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Z	57	Total	C	N	O	S	0	0	0
			444	273	91	75	5			

- Molecule 27 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	1	53	Total	C	N	O	S	0	0	0
			427	271	79	76	1			

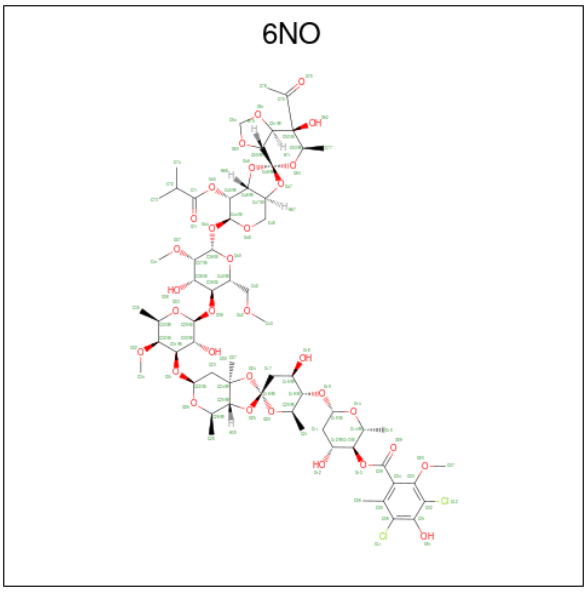
- Molecule 28 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	2	46	Total	C	N	O	S	0	0	0
			383	230	91	60	2			

- Molecule 29 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	3	59	Total	C	N	O	S	0	0	0
			453	285	92	73	3			

- Molecule 30 is Avilamycin (three-letter code: 6NO) (formula: $C_{61}H_{88}Cl_2O_{32}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	X	1	Total	C	Cl	O	0	0
			95	61	2	32		

- Molecule 31 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
31	X	420	Total	Mg	0	0
			420	420		

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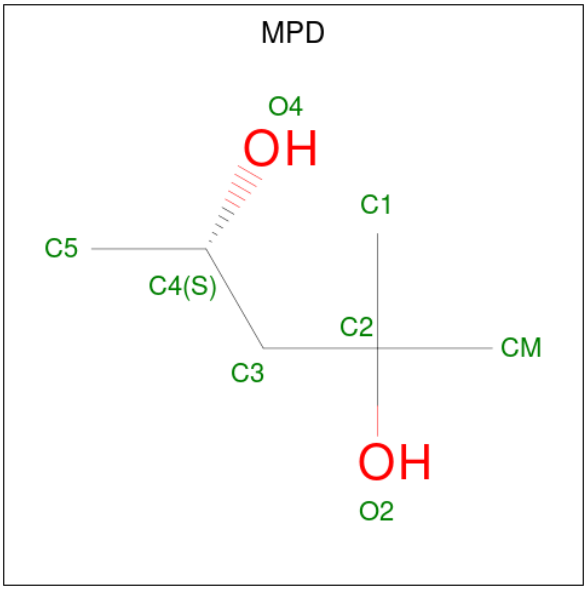
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	Y	19	Total Mg 19 19	0	0
31	A	1	Total Mg 1 1	0	0
31	J	1	Total Mg 1 1	0	0
31	K	1	Total Mg 1 1	0	0
31	M	1	Total Mg 1 1	0	0
31	N	1	Total Mg 1 1	0	0
31	T	1	Total Mg 1 1	0	0
31	3	1	Total Mg 1 1	0	0

- Molecule 32 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	X	1	Total C O 8 6 2	0	0
32	X	1	Total C O 8 6 2	0	0
32	X	1	Total C O 8 6 2	0	0

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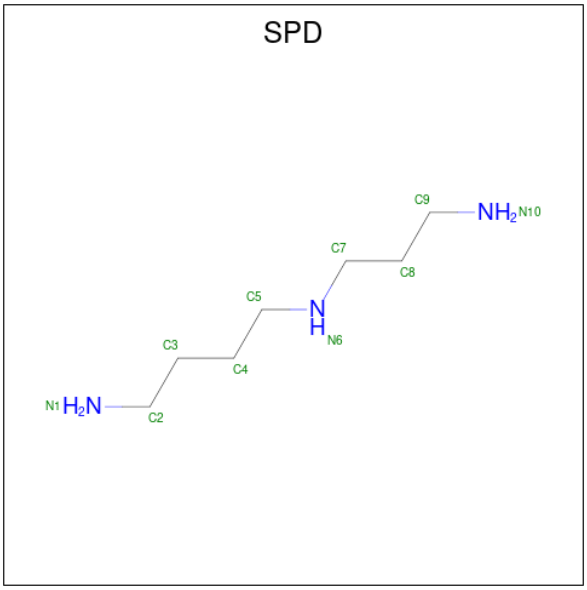
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	X	1	Total C O 8 6 2	0	0
32	X	1	Total C O 8 6 2	0	0

- Molecule 33 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$).



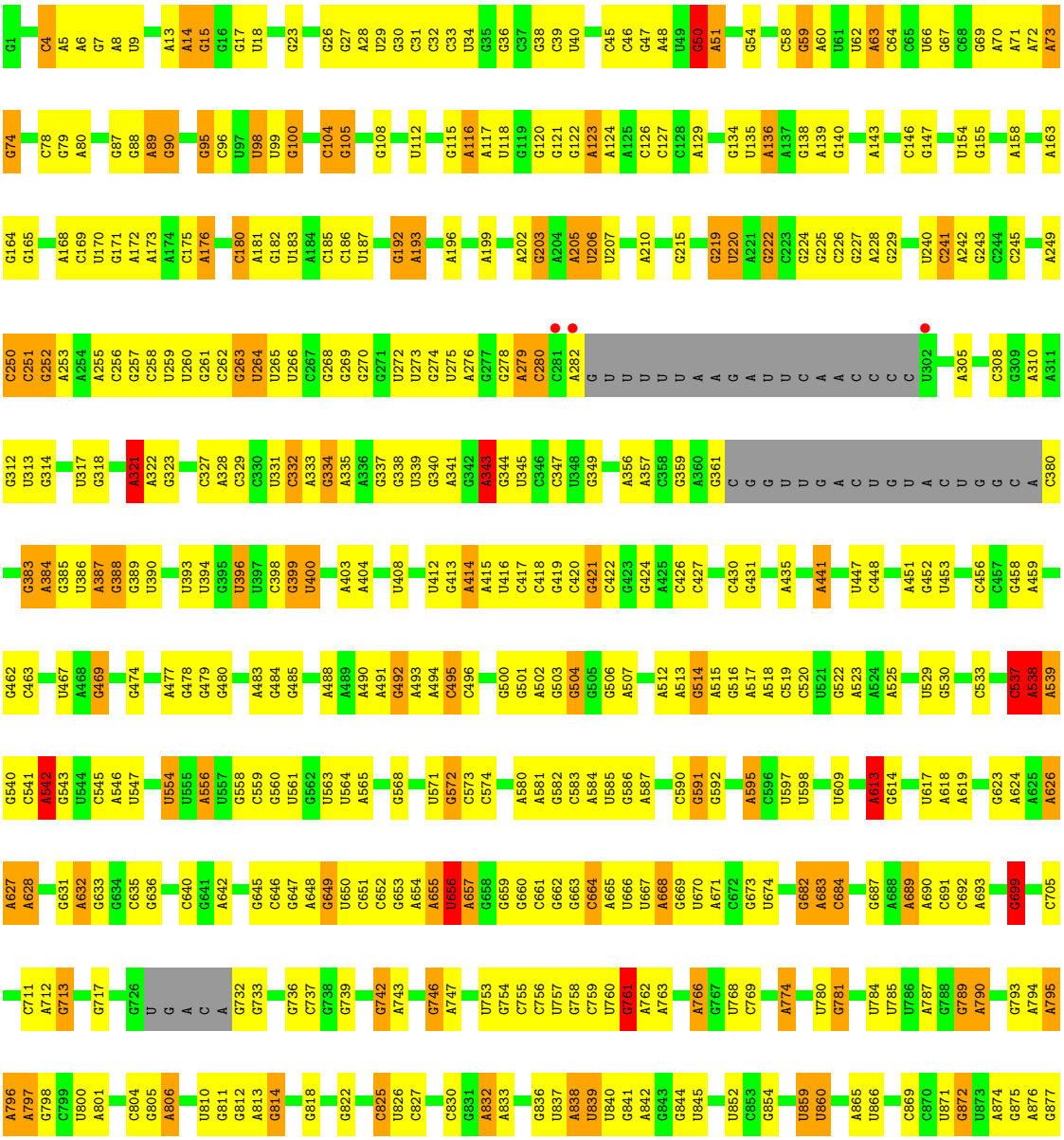
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	X	1	Total C N 10 7 3	0	0
33	X	1	Total C N 10 7 3	0	0
33	X	1	Total C N 10 7 3	0	0

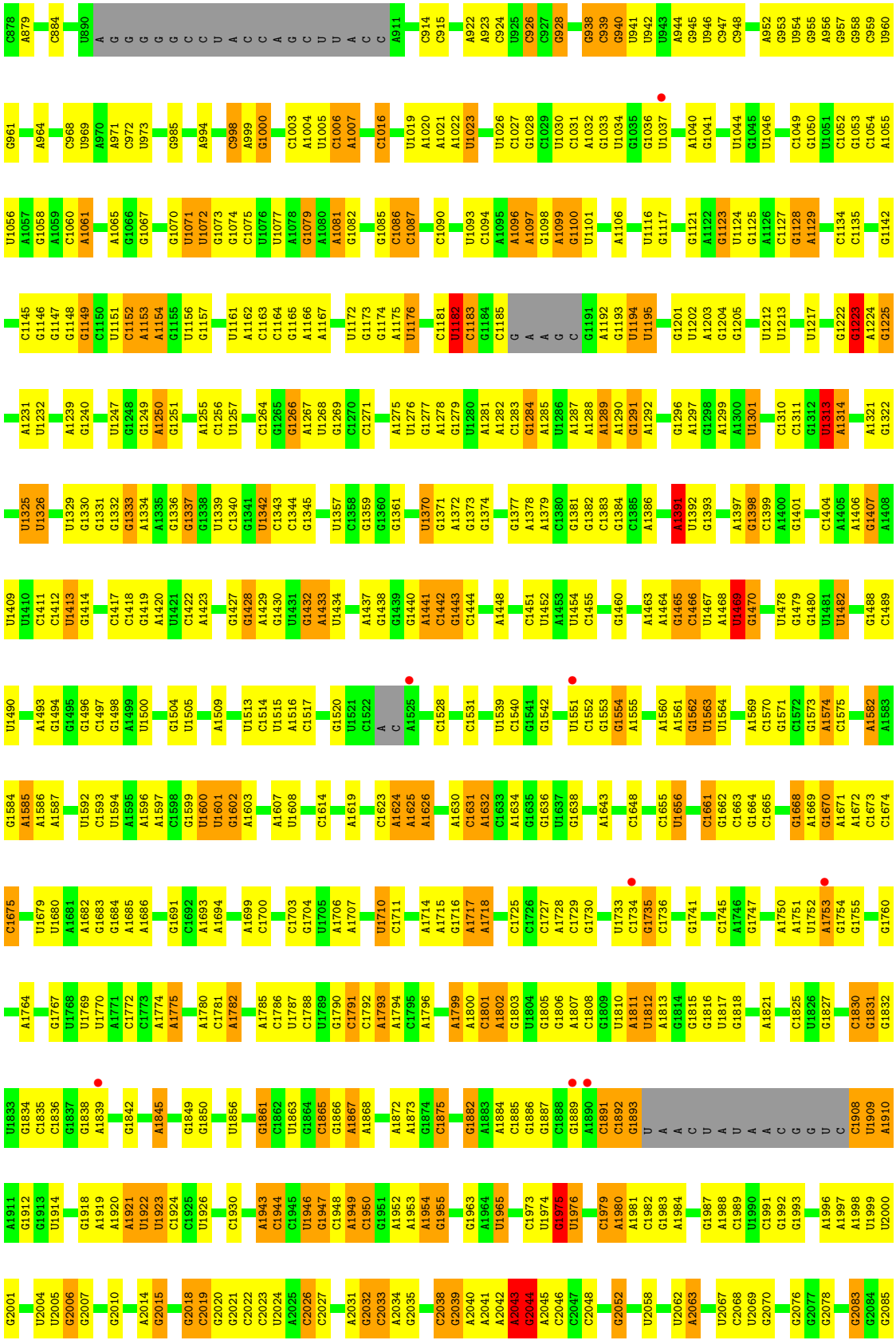
3 Residue-property plots (i)

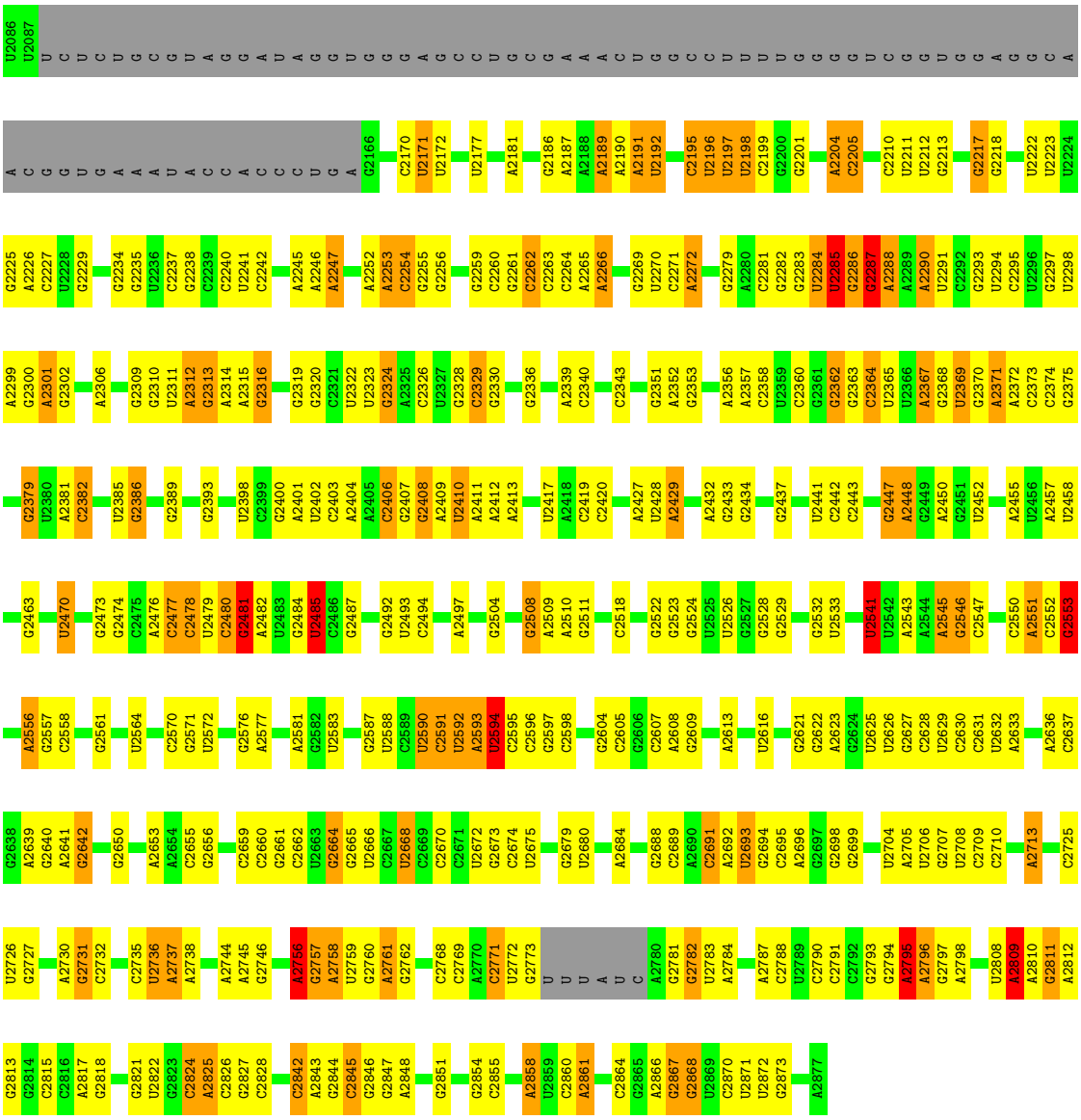
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: 23S ribosomal RNA

Chain X:

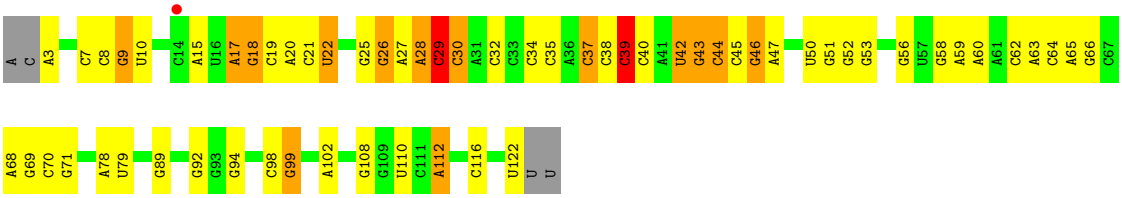






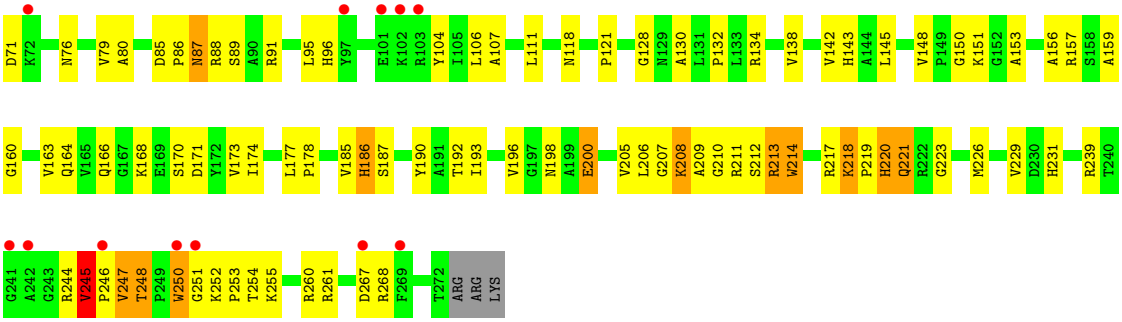
• Molecule 2: 5S ribosomal RNA

Chain Y:



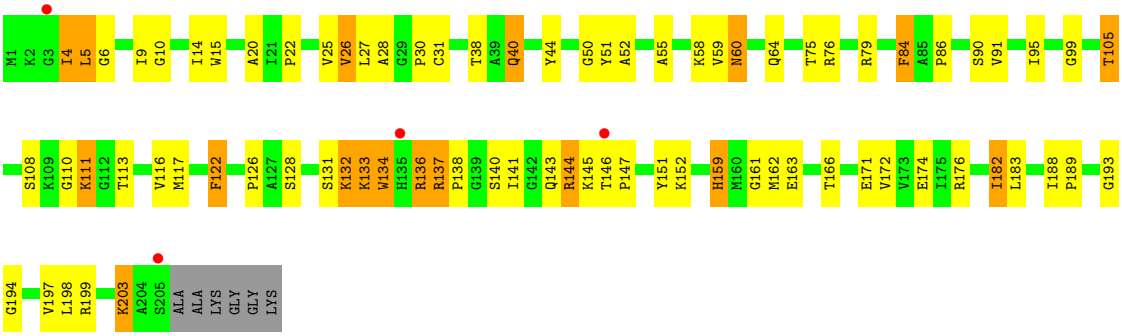
• Molecule 3: 50S ribosomal protein L2

Chain A:



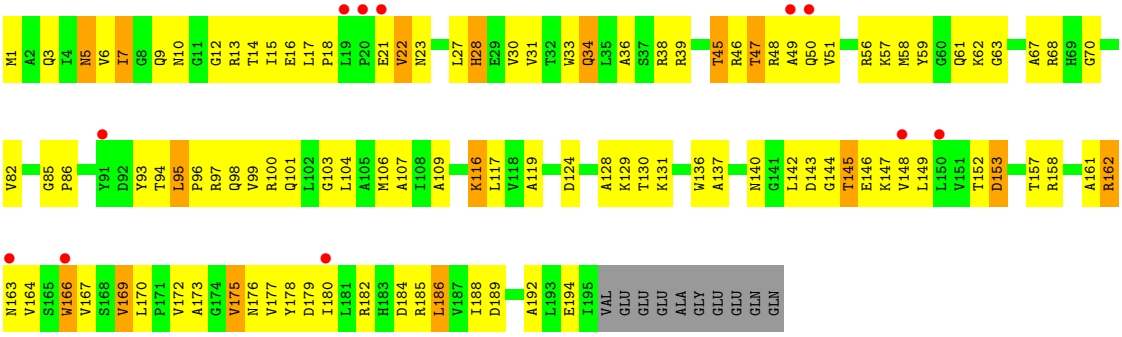
• Molecule 4: 50S ribosomal protein L3

Chain B:



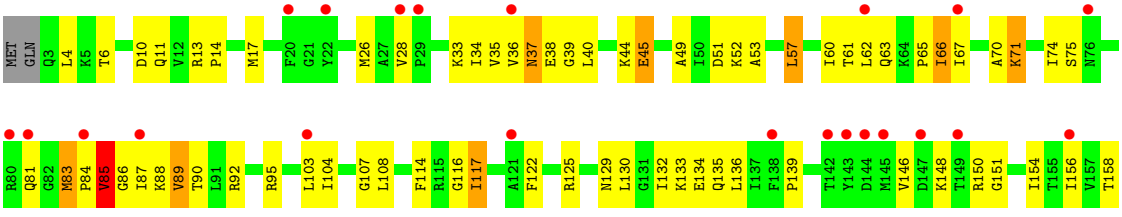
• Molecule 5: 50S ribosomal protein L4

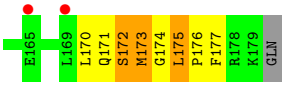
Chain C:



• Molecule 6: 50S ribosomal protein L5

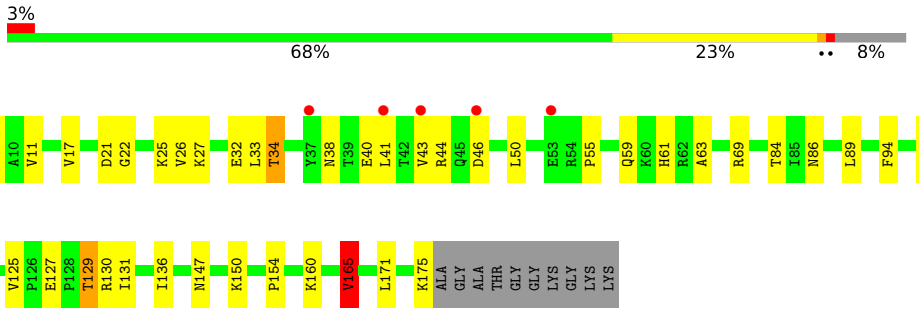
Chain D:





• Molecule 7: 50S ribosomal protein L6

Chain E:



• Molecule 8: 50S ribosomal protein L11

Chain F:

• Molecule 9: 50S ribosomal protein L13

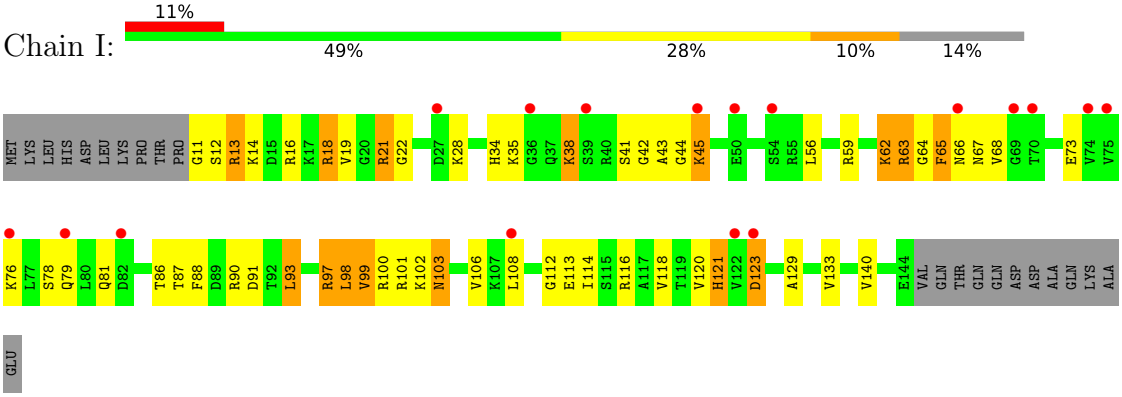
Chain G:

• Molecule 10: 50S ribosomal protein L14

Chain H:

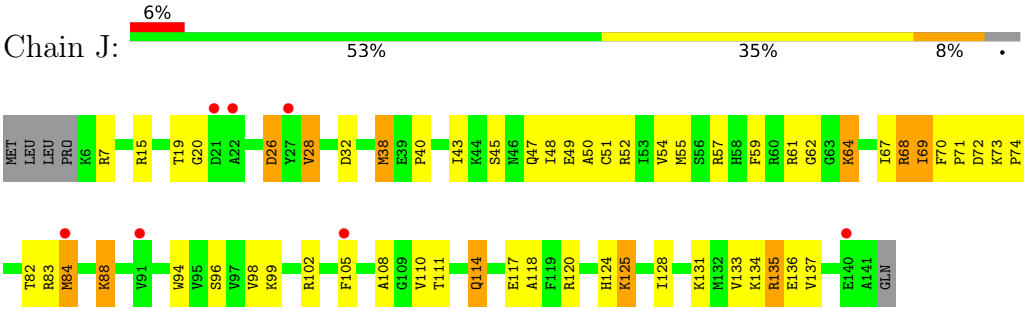
• Molecule 11: 50S ribosomal protein L15

Chain I:



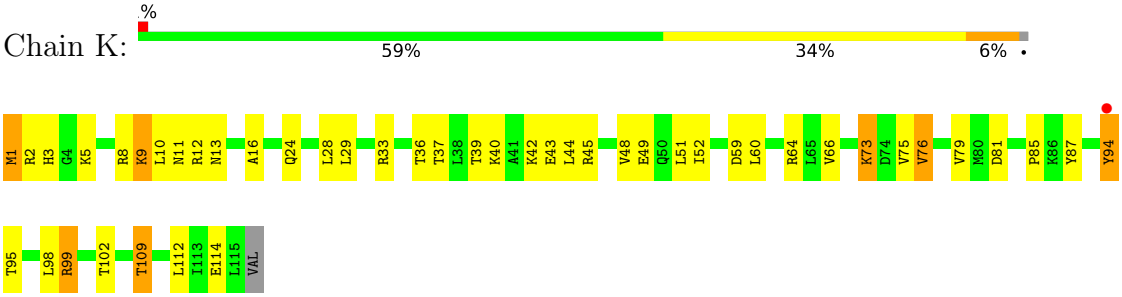
• Molecule 12: 50S ribosomal protein L16

Chain J:



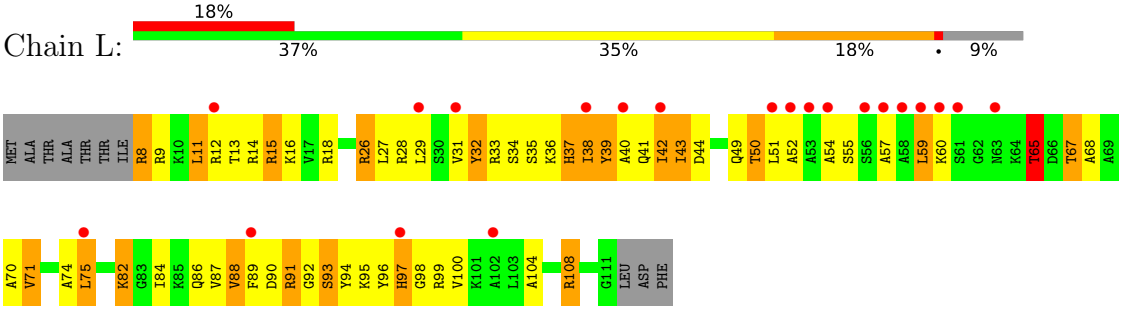
• Molecule 13: 50S ribosomal protein L17

Chain K:



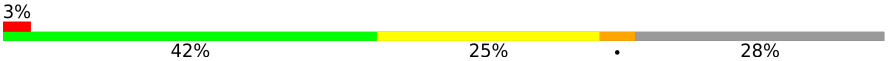
• Molecule 14: 50S ribosomal protein L18

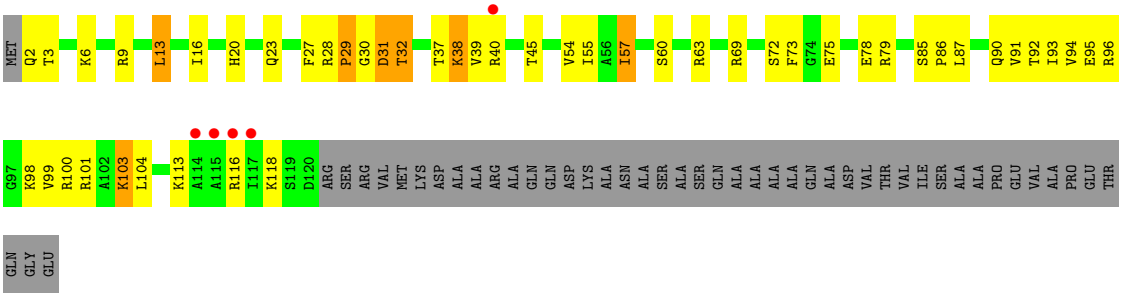
Chain L:



• Molecule 15: 50S ribosomal protein L19

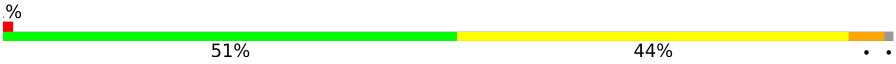
Chain M:

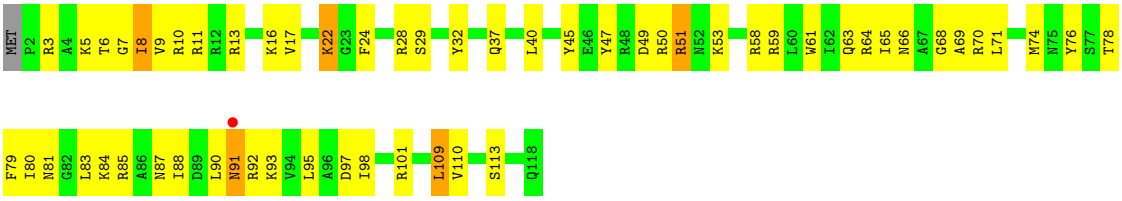




• Molecule 16: 50S ribosomal protein L20

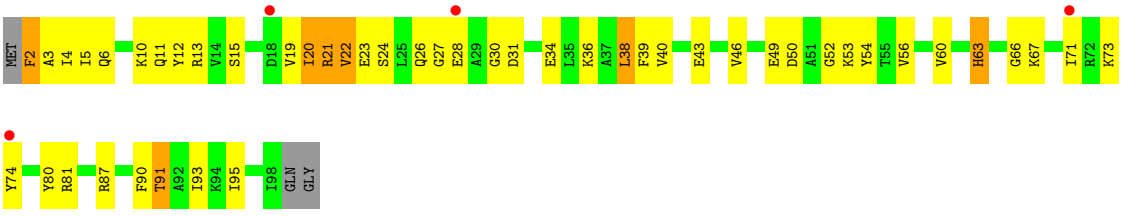
Chain N:





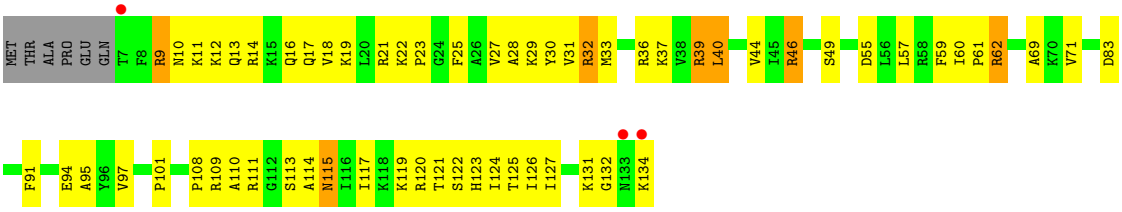
• Molecule 17: 50S ribosomal protein L21

Chain O:



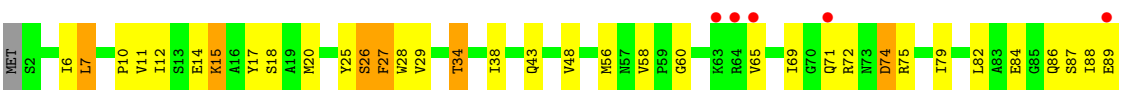
• Molecule 18: 50S ribosomal protein L22

Chain P:



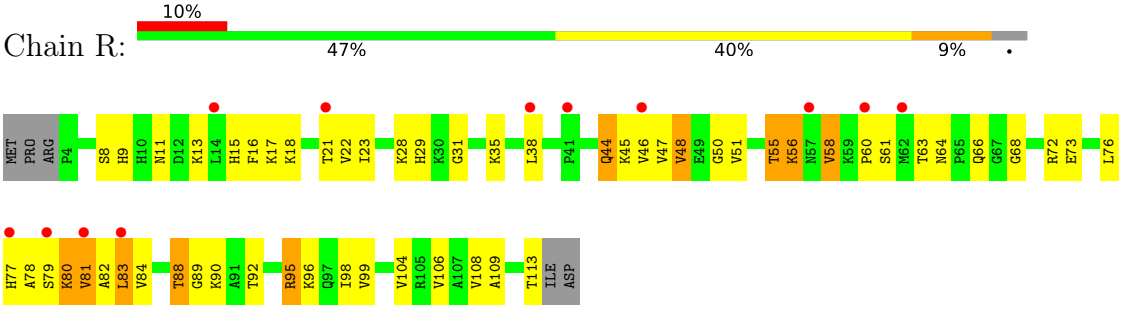
• Molecule 19: 50S ribosomal protein L23

Chain Q:



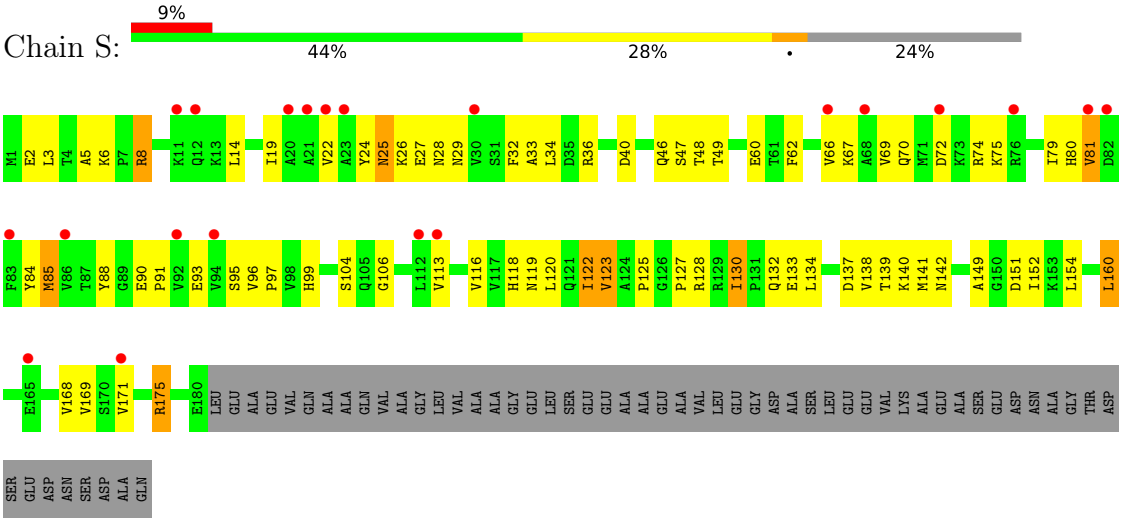
• Molecule 20: 50S ribosomal protein L24

Chain R:



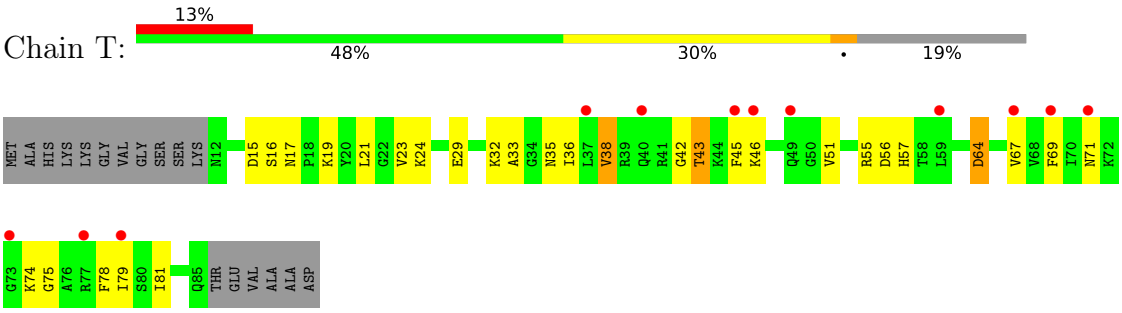
• Molecule 21: 50S ribosomal protein L25

Chain S:



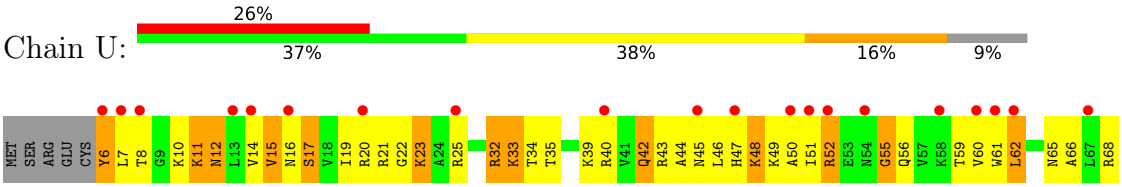
• Molecule 22: 50S ribosomal protein L27

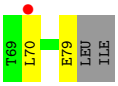
Chain T:



• Molecule 23: 50S ribosomal protein L28

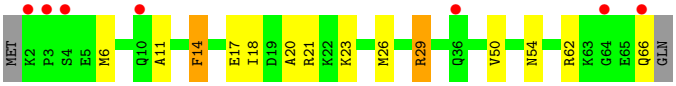
Chain U:





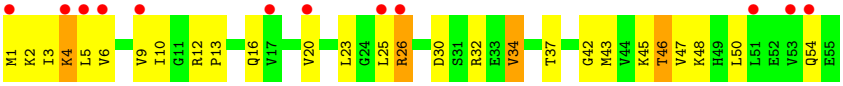
• Molecule 24: 50S ribosomal protein L29

Chain V:



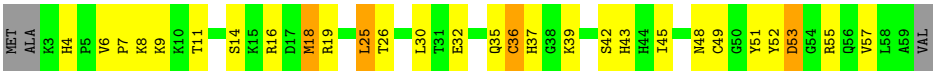
• Molecule 25: 50S ribosomal protein L30

Chain W:



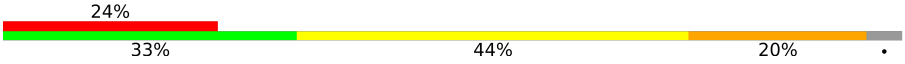
• Molecule 26: 50S ribosomal protein L32

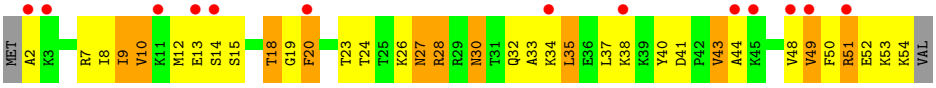
Chain Z:



• Molecule 27: 50S ribosomal protein L33

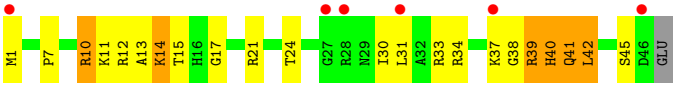
Chain 1:





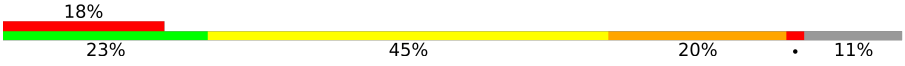
• Molecule 28: 50S ribosomal protein L34

Chain 2:



• Molecule 29: 50S ribosomal protein L35

Chain 3:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	170.03Å 412.63Å 698.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.55 – 3.43 51.02 – 3.43	Depositor EDS
% Data completeness (in resolution range)	88.9 (49.55-3.43) 88.9 (51.02-3.43)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.61 (at 3.40Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.211 , 0.253 0.214 , 0.255	Depositor DCC
R_{free} test set	14626 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	99.1	Xtriage
Anisotropy	0.729	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.18 , 65.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	85766	wwPDB-VP
Average B, all atoms (Å^2)	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 6NO, MPD, SPD, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	X	0.45	3/65161 (0.0%)	0.98	120/101636 (0.1%)
2	Y	0.32	0/2863	0.82	2/4461 (0.0%)
3	A	0.34	0/2127	0.66	3/2864 (0.1%)
4	B	0.41	0/1567	0.69	0/2105
5	C	0.34	0/1512	0.61	0/2046
6	D	0.25	0/1385	0.54	0/1862
7	E	0.25	0/1308	0.47	0/1771
8	F	0.24	0/455	0.48	0/611
9	G	0.39	0/1138	0.70	0/1539
10	H	0.40	0/1007	0.68	0/1352
11	I	0.39	0/991	0.69	0/1328
12	J	0.41	0/1083	0.64	0/1451
13	K	0.43	0/905	0.68	0/1212
14	L	0.35	0/785	0.64	0/1048
15	M	0.45	0/952	0.72	1/1277 (0.1%)
16	N	0.36	0/994	0.58	0/1323
17	O	0.35	0/768	0.66	1/1025 (0.1%)
18	P	0.43	0/1028	0.65	0/1375
19	Q	0.35	0/737	0.60	0/988
20	R	0.37	0/819	0.71	0/1103
21	S	0.27	0/1395	0.57	0/1897
22	T	0.37	0/563	0.66	0/747
23	U	0.36	0/553	0.73	0/741
24	V	0.25	0/529	0.48	0/704
25	W	0.32	0/426	0.52	0/568
26	Z	0.38	0/456	0.64	0/613
27	1	0.37	0/434	0.76	1/579 (0.2%)
28	2	0.37	0/387	0.72	0/509
29	3	0.40	0/459	0.72	0/604
All	All	0.43	3/92787 (0.0%)	0.90	128/139339 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
6	D	0	2
9	G	0	2
11	I	0	2
14	L	0	2
15	M	0	1
21	S	0	1
22	T	0	1
23	U	0	3
27	1	0	1
28	2	0	1
29	3	0	3
All	All	0	19

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	774	A	N9-C4	7.85	1.42	1.37
1	X	774	A	N7-C5	6.14	1.43	1.39
1	X	774	A	C6-N1	-5.13	1.31	1.35

All (128) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	1670	G	N1-C6-O6	-12.98	112.11	119.90
1	X	774	A	N1-C6-N6	-12.65	111.01	118.60
1	X	1675	C	O5'-P-OP1	-12.45	94.49	105.70
1	X	1670	G	C5-C6-O6	9.99	134.60	128.60
1	X	1670	G	C6-C5-N7	9.02	135.81	130.40
1	X	1670	G	C4-C5-N7	-8.65	107.34	110.80
1	X	538	A	C2-N3-C4	8.27	114.73	110.60
1	X	1718[A]	A	OP1-P-O3'	7.98	122.76	105.20
1	X	1718[B]	A	OP1-P-O3'	7.98	122.76	105.20
1	X	1718[A]	A	OP2-P-O3'	-7.87	87.89	105.20
1	X	1718[B]	A	OP2-P-O3'	-7.87	87.89	105.20
17	O	38	LEU	CA-CB-CG	7.77	133.17	115.30
1	X	2550	C	C6-N1-C2	-7.26	117.40	120.30
1	X	1469	U	C2-N1-C1'	7.13	126.26	117.70
1	X	537	C	C6-N1-C2	-7.05	117.48	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	699	G	C4-C5-N7	7.04	113.62	110.80
1	X	2285	U	C2-N1-C1'	7.03	126.13	117.70
1	X	1292	A	C8-N9-C4	7.02	108.61	105.80
1	X	537	C	O4'-C1'-N1	6.70	113.56	108.20
1	X	2285	U	N1-C2-O2	6.68	127.48	122.80
1	X	1670	G	C5-N7-C8	6.65	107.62	104.30
1	X	2867	G	N3-C4-C5	6.61	131.90	128.60
1	X	746	G	N3-C4-C5	-6.46	125.37	128.60
1	X	1670	G	N7-C8-N9	-6.41	109.89	113.10
1	X	2044	G	O5'-P-OP2	-6.32	100.01	105.70
1	X	2670	C	C6-N1-C2	-6.28	117.79	120.30
1	X	542	A	N1-C6-N6	6.24	122.34	118.60
1	X	774	A	C5-C6-N6	6.19	128.65	123.70
1	X	1391	A	P-O3'-C3'	6.14	127.07	119.70
1	X	796	A	C2-N3-C4	-6.11	107.54	110.60
1	X	1333	G	N3-C4-N9	-6.08	122.35	126.00
1	X	1975	G	P-O3'-C3'	5.98	126.87	119.70
1	X	1469	U	C5-C6-N1	5.97	125.69	122.70
1	X	2594	U	C5-C6-N1	5.93	125.66	122.70
1	X	2033	C	C6-N1-C2	-5.93	117.93	120.30
1	X	774	A	C2-N3-C4	5.91	113.56	110.60
1	X	1313	U	P-O3'-C3'	5.90	126.78	119.70
1	X	2018	G	C4-C5-N7	5.88	113.15	110.80
3	A	33	LEU	N-CA-C	-5.86	95.17	111.00
15	M	31	ASP	N-CA-C	5.84	126.77	111.00
1	X	1182	U	OP1-P-O3'	5.80	117.97	105.20
1	X	2815	C	C6-N1-C2	5.75	122.60	120.30
1	X	2553	G	N3-C4-C5	5.74	131.47	128.60
1	X	689	A	C5-N7-C8	-5.70	101.05	103.90
1	X	1770	U	O4'-C1'-N1	5.67	112.74	108.20
1	X	2590	U	N3-C2-O2	-5.64	118.25	122.20
1	X	2043	A	OP2-P-O3'	5.63	117.58	105.20
1	X	1683	G	C4-N9-C1'	-5.62	119.20	126.50
1	X	762	A	N1-C6-N6	5.61	121.96	118.60
1	X	1223	G	C6-C5-N7	-5.60	127.04	130.40
1	X	699	G	C5-N7-C8	-5.59	101.51	104.30
1	X	1326	U	C2-N1-C1'	5.58	124.39	117.70
1	X	2316	G	N3-C4-N9	5.58	129.34	126.00
1	X	1223	G	C4-N9-C1'	5.57	133.74	126.50
1	X	321	A	O4'-C1'-N9	5.54	112.63	108.20
1	X	1291	G	N7-C8-N9	-5.51	110.34	113.10
1	X	746	G	N3-C4-N9	5.51	129.31	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	746	G	C4-N9-C1'	5.50	133.66	126.50
1	X	2756	A	P-O3'-C3'	5.48	126.28	119.70
1	X	2285	U	N3-C2-O2	-5.48	118.36	122.20
1	X	2410	U	N3-C2-O2	-5.48	118.37	122.20
1	X	2018	G	C5-N7-C8	-5.46	101.57	104.30
1	X	774	A	N9-C4-C5	5.46	107.98	105.80
1	X	1333	G	N3-C4-C5	5.45	131.32	128.60
1	X	761	G	C4-N9-C1'	-5.43	119.44	126.50
1	X	2316	G	C4-N9-C1'	5.43	133.56	126.50
1	X	1675	C	O5'-P-OP2	5.43	117.22	110.70
1	X	522	G	O4'-C1'-N9	5.43	112.54	108.20
1	X	1718[A]	A	P-O3'-C3'	5.42	126.20	119.70
1	X	1718[B]	A	P-O3'-C3'	5.42	126.20	119.70
1	X	742	G	C4-N9-C1'	5.39	133.51	126.50
1	X	656	U	P-O3'-C3'	5.38	126.15	119.70
1	X	955	G	C4-N9-C1'	5.37	133.48	126.50
1	X	2485	U	C2-N1-C1'	5.36	124.14	117.70
1	X	1292	A	N7-C8-N9	-5.36	111.12	113.80
1	X	699	G	C6-C5-N7	-5.35	127.19	130.40
1	X	796	A	C5-C6-N1	-5.34	115.03	117.70
1	X	1683	G	C8-N9-C1'	5.34	133.94	127.00
1	X	1182	U	P-O3'-C3'	5.33	126.10	119.70
2	Y	39	C	C2-N1-C1'	5.33	124.67	118.80
1	X	343	A	C6-C5-N7	-5.32	128.57	132.30
1	X	343	A	C4-N9-C1'	5.31	135.85	126.30
1	X	1923	U	P-O3'-C3'	5.31	126.07	119.70
1	X	2485	U	C5-C6-N1	5.30	125.35	122.70
27	1	19	GLY	N-CA-C	5.29	126.33	113.10
1	X	774	A	C6-C5-N7	5.29	136.00	132.30
1	X	2699	G	N1-C6-O6	5.29	123.07	119.90
1	X	343	A	N7-C8-N9	5.28	116.44	113.80
3	A	221	GLN	N-CA-C	5.28	125.27	111.00
1	X	2590	U	C2-N1-C1'	5.28	124.04	117.70
3	A	245	VAL	N-CA-C	5.27	125.24	111.00
1	X	2478	C	C6-N1-C2	-5.27	118.19	120.30
1	X	2655	C	C6-N1-C2	5.27	122.41	120.30
1	X	2481	G	C8-N9-C4	-5.26	104.29	106.40
1	X	2594	U	C2-N1-C1'	5.26	124.01	117.70
1	X	2018	G	O4'-C1'-N9	5.25	112.40	108.20
1	X	2287	G	P-O3'-C3'	5.24	125.99	119.70
1	X	2478	C	C5-C6-N1	5.22	123.61	121.00
1	X	2316	G	C8-N9-C1'	-5.22	120.22	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	955	G	N3-C4-N9	5.20	129.12	126.00
1	X	1683	G	N3-C4-N9	-5.19	122.89	126.00
1	X	742	G	C8-N9-C1'	-5.18	120.26	127.00
1	X	50	G	P-O3'-C3'	5.17	125.91	119.70
1	X	2018	G	N7-C8-N9	5.16	115.68	113.10
1	X	923	A	O4'-C1'-N9	5.15	112.32	108.20
1	X	1291	G	C8-N9-C4	5.15	108.46	106.40
1	X	2019	C	C6-N1-C2	-5.15	118.24	120.30
1	X	2541	U	N3-C2-O2	-5.14	118.60	122.20
1	X	2809	A	C6-C5-N7	-5.14	128.70	132.30
1	X	774	A	C4-C5-N7	-5.14	108.13	110.70
1	X	928	G	C6-C5-N7	-5.13	127.32	130.40
1	X	2795	A	P-O3'-C3'	5.11	125.83	119.70
2	Y	29	C	C6-N1-C2	-5.11	118.26	120.30
1	X	542	A	C5-N7-C8	-5.10	101.35	103.90
1	X	2655	C	C5-C6-N1	-5.10	118.45	121.00
1	X	1223	G	C8-N9-C1'	-5.08	120.39	127.00
1	X	746	G	C4-C5-C6	5.08	121.85	118.80
1	X	689	A	N1-C6-N6	5.06	121.64	118.60
1	X	343	A	O4'-C1'-N9	5.06	112.25	108.20
1	X	2437	G	C8-N9-C4	-5.06	104.38	106.40
1	X	774	A	C5-C6-N1	5.05	120.23	117.70
1	X	2845	C	C6-N1-C2	-5.04	118.28	120.30
1	X	1407	G	C4-N9-C1'	5.03	133.04	126.50
1	X	2699	G	N3-C4-C5	5.02	131.11	128.60
1	X	774	A	N3-C4-C5	-5.01	123.29	126.80
1	X	2809	A	N1-C6-N6	5.01	121.61	118.60
1	X	742	G	N3-C4-N9	5.01	129.01	126.00
1	X	613	A	C2-N3-C4	5.01	113.11	110.60

There are no chirality outliers.

All (19) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
27	1	18	THR	Peptide
28	2	37	LYS	Peptide
29	3	39	ASP	Peptide
29	3	60	LEU	Peptide
29	3	61	MET	Peptide
6	D	81	GLN	Peptide
6	D	83	MET	Peptide
9	G	107	GLN	Peptide

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Mol	Chain	Res	Type	Group
9	G	113	GLU	Peptide
11	I	38	LYS	Peptide
11	I	44	GLY	Peptide
14	L	59	LEU	Peptide
14	L	65	THR	Peptide
15	M	30	GLY	Peptide
21	S	90	GLU	Peptide
22	T	71	ASN	Peptide
23	U	32	ARG	Peptide
23	U	33	LYS	Peptide
23	U	55	GLY	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	X	58191	0	29325	964	0
2	Y	2561	0	1306	45	0
3	A	2085	0	2158	110	0
4	B	1539	0	1600	84	0
5	C	1489	0	1516	87	0
6	D	1367	0	1408	59	0
7	E	1286	0	1336	25	0
8	F	451	0	474	9	0
9	G	1114	0	1144	69	0
10	H	997	0	1046	34	0
11	I	982	0	1002	54	0
12	J	1060	0	1073	40	0
13	K	897	0	955	48	0
14	L	779	0	820	62	0
15	M	939	0	964	38	0
16	N	978	0	1020	55	0
17	O	759	0	774	38	0
18	P	1015	0	1094	47	0
19	Q	726	0	753	22	0
20	R	809	0	848	45	0
21	S	1370	0	1385	41	0
22	T	556	0	579	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	U	549	0	584	40	0
24	V	525	0	546	7	0
25	W	424	0	470	17	0
26	Z	444	0	440	28	0
27	1	427	0	445	33	0
28	2	383	0	414	21	0
29	3	453	0	488	37	0
30	X	95	0	0	2	0
31	3	1	0	0	0	0
31	A	1	0	0	0	0
31	J	1	0	0	0	0
31	K	1	0	0	0	0
31	M	1	0	0	0	0
31	N	1	0	0	0	0
31	T	1	0	0	0	0
31	X	420	0	0	0	0
31	Y	19	0	0	0	0
32	X	40	0	70	15	0
33	X	30	0	57	7	0
All	All	85766	0	56094	1897	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 14.

All (1897) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1277:G:OP1	26:Z:19:ARG:NH2	1.99	0.95
1:X:1669:A:OP2	13:K:9:LYS:NZ	2.00	0.95
1:X:2757:G:H5"	1:X:2758:A:H5'	1.49	0.94
1:X:2015:G:N7	32:X:3316:MPD:O4	2.00	0.93
10:H:28:GLY:HA2	10:H:50:ILE:HD11	1.52	0.91
18:P:28:ALA:HB2	18:P:71:VAL:HG21	1.52	0.90
1:X:1976:U:H4'	4:B:128:SER:HB3	1.54	0.89
1:X:1283:C:H5"	1:X:1284:G:H5'	1.57	0.87
3:A:217:ARG:HG2	3:A:219:PRO:HD3	1.56	0.86
1:X:1264:C:H5"	16:N:13:ARG:HH12	1.41	0.85
1:X:278:G:H1	1:X:380:C:H42	1.25	0.84
1:X:477:A:H4'	28:2:30:ILE:HD13	1.60	0.83
1:X:699:G:H1	28:2:12:ARG:HD3	1.44	0.83
3:A:53:PHE:HB3	3:A:218:LYS:HA	1.62	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:116:LYS:HZ2	5:C:117:LEU:H	1.27	0.82
4:B:174:GLU:HB3	4:B:183:LEU:HD12	1.62	0.82
16:N:5:LYS:HG3	16:N:7:GLY:H	1.45	0.82
1:X:1075:C:H42	1:X:1085:G:H1	1.26	0.81
1:X:1373:G:H22	1:X:2192:U:H3	1.28	0.81
1:X:1322:G:H4'	28:2:7:PRO:HB2	1.63	0.81
1:X:2757:G:OP2	1:X:2761:A:O2'	1.98	0.80
3:A:17:THR:HB	3:A:205:VAL:H	1.46	0.80
1:X:251:C:H3'	1:X:252:G:H5"	1.64	0.79
1:X:459:A:H2'	32:X:3315:MPD:H13	1.62	0.79
10:H:17:ARG:H	10:H:58:ALA:HA	1.46	0.79
15:M:57:ILE:HD12	15:M:103:LYS:HE3	1.64	0.79
1:X:2379:G:H4'	27:1:20:PHE:HB2	1.64	0.79
7:E:86:ASN:HB2	7:E:165:VAL:HG22	1.64	0.79
24:V:26:MET:HA	24:V:29:ARG:HE	1.48	0.79
1:X:2659:C:H5'	4:B:189:PRO:HA	1.65	0.78
10:H:75:VAL:HG12	10:H:118:LEU:HD21	1.66	0.78
9:G:110:LEU:O	9:G:112:THR:OG1	2.01	0.78
1:X:215:G:H21	1:X:632:A:H8	1.31	0.77
1:X:1429:A:N7	1:X:1600:U:O2'	2.15	0.77
29:3:39:ASP:O	29:3:41:ILE:N	2.11	0.77
1:X:2795:A:H4'	13:K:3:HIS:HD2	1.49	0.77
1:X:220:U:H5'	29:3:62:LEU:HD22	1.67	0.77
6:D:116:GLY:HA3	6:D:176:PRO:HB2	1.65	0.77
23:U:11:LYS:H	23:U:11:LYS:HD3	1.50	0.77
1:X:349:G:OP1	20:R:13:LYS:NZ	2.17	0.76
1:X:1668:G:OP2	13:K:40:LYS:NZ	2.18	0.76
25:W:25:LEU:HD22	25:W:30:ASP:HB3	1.66	0.76
1:X:1791:C:OP1	3:A:261:ARG:NH1	2.19	0.76
5:C:124:ASP:HB2	5:C:136:TRP:HD1	1.51	0.76
9:G:67:ARG:HD3	9:G:70:PHE:HA	1.67	0.75
1:X:2672:U:H2'	1:X:2673:G:H8	1.51	0.75
1:X:1623:C:N4	1:X:1638:G:OP2	2.20	0.75
26:Z:45:ILE:HG22	26:Z:52:TYR:HB2	1.69	0.75
1:X:2795:A:H4'	13:K:3:HIS:CD2	2.21	0.75
1:X:2264:C:OP2	27:1:28:ARG:NH1	2.21	0.74
1:X:640:C:O2	1:X:650:U:O2'	2.03	0.74
1:X:2362:G:N2	1:X:2363:G:N3	2.36	0.74
1:X:339:U:H3	1:X:343:A:H2	1.33	0.74
1:X:2795:A:N1	15:M:2:GLN:N	2.36	0.74
9:G:99:VAL:HA	9:G:115:ALA:HB1	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:U:19:ILE:HG22	23:U:42:GLN:HG3	1.69	0.74
25:W:45:LYS:HD3	25:W:48:LYS:HD3	1.69	0.74
1:X:833:A:N3	1:X:954:U:O2'	2.20	0.74
1:X:538:A:O2'	1:X:539:A:O5'	2.04	0.73
1:X:2264:C:OP2	27:1:30:ASN:ND2	2.21	0.73
3:A:55:GLY:H	3:A:217:ARG:HB3	1.54	0.73
28:2:38:GLY:C	28:2:40:HIS:H	1.90	0.73
3:A:28:ARG:HE	3:A:29:PRO:HD2	1.52	0.73
11:I:102:LYS:O	11:I:103:ASN:ND2	2.21	0.73
16:N:88:ILE:HG23	17:O:49:GLU:HB2	1.68	0.73
1:X:1963:G:O2'	1:X:1965:U:OP2	2.05	0.73
14:L:11:LEU:HD23	14:L:14:ARG:HH12	1.53	0.73
27:1:18:THR:HA	27:1:20:PHE:H	1.53	0.73
1:X:2809:A:H8	1:X:2858:A:H62	1.37	0.73
21:S:47:SER:OG	21:S:48:THR:N	2.19	0.73
1:X:263:G:N2	1:X:264:U:O4	2.21	0.73
1:X:2450:A:N3	30:X:2901:6NO:O30	2.22	0.73
9:G:32:TYR:HB3	16:N:64:ARG:HH22	1.53	0.72
11:I:66:ASN:HB2	29:3:11:LYS:HE3	1.71	0.72
1:X:1342:U:H5"	1:X:1343:C:H5	1.55	0.72
1:X:2336:G:N2	1:X:2339:A:OP2	2.23	0.72
1:X:1030:U:H3	1:X:1153:A:H62	1.35	0.72
21:S:67:LYS:HD2	21:S:84:TYR:HB2	1.72	0.72
27:1:18:THR:HA	27:1:20:PHE:N	2.04	0.72
2:Y:30:C:OP1	14:L:37:HIS:NE2	2.22	0.71
21:S:104:SER:HA	21:S:139:THR:HA	1.72	0.71
1:X:387:A:HO2'	1:X:388:G:P	2.14	0.71
1:X:793:G:H21	1:X:796:A:H62	1.38	0.71
1:X:1202:U:H2'	1:X:1203:A:H8	1.55	0.71
1:X:1811:A:H3'	3:A:178:PRO:HB2	1.72	0.71
1:X:2038:C:N3	32:X:3316:MPD:H13	2.05	0.71
1:X:1562:G:H5'	1:X:1563:U:H5'	1.73	0.71
19:Q:10:PRO:HA	19:Q:27:PHE:HB3	1.73	0.71
23:U:47:HIS:O	23:U:48:LYS:NZ	2.15	0.71
15:M:29:PRO:O	15:M:96:ARG:NH2	2.22	0.71
18:P:9:ARG:HG3	18:P:13:GLN:HG3	1.72	0.71
25:W:23:LEU:HD21	25:W:43:MET:HB3	1.71	0.71
13:K:102:THR:HA	13:K:109:THR:HA	1.70	0.71
20:R:63:THR:O	20:R:66:GLN:NE2	2.24	0.71
4:B:183:LEU:HD21	15:M:16:ILE:HG12	1.73	0.71
20:R:55:THR:HG21	20:R:72:ARG:HD3	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:653:G:H21	1:X:656:U:H5	1.37	0.71
2:Y:51:G:H2'	2:Y:52:G:H8	1.56	0.71
11:I:86:THR:HG21	11:I:116:ARG:HB3	1.72	0.71
26:Z:36:CYS:SG	26:Z:49:CYS:N	2.63	0.71
14:L:16:LYS:NZ	14:L:90:ASP:OD2	2.24	0.70
27:1:14:SER:OG	27:1:23:THR:N	2.24	0.70
1:X:507:A:OP2	18:P:19:LYS:NZ	2.19	0.70
1:X:2417:U:O2'	1:X:2419:C:OP1	2.09	0.70
9:G:84:ASN:O	9:G:86:ALA:N	2.18	0.70
1:X:403:A:H4'	1:X:404:A:H5'	1.73	0.70
1:X:2083:G:H1	1:X:2172:U:H3	1.39	0.70
3:A:41:GLY:O	3:A:43:ARG:NH1	2.25	0.70
1:X:1073:G:H1	1:X:1087:C:H42	1.38	0.70
21:S:25:ASN:ND2	21:S:28:ASN:OD1	2.24	0.70
1:X:1584:G:H5"	3:A:61:LEU:HG	1.72	0.70
2:Y:3:A:H61	2:Y:122:U:H3	1.37	0.70
1:X:2526:U:O2	10:H:23:ARG:NH1	2.25	0.69
14:L:82:LYS:HB3	14:L:84:ILE:HD12	1.72	0.69
10:H:120:ASP:OD1	10:H:120:ASP:N	2.20	0.69
5:C:3:GLN:HB3	5:C:13:ARG:HG3	1.75	0.69
17:O:3:ALA:HB3	17:O:13:ARG:HB2	1.73	0.69
1:X:1882:G:H21	1:X:1885:C:N4	1.91	0.69
7:E:127:GLU:HB2	7:E:130:ARG:HB3	1.74	0.69
13:K:24:GLN:HB3	13:K:44:LEU:HD22	1.73	0.69
1:X:517:A:H5"	1:X:518:A:H5'	1.75	0.69
6:D:172:SER:OG	6:D:173:MET:SD	2.49	0.69
1:X:224:G:OP2	1:X:226:C:N4	2.23	0.69
1:X:1377:G:N7	23:U:6:TYR:N	2.41	0.69
1:X:673:G:N2	11:I:21:ARG:O	2.26	0.69
1:X:1222:G:O2'	1:X:1250:A:N6	2.26	0.69
3:A:34:THR:OG1	3:A:35:GLU:N	2.23	0.69
1:X:1561:A:O2'	1:X:1562:G:O4'	2.11	0.69
1:X:1831:G:H2'	1:X:1832:G:H8	1.58	0.68
4:B:143:GLN:NE2	4:B:151:TYR:OH	2.26	0.68
1:X:757:U:OP1	4:B:132:LYS:NZ	2.19	0.68
1:X:2622:G:OP2	33:X:3321:SPD:N1	2.25	0.68
3:A:13:ARG:HA	3:A:16:MET:HB3	1.74	0.68
4:B:111:LYS:HD2	13:K:3:HIS:CE1	2.29	0.68
11:I:91:ASP:HA	11:I:121:HIS:HB2	1.75	0.68
18:P:97:VAL:HG22	18:P:124:ILE:HG23	1.74	0.68
1:X:1769:U:H2'	1:X:1775:A:H62	1.57	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1469:U:H1'	13:K:60:LEU:HD13	1.75	0.68
1:X:1582:A:OP1	3:A:211:ARG:NH1	2.25	0.68
6:D:14:PRO:HA	6:D:17:MET:HB3	1.75	0.68
17:O:23:GLU:HG2	17:O:91:THR:HG21	1.75	0.68
1:X:318:G:N2	1:X:321:A:OP2	2.25	0.68
1:X:1673:C:H5"	4:B:136:ARG:HG2	1.76	0.68
9:G:31:THR:HG22	16:N:61:TRP:CH2	2.29	0.68
1:X:168:A:H2'	1:X:169:C:C6	2.29	0.68
1:X:337:G:HO2'	20:R:9:HIS:HD1	1.41	0.68
1:X:1478:U:H2'	1:X:1479:G:C8	2.29	0.68
20:R:96:LYS:HB3	20:R:98:ILE:HG12	1.76	0.68
1:X:1673:C:H2'	1:X:1674:C:H6	1.57	0.68
1:X:1806:G:OP1	3:A:43:ARG:NH1	2.26	0.68
5:C:162:ARG:O	5:C:162:ARG:NE	2.25	0.68
15:M:29:PRO:HA	15:M:54:VAL:HG13	1.76	0.68
1:X:865:A:H5'	25:W:42:GLY:HA3	1.75	0.67
7:E:11:VAL:HG21	7:E:50:LEU:HD13	1.75	0.67
3:A:244:ARG:O	3:A:252:LYS:NZ	2.21	0.67
4:B:52:ALA:O	4:B:76:ARG:N	2.21	0.67
24:V:50:VAL:O	24:V:54:ASN:ND2	2.28	0.67
1:X:469:G:H2'	28:2:38:GLY:HA2	1.76	0.67
1:X:2551:A:H5"	1:X:2553:G:H4'	1.77	0.67
3:A:210:GLY:HA2	3:A:213:ARG:HB2	1.77	0.67
29:3:16:ILE:N	29:3:64:ARG:O	2.28	0.67
1:X:1004:A:OP1	16:N:50:ARG:NH1	2.28	0.66
1:X:1116:U:H2'	1:X:1117:G:H8	1.60	0.66
1:X:2485:U:OP1	4:B:144:ARG:NH2	2.28	0.66
9:G:41:TRP:HB2	9:G:164:GLN:HB2	1.76	0.66
23:U:70:LEU:HD12	23:U:79:GLU:HA	1.77	0.66
1:X:1849:G:O6	1:X:1850:G:N2	2.28	0.66
13:K:33:ARG:HG3	13:K:114:GLU:HB3	1.76	0.66
1:X:623:G:O2'	1:X:626:A:N6	2.24	0.66
1:X:2528:G:H2'	1:X:2529:G:H8	1.61	0.66
1:X:1856:U:OP1	1:X:2389:G:O2'	2.13	0.66
29:3:6:THR:HG23	29:3:8:LYS:H	1.61	0.66
1:X:787:A:H2	1:X:800:U:HO2'	1.42	0.66
1:X:1856:U:H3	1:X:1861:G:H1	1.44	0.66
1:X:2598:C:OP1	4:B:152:LYS:NZ	2.19	0.66
21:S:49:THR:HB	21:S:132:GLN:HA	1.77	0.66
1:X:2237:C:O2'	1:X:2406:C:OP2	2.14	0.66
11:I:133:VAL:HG11	11:I:140:VAL:HG23	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:T:64:ASP:OD1	22:T:64:ASP:N	2.28	0.66
1:X:1718[A]:A:H8	1:X:1718[A]:A:OP2	1.78	0.66
20:R:48:VAL:HG13	20:R:50:GLY:H	1.60	0.66
3:A:34:THR:HA	3:A:63:ARG:HA	1.77	0.66
10:H:47:VAL:HG23	10:H:77:THR:HG23	1.78	0.66
19:Q:14:GLU:O	19:Q:18:SER:OG	2.12	0.66
1:X:494:A:O2'	20:R:68:GLY:N	2.23	0.66
13:K:9:LYS:HD2	13:K:11:ASN:H	1.60	0.66
1:X:2781:G:O2'	1:X:2782:G:N2	2.28	0.65
3:A:32:ALA:HB1	3:A:35:GLU:HG2	1.79	0.65
1:X:1264:C:OP1	16:N:13:ARG:NH1	2.29	0.65
22:T:42:GLY:O	22:T:57:HIS:ND1	2.29	0.65
29:3:58:MET:SD	29:3:58:MET:N	2.58	0.65
21:S:70:GLN:HB3	21:S:80:HIS:HB3	1.78	0.65
12:J:61:ARG:HD2	21:S:175:ARG:HH21	1.62	0.65
24:V:62:ARG:O	24:V:66:GLN:N	2.30	0.65
25:W:46:THR:HG22	25:W:47:VAL:HG13	1.77	0.65
1:X:2264:C:H41	27:1:26:LYS:HD2	1.61	0.65
1:X:797:A:C5	3:A:229:VAL:HG21	2.32	0.65
5:C:163:ASN:H	5:C:167:VAL:HB	1.62	0.65
9:G:99:VAL:HA	9:G:115:ALA:CB	2.26	0.65
12:J:28:VAL:HG11	12:J:135:ARG:HG2	1.78	0.65
12:J:82:THR:HG23	12:J:84:MET:H	1.62	0.65
21:S:25:ASN:HD22	21:S:27:GLU:HB2	1.60	0.65
1:X:2225:G:H2'	1:X:2226:A:H8	1.61	0.64
3:A:223:GLY:HA2	3:A:226:MET:HG3	1.79	0.64
1:X:657:A:N3	1:X:2329:C:O2'	2.31	0.64
1:X:833:A:H1'	1:X:954:U:H1'	1.80	0.64
1:X:2034:A:OP1	4:B:137:ARG:HD2	1.96	0.64
7:E:44:ARG:HH22	7:E:46:ASP:HB2	1.62	0.64
1:X:627:A:H2'	1:X:628:A:C8	2.32	0.64
1:X:1276:U:OP1	26:Z:16:ARG:NH1	2.30	0.64
14:L:68:ALA:HA	14:L:71:VAL:HG13	1.80	0.64
27:1:15:SER:HB3	27:1:51:ARG:O	1.97	0.64
3:A:244:ARG:HB2	3:A:246:PRO:HD3	1.80	0.64
20:R:46:VAL:N	20:R:76:LEU:O	2.26	0.64
9:G:114:THR:HA	9:G:116:ARG:HE	1.61	0.64
19:Q:48:VAL:HG21	19:Q:82:LEU:HD13	1.80	0.64
1:X:2369:U:OP2	27:1:2:ALA:N	2.31	0.64
1:X:2371:A:H2	1:X:2403:C:H42	1.46	0.64
1:X:2371:A:OP2	29:3:32:GLN:NE2	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:136:TRP:O	5:C:140:ASN:ND2	2.28	0.64
11:I:108:LEU:HD22	11:I:120:VAL:HG11	1.80	0.64
4:B:134:TRP:H	4:B:134:TRP:HD1	1.44	0.63
10:H:97:VAL:HG11	10:H:126:ILE:HD11	1.79	0.63
27:1:30:ASN:N	27:1:30:ASN:OD1	2.31	0.63
1:X:2285:U:H5'	1:X:2286:G:C8	2.33	0.63
1:X:2287:G:O2'	1:X:2288:A:O5'	2.15	0.63
29:3:30:ARG:HG3	29:3:31:HIS:H	1.62	0.63
1:X:1093:U:H4'	8:F:117:ALA:HA	1.81	0.63
1:X:2211:U:OP1	23:U:43:ARG:NH1	2.31	0.63
1:X:2283:G:N2	1:X:2284:U:O4	2.32	0.63
1:X:684:C:H41	11:I:43:ALA:HB1	1.62	0.63
1:X:812:G:H3'	1:X:813:A:H2'	1.79	0.63
9:G:31:THR:HG22	16:N:61:TRP:HH2	1.63	0.63
13:K:9:LYS:HE3	13:K:10:LEU:H	1.64	0.63
1:X:2796:A:H2'	1:X:2797:G:H8	1.63	0.63
9:G:69:ASP:OD1	9:G:69:ASP:N	2.31	0.63
12:J:54:VAL:HG21	12:J:125:LYS:HD3	1.80	0.63
28:2:41:GLN:OE1	28:2:41:GLN:N	2.31	0.63
5:C:5:ASN:N	5:C:5:ASN:OD1	2.31	0.63
1:X:517:A:C5'	1:X:518:A:H5'	2.29	0.63
15:M:39:VAL:HG12	15:M:45:THR:HG23	1.80	0.63
27:1:9:ILE:HA	27:1:28:ARG:HA	1.79	0.63
1:X:646:C:O2'	1:X:650:U:OP1	2.16	0.63
1:X:2262:C:OP1	27:1:7:ARG:NH2	2.32	0.63
5:C:152:THR:OG1	5:C:153:ASP:N	2.32	0.63
9:G:31:THR:OG1	9:G:32:TYR:N	2.31	0.63
16:N:66:ASN:HD22	16:N:70:ARG:HH22	1.45	0.63
10:H:10:VAL:HG22	10:H:19:ILE:HG22	1.80	0.62
17:O:36:LYS:HD2	17:O:54:TYR:HB2	1.81	0.62
1:X:837:U:H2'	1:X:838:A:C8	2.35	0.62
1:X:1313:U:H4'	1:X:1314:A:H5'	1.81	0.62
1:X:1382:G:O4'	1:X:1799:A:N6	2.31	0.62
2:Y:21:C:H42	2:Y:66:G:H1	1.47	0.62
3:A:53:PHE:CZ	3:A:220:HIS:HA	2.35	0.62
12:J:15:ARG:HB2	12:J:15:ARG:HH11	1.65	0.62
1:X:1675:C:OP1	4:B:134:TRP:NE1	2.32	0.62
1:X:2281:C:H42	1:X:2293:G:H1	1.46	0.62
1:X:2796:A:OP2	4:B:111:LYS:NZ	2.32	0.62
5:C:45:THR:OG1	5:C:86:PRO:O	2.16	0.62
14:L:12:ARG:NH1	14:L:91:ARG:O	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:U:14:VAL:HG23	23:U:15:VAL:HG23	1.81	0.62
6:D:37:ASN:ND2	6:D:87:ILE:O	2.30	0.62
6:D:122:PHE:HD2	6:D:129:ASN:H	1.47	0.62
7:E:41:LEU:HD12	7:E:55:PRO:HD3	1.82	0.62
17:O:27:GLY:HA3	17:O:30:GLY:HA3	1.81	0.62
1:X:387:A:O2'	1:X:388:G:O5'	2.12	0.62
1:X:746:G:N7	1:X:774:A:C6	2.67	0.62
1:X:2636:A:O3'	7:E:160:LYS:NZ	2.32	0.62
1:X:2713:A:H61	4:B:203:LYS:HE3	1.65	0.62
3:A:213:ARG:HD2	3:A:217:ARG:HG3	1.82	0.62
5:C:56:ARG:HG2	5:C:57:LYS:H	1.65	0.62
1:X:2311:U:O2'	1:X:2315:A:N7	2.33	0.62
1:X:854:G:H1	1:X:948:C:H42	1.47	0.62
8:F:75:SER:HA	8:F:78:ILE:HB	1.81	0.62
12:J:26:ASP:HB2	12:J:68:ARG:HH22	1.65	0.62
1:X:1225:G:H2'	1:X:1249:G:N2	2.14	0.62
1:X:2286:G:H1	6:D:39:GLY:HA3	1.65	0.62
1:X:1787:U:H2'	1:X:1788:C:C6	2.35	0.61
3:A:12:SER:OG	3:A:13:ARG:N	2.32	0.61
6:D:103:LEU:HD12	6:D:107:GLY:HA3	1.81	0.61
21:S:24:TYR:HB3	21:S:29:ASN:HB3	1.80	0.61
26:Z:30:LEU:HD22	26:Z:39:LYS:HB3	1.82	0.61
1:X:387:A:O2'	1:X:388:G:H8	1.83	0.61
13:K:60:LEU:HD11	13:K:64:ARG:HE	1.64	0.61
16:N:91:ASN:HB3	16:N:95:LEU:HD13	1.82	0.61
1:X:580:A:H4'	1:X:581:A:OP1	2.00	0.61
1:X:1919:A:H62	1:X:1946:U:H3	1.48	0.61
4:B:143:GLN:N	4:B:143:GLN:OE1	2.33	0.61
14:L:97:HIS:CG	14:L:98:GLY:N	2.68	0.61
12:J:49:GLU:OE2	12:J:52:ARG:NH2	2.34	0.61
13:K:8:ARG:HD3	13:K:43:GLU:HG2	1.82	0.61
1:X:50:G:H4'	1:X:51:A:O5'	2.00	0.61
4:B:5:LEU:HD13	4:B:51:TYR:HB2	1.81	0.61
1:X:222:G:OP2	11:I:66:ASN:ND2	2.33	0.61
1:X:2085:G:N1	1:X:2171:U:O2	2.34	0.61
1:X:2824:C:P	15:M:100:ARG:HH11	2.24	0.61
1:X:2295:C:O2'	6:D:125:ARG:NH2	2.33	0.61
1:X:661:C:N3	1:X:662:G:N1	2.48	0.61
22:T:51:VAL:HG21	22:T:79:ILE:HG22	1.83	0.61
1:X:1954:A:O2'	1:X:1955:G:OP1	2.16	0.61
1:X:2796:A:H2'	1:X:2797:G:C8	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:251:GLY:C	3:A:255:LYS:HZ1	2.04	0.61
1:X:1007:A:H1'	17:O:6:GLN:HG3	1.83	0.61
1:X:1704:G:H21	1:X:1718[B]:A:H2	1.48	0.61
1:X:1975:G:N2	1:X:1979:C:O2'	2.34	0.60
5:C:147:LYS:HA	5:C:166:TRP:HB2	1.81	0.60
3:A:70:ARG:HH21	3:A:150:GLY:H	1.47	0.60
14:L:54:ALA:HB2	14:L:75:LEU:HB2	1.84	0.60
1:X:954:U:OP2	11:I:38:LYS:NZ	2.16	0.60
1:X:1624:A:H1'	1:X:1626:A:OP2	2.01	0.60
4:B:9:ILE:O	15:M:9:ARG:NH1	2.34	0.60
22:T:23:VAL:HG13	22:T:38:VAL:HG23	1.83	0.60
1:X:755:C:H2'	1:X:756:C:H6	1.66	0.60
1:X:2662:C:O2	10:H:82:LYS:NZ	2.34	0.60
20:R:61:SER:OG	20:R:64:ASN:O	2.18	0.60
1:X:135:U:H2'	1:X:136:A:C8	2.37	0.60
1:X:1073:G:H1	1:X:1087:C:N4	1.99	0.60
3:A:134:ARG:HB3	3:A:187:SER:HB2	1.81	0.60
20:R:28:LYS:HG2	20:R:29:HIS:HD2	1.66	0.60
1:X:590:C:H2'	1:X:591:G:H8	1.66	0.60
1:X:2035:G:H4'	4:B:143:GLN:O	2.01	0.60
1:X:478:G:OP1	28:2:33:ARG:HD2	2.01	0.60
1:X:1264:C:H5"	16:N:13:ARG:NH1	2.15	0.60
1:X:2352:A:H2'	1:X:2353:G:C8	2.37	0.60
4:B:14:ILE:HG12	15:M:20:HIS:CD2	2.36	0.60
14:L:8:ARG:HG3	14:L:9:ARG:H	1.66	0.60
1:X:2001:G:OP1	26:Z:9:LYS:NZ	2.23	0.60
6:D:62:LEU:O	6:D:95:ARG:NH1	2.35	0.60
1:X:4:C:H42	1:X:2873:G:H1	1.48	0.60
1:X:29:U:H5	32:X:3315:MPD:H51	1.67	0.60
1:X:48:A:H61	1:X:154:U:H2'	1.66	0.60
1:X:687:G:H5"	5:C:70:GLY:H	1.67	0.60
1:X:1636:G:O4'	28:2:1:MET:N	2.34	0.59
1:X:1212:U:H2'	1:X:1213:U:C6	2.37	0.59
1:X:1225:G:H2'	1:X:1249:G:H22	1.66	0.59
1:X:1329:U:H2'	1:X:1330:G:H8	1.67	0.59
1:X:1643:A:H61	1:X:1656:U:H3	1.50	0.59
1:X:2265:A:H4'	1:X:2266:A:O4'	2.01	0.59
1:X:1679:U:H1'	1:X:2666:U:H5'	1.84	0.59
1:X:2623:A:H62	33:X:3321:SPD:H22	1.67	0.59
12:J:19:THR:HG21	12:J:40:PRO:HB3	1.85	0.59
14:L:26:ARG:HE	14:L:86:GLN:HB3	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:674:U:H1'	11:I:22:GLY:HA3	1.84	0.59
10:H:13:ASN:ND2	10:H:108:THR:OG1	2.35	0.59
16:N:37:GLN:HA	16:N:40:LEU:HD23	1.84	0.59
1:X:1478:U:H2'	1:X:1479:G:H8	1.67	0.59
4:B:38:THR:HG22	4:B:40:GLN:H	1.66	0.59
5:C:45:THR:HG21	5:C:85:GLY:HA3	1.85	0.59
1:X:1816:G:OP1	3:A:52:ARG:HD3	2.01	0.59
4:B:126:PRO:HG2	4:B:131:SER:HB2	1.83	0.59
9:G:102:ARG:O	9:G:103:TYR:HB2	2.02	0.59
29:3:29:LYS:HD3	29:3:34:THR:HA	1.83	0.59
1:X:1000:G:H5"	25:W:10:ILE:HD11	1.82	0.59
1:X:1675:C:OP1	4:B:134:TRP:CE2	2.56	0.59
1:X:968:C:H5'	12:J:77:LYS:HD2	1.84	0.59
1:X:1288:A:OP2	1:X:1663:C:N4	2.35	0.59
14:L:55:SER:HB3	14:L:57:ALA:H	1.66	0.59
14:L:65:THR:HA	14:L:67:THR:HG23	1.84	0.59
21:S:19:ILE:HD11	21:S:36:ARG:HD3	1.85	0.59
1:X:226:C:OP2	1:X:2373:C:O2'	2.20	0.59
1:X:313:U:H2'	1:X:314:G:H8	1.67	0.59
1:X:2374:C:O2'	23:U:33:LYS:HD3	2.02	0.59
13:K:33:ARG:HH11	13:K:112:LEU:HD13	1.67	0.59
25:W:1:MET:N	25:W:34:VAL:O	2.36	0.59
1:X:163:A:H2'	1:X:164:G:C8	2.38	0.59
1:X:2594:U:C2	26:Z:7:PRO:HA	2.36	0.59
2:Y:9:G:H5'	14:L:32:TYR:CZ	2.38	0.59
4:B:108:SER:HB3	4:B:163:GLU:H	1.67	0.59
6:D:13:ARG:HG3	6:D:28:VAL:HG21	1.85	0.59
29:3:30:ARG:HG3	29:3:31:HIS:N	2.18	0.59
1:X:2253:A:H5'	1:X:2254:C:OP2	2.03	0.58
1:X:1437:A:H2'	1:X:1438:G:H8	1.68	0.58
1:X:1509:A:N3	1:X:2189:A:O2'	2.35	0.58
1:X:655:A:H2'	1:X:656:U:H5'	1.85	0.58
1:X:872:G:O2'	1:X:928:G:O6	2.20	0.58
4:B:50:GLY:HA3	4:B:75:THR:HG21	1.84	0.58
1:X:2311:U:H4'	1:X:2315:A:H62	1.67	0.58
1:X:2674:C:H2'	1:X:2675:U:C6	2.38	0.58
7:E:25:LYS:HG3	7:E:34:THR:HG22	1.86	0.58
1:X:5:A:H2'	1:X:6:A:C8	2.39	0.58
1:X:317:U:O2'	1:X:1224:A:N7	2.37	0.58
1:X:504:G:H4'	18:P:27:VAL:HG13	1.85	0.58
26:Z:53:ASP:OD1	26:Z:53:ASP:N	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:692:C:H2'	1:X:693:A:H8	1.69	0.58
1:X:841:G:H2'	1:X:842:A:C8	2.39	0.58
1:X:1067:G:H4'	1:X:1097:A:H8	1.69	0.58
1:X:2408:G:O6	11:I:59:ARG:NH2	2.30	0.58
6:D:171:GLN:O	6:D:172:SER:OG	2.22	0.58
14:L:37:HIS:ND1	14:L:37:HIS:O	2.32	0.58
21:S:95:SER:HB3	21:S:119:ASN:HB3	1.86	0.58
6:D:63:GLN:HE21	6:D:89:VAL:HG12	1.68	0.58
11:I:62:LYS:HB3	29:3:12:ARG:HA	1.86	0.58
16:N:66:ASN:HB3	16:N:76:TYR:HB2	1.86	0.58
1:X:1673:C:H2'	1:X:1674:C:C6	2.39	0.58
14:L:28:ARG:HG3	14:L:90:ASP:HB2	1.85	0.58
23:U:47:HIS:CG	23:U:48:LYS:H	2.21	0.58
1:X:7:G:H2'	1:X:8:A:H8	1.68	0.58
1:X:1281:A:H2'	1:X:1282:A:O4'	2.03	0.58
1:X:1296:G:H22	1:X:1299:A:H5'	1.69	0.58
1:X:1919:A:H2	1:X:1926:U:N3	2.01	0.58
1:X:2229:G:C6	12:J:83:ARG:HG2	2.38	0.58
1:X:2522:G:H2'	1:X:2523:G:C8	2.38	0.58
4:B:111:LYS:HD2	13:K:3:HIS:NE2	2.19	0.58
5:C:95:LEU:O	5:C:100:ARG:NH2	2.37	0.58
27:1:32:GLN:HB3	27:1:34:LYS:HG2	1.86	0.58
1:X:73:A:H5"	1:X:74:G:O4'	2.04	0.57
1:X:859:U:HO2'	1:X:860:U:P	2.25	0.57
4:B:55:ALA:H	4:B:58:LYS:HE2	1.69	0.57
1:X:1099:A:N6	8:F:133:SER:OG	2.37	0.57
1:X:1465:G:H2'	1:X:1466:C:C6	2.39	0.57
1:X:1573:G:H3'	1:X:1574:A:H5"	1.86	0.57
1:X:2272:A:OP1	1:X:2356:A:N6	2.35	0.57
1:X:2668:U:OP2	1:X:2847:G:N2	2.36	0.57
1:X:154:U:H3'	1:X:155:G:H8	1.69	0.57
1:X:400:U:OP2	23:U:21:ARG:NH1	2.35	0.57
1:X:1297:A:H62	33:X:3322:SPD:H22	1.68	0.57
1:X:2570:C:OP1	3:A:239:ARG:HD2	2.05	0.57
1:X:2596:C:H2'	1:X:2597:G:H8	1.69	0.57
33:X:3320:SPD:H31	33:X:3320:SPD:H71	1.87	0.57
12:J:64:LYS:HB3	12:J:108:ALA:HB3	1.84	0.57
16:N:17:VAL:HG21	16:N:32:TYR:HE1	1.69	0.57
29:3:6:THR:HG23	29:3:8:LYS:N	2.18	0.57
1:X:754:G:H2'	1:X:755:C:C6	2.40	0.57
11:I:81:GLN:HB3	11:I:114:ILE:HG22	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:O:22:VAL:HA	17:O:91:THR:HG22	1.87	0.57
23:U:21:ARG:HH21	23:U:23:LYS:HG2	1.68	0.57
29:3:24:ALA:O	29:3:47:GLY:N	2.36	0.57
1:X:2640:G:H2'	1:X:2641:A:C8	2.40	0.57
1:X:2691:C:O2'	1:X:2693:U:H5'	2.05	0.57
23:U:49:LYS:HB2	23:U:61:TRP:CZ3	2.40	0.57
29:3:15:LYS:O	29:3:23:MET:N	2.33	0.57
1:X:859:U:O2'	1:X:860:U:O5'	2.18	0.57
1:X:876:A:H2	1:X:926:C:H41	1.53	0.57
1:X:1046:U:H5'	7:E:59:GLN:HG2	1.85	0.57
3:A:95:LEU:O	3:A:96:HIS:ND1	2.38	0.57
17:O:15:SER:HA	17:O:95:ILE:O	2.05	0.57
1:X:2639:A:H2'	1:X:2640:G:O4'	2.05	0.57
1:X:837:U:H2'	1:X:838:A:H8	1.69	0.57
10:H:25:LEU:HD11	10:H:52:VAL:HG23	1.87	0.57
1:X:339:U:H4'	20:R:77:HIS:CD2	2.40	0.56
1:X:1339:U:HO2'	1:X:1993:G:HO2'	1.50	0.56
11:I:13:ARG:HH21	11:I:14:LYS:HG3	1.69	0.56
16:N:79:PHE:HE1	16:N:110:VAL:HA	1.69	0.56
21:S:106:GLY:HA3	21:S:142:ASN:HA	1.88	0.56
23:U:11:LYS:HG2	23:U:12:ASN:H	1.70	0.56
1:X:492:G:H1'	1:X:516:G:N2	2.20	0.56
1:X:2319:G:H2'	1:X:2320:G:H8	1.70	0.56
16:N:50:ARG:HH12	17:O:71:ILE:HG13	1.69	0.56
18:P:132:GLY:O	18:P:134:LYS:NZ	2.38	0.56
1:X:1693:A:C2	1:X:1976:U:H5'	2.40	0.56
1:X:2272:A:O3'	14:L:95:LYS:NZ	2.36	0.56
1:X:2594:U:H5'	1:X:2595:C:OP2	2.06	0.56
1:X:2867:G:H4'	1:X:2868:G:O4'	2.06	0.56
7:E:17:VAL:HG22	7:E:26:VAL:HG22	1.87	0.56
14:L:29:LEU:HB3	14:L:89:PHE:HA	1.87	0.56
15:M:29:PRO:HB2	15:M:99:VAL:HG11	1.88	0.56
16:N:66:ASN:HB3	16:N:76:TYR:H	1.71	0.56
1:X:789:G:N2	1:X:806:A:O2'	2.38	0.56
1:X:1342:U:H5"	1:X:1343:C:C5	2.38	0.56
1:X:1542:G:H22	1:X:1562:G:H1	1.53	0.56
1:X:2043:A:O2'	1:X:2044:G:OP2	2.22	0.56
1:X:2736:U:H1'	1:X:2737:A:H5"	1.86	0.56
1:X:568:G:N2	16:N:49:ASP:OD1	2.39	0.56
1:X:1803:G:H21	3:A:46:ARG:HG3	1.70	0.56
1:X:2286:G:O6	6:D:150:ARG:NH2	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:4:ILE:HD13	4:B:28:ALA:HB1	1.86	0.56
17:O:4:ILE:HG22	17:O:5:ILE:H	1.69	0.56
1:X:1872:A:H2'	1:X:1873:A:C8	2.41	0.56
2:Y:32:C:H1'	2:Y:59:A:H61	1.68	0.56
23:U:21:ARG:HD3	23:U:23:LYS:HG2	1.88	0.56
1:X:495:C:H2'	1:X:496:C:H6	1.70	0.56
1:X:495:C:H2'	1:X:496:C:C6	2.41	0.56
1:X:1850:G:O2'	1:X:1867:A:N6	2.38	0.56
9:G:104:THR:HG22	9:G:106:TYR:H	1.71	0.56
16:N:98:ILE:HD12	16:N:98:ILE:H	1.69	0.56
27:1:18:THR:CA	27:1:20:PHE:H	2.19	0.56
1:X:469:G:H5'	28:2:39:ARG:HB3	1.88	0.56
1:X:2286:G:O2'	1:X:2287:G:N7	2.38	0.56
5:C:146:GLU:OE2	5:C:185:ARG:NH2	2.39	0.56
7:E:104:GLU:HA	7:E:114:ILE:HG22	1.88	0.56
15:M:32:THR:HA	15:M:92:THR:O	2.05	0.56
1:X:493:A:H4'	20:R:56:LYS:HG3	1.88	0.56
4:B:4:ILE:HG12	4:B:5:LEU:H	1.71	0.56
14:L:27:LEU:HD22	14:L:44:ASP:HA	1.88	0.56
1:X:339:U:N3	1:X:343:A:H2	2.03	0.56
1:X:1223:G:H5'	1:X:1225:G:O4'	2.04	0.56
1:X:1674:C:H2'	1:X:1675:C:C6	2.41	0.56
1:X:2621:G:OP1	9:G:104:THR:HG21	2.05	0.56
3:A:45:ASN:HD21	3:A:50:THR:HG23	1.70	0.56
17:O:66:GLY:O	17:O:87:ARG:NH2	2.28	0.56
9:G:67:ARG:HB2	9:G:70:PHE:HA	1.87	0.55
1:X:1256:C:O3'	11:I:16:ARG:NH2	2.39	0.55
1:X:1670:G:O6	13:K:9:LYS:HD3	2.06	0.55
1:X:1745:C:P	15:M:101:ARG:HH22	2.29	0.55
1:X:2285:U:H5'	1:X:2286:G:H8	1.69	0.55
1:X:2637:C:P	7:E:160:LYS:HZ1	2.29	0.55
2:Y:28:A:H2'	2:Y:28:A:OP2	2.06	0.55
10:H:109:ARG:HA	10:H:129:LEU:HD13	1.87	0.55
21:S:14:LEU:HD22	21:S:36:ARG:HH12	1.71	0.55
1:X:1370:U:H3'	1:X:1371:G:C8	2.40	0.55
3:A:91:ARG:HB2	3:A:107:ALA:HB3	1.88	0.55
9:G:93:LYS:HD3	9:G:93:LYS:H	1.72	0.55
18:P:39:ARG:HD3	18:P:97:VAL:HB	1.89	0.55
1:X:506:G:H4'	18:P:21:ARG:HH12	1.69	0.55
1:X:661:C:OP1	29:3:19:THR:OG1	2.22	0.55
1:X:1337:G:H4'	1:X:1632:A:N7	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1922:U:H5	1:X:1950:C:HO2'	1.55	0.55
12:J:48:ILE:HA	12:J:51:CYS:HB2	1.88	0.55
12:J:79:PRO:HD3	12:J:88:LYS:HD3	1.89	0.55
18:P:94:GLU:HG3	18:P:127:ILE:HB	1.88	0.55
29:3:36:LYS:HG3	29:3:37:SER:H	1.71	0.55
1:X:99:U:H3'	1:X:100:G:H5'	1.89	0.55
1:X:343:A:O2'	1:X:345:U:OP2	2.24	0.55
1:X:684:C:H41	11:I:43:ALA:CB	2.20	0.55
1:X:1774:A:H5'	1:X:2587:G:H4'	1.87	0.55
1:X:1827:G:H1'	1:X:1914:U:C2	2.41	0.55
1:X:2379:G:H4'	27:1:20:PHE:CB	2.35	0.55
1:X:2508:G:H5"	1:X:2509:A:H5"	1.88	0.55
30:X:2901:6NO:C44	30:X:2901:6NO:O37	2.54	0.55
12:J:28:VAL:HG21	12:J:135:ARG:HB3	1.89	0.55
1:X:692:C:H2'	1:X:693:A:C8	2.41	0.55
1:X:1718[A]:A:OP2	1:X:1718[A]:A:H2'	2.06	0.55
1:X:2024:U:OP1	9:G:102:ARG:NH2	2.39	0.55
2:Y:63:A:H2'	2:Y:64:C:C6	2.42	0.55
3:A:43:ARG:O	3:A:49:ILE:HA	2.06	0.55
13:K:75:VAL:O	13:K:79:VAL:HG13	2.07	0.55
1:X:711:C:O2'	1:X:747:A:N6	2.39	0.55
1:X:2225:G:H2'	1:X:2226:A:C8	2.40	0.55
13:K:12:ARG:HB2	13:K:16:ALA:HB3	1.88	0.55
16:N:83:LEU:HD13	16:N:113:SER:HB2	1.88	0.55
29:3:8:LYS:HA	29:3:8:LYS:NZ	2.22	0.55
5:C:22:VAL:HG12	5:C:23:ASN:H	1.72	0.55
16:N:24:PHE:O	16:N:29:SER:HB3	2.06	0.55
20:R:23:ILE:HG23	20:R:31:GLY:HA2	1.88	0.55
1:X:78:C:H2'	1:X:79:G:H8	1.72	0.55
1:X:1422:C:H2'	1:X:1423:A:C8	2.42	0.55
5:C:161:ALA:C	5:C:162:ARG:HG3	2.27	0.55
3:A:69:ARG:CZ	3:A:130:ALA:HB2	2.37	0.55
1:X:1982:C:O2	1:X:2666:U:O2'	2.22	0.54
27:1:9:ILE:HG13	27:1:10:VAL:N	2.21	0.54
1:X:2447:G:HO2'	1:X:2448:A:H8	1.55	0.54
1:X:2621:G:OP2	9:G:110:LEU:HD22	2.07	0.54
2:Y:64:C:H2'	2:Y:65:A:C8	2.42	0.54
5:C:153:ASP:HA	5:C:172:VAL:HG22	1.90	0.54
5:C:173:ALA:HA	5:C:175:VAL:HG12	1.89	0.54
18:P:57:LEU:HD13	18:P:69:ALA:HA	1.88	0.54
20:R:108:VAL:HG13	20:R:109:ALA:H	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1098:G:C8	1:X:1100:G:H1'	2.43	0.54
1:X:2629:U:H2'	1:X:2630:C:H6	1.71	0.54
6:D:117:ILE:HD12	6:D:117:ILE:H	1.72	0.54
16:N:47:TYR:HE2	17:O:73:LYS:HE2	1.72	0.54
17:O:2:PHE:HE1	17:O:40:VAL:HG11	1.72	0.54
23:U:51:ILE:HG23	23:U:52:ARG:H	1.73	0.54
24:V:20:ALA:HA	24:V:23:LYS:HD3	1.89	0.54
25:W:25:LEU:HD21	25:W:32:ARG:HG2	1.89	0.54
26:Z:36:CYS:SG	26:Z:48:ASN:HB2	2.47	0.54
1:X:413:G:N7	23:U:68:ARG:NH1	2.55	0.54
1:X:673:G:H21	11:I:21:ARG:HG2	1.73	0.54
1:X:757:U:P	4:B:132:LYS:HZ1	2.28	0.54
1:X:1448:A:H61	1:X:1574:A:H61	1.55	0.54
1:X:1451:C:H2'	1:X:1452:U:C6	2.42	0.54
1:X:2492:G:H2'	1:X:2493:U:C6	2.41	0.54
1:X:2812:A:H2'	1:X:2813:G:C8	2.42	0.54
11:I:76:LYS:HB3	11:I:79:GLN:HG2	1.90	0.54
13:K:28:LEU:HD23	13:K:48:VAL:HG11	1.90	0.54
1:X:687:G:H21	5:C:68:ARG:HH22	1.56	0.54
1:X:1071:U:P	8:F:74:MET:HB2	2.48	0.54
1:X:1287:A:N1	1:X:1661:C:O2'	2.33	0.54
3:A:121:PRO:HA	3:A:132:PRO:HD2	1.89	0.54
15:M:69:ARG:HB2	15:M:78:GLU:HG2	1.89	0.54
17:O:10:LYS:HG3	17:O:11:GLN:HG2	1.89	0.54
19:Q:7:LEU:HA	19:Q:29:VAL:HA	1.89	0.54
29:3:21:LYS:HA	29:3:50:LEU:HD21	1.89	0.54
1:X:590:C:H2'	1:X:591:G:C8	2.42	0.54
1:X:1070:G:H5"	1:X:1071:U:H2'	1.89	0.54
1:X:2043:A:H3'	5:C:62:LYS:NZ	2.23	0.54
11:I:79:GLN:HG3	11:I:98:LEU:HD11	1.88	0.54
23:U:11:LYS:HD2	23:U:66:ALA:HB2	1.90	0.54
27:1:13:GLU:HA	27:1:24:THR:HG22	1.89	0.54
1:X:547:U:OP1	1:X:1006:C:N4	2.39	0.54
4:B:144:ARG:CG	4:B:145:LYS:H	2.20	0.54
17:O:22:VAL:HG23	17:O:24:SER:H	1.73	0.54
1:X:1983:G:H5"	13:K:2:ARG:HH21	1.72	0.54
2:Y:46:G:N2	2:Y:50:U:O2	2.41	0.54
5:C:116:LYS:HZ2	5:C:117:LEU:N	2.03	0.54
6:D:60:ILE:HG13	6:D:61:THR:HG23	1.89	0.54
9:G:45:ASP:HB2	9:G:167:LYS:HZ1	1.73	0.54
13:K:49:GLU:O	13:K:52:ILE:HG12	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:P:31:VAL:HG21	18:P:124:ILE:HD11	1.90	0.54
1:X:78:C:H2'	1:X:79:G:C8	2.43	0.54
1:X:1454:U:H2'	1:X:1455:C:C6	2.43	0.54
1:X:2357:A:H4'	14:L:87:VAL:HG21	1.90	0.54
25:W:2:LYS:HB3	25:W:54:GLN:HB3	1.89	0.54
26:Z:14:SER:O	26:Z:18:MET:HB2	2.07	0.54
1:X:860:U:H3	1:X:945:G:N2	2.06	0.54
1:X:1329:U:H2'	1:X:1330:G:C8	2.43	0.54
1:X:2212:U:H2'	1:X:2213:G:C8	2.43	0.54
1:X:2594:U:H1'	26:Z:7:PRO:HB3	1.90	0.54
8:F:81:ALA:HB3	8:F:103:GLN:HE22	1.72	0.54
15:M:98:LYS:HB3	15:M:118:LYS:HB3	1.90	0.54
1:X:1463:A:H2'	1:X:1464:A:C8	2.43	0.53
14:L:41:GLN:OE1	14:L:50:THR:HG21	2.08	0.53
18:P:59:PHE:CD2	26:Z:30:LEU:HD21	2.43	0.53
1:X:492:G:O2'	1:X:517:A:N6	2.40	0.53
1:X:617:U:H5	1:X:632:A:C2	2.27	0.53
1:X:1193:G:H2'	1:X:1194:U:C6	2.43	0.53
3:A:43:ARG:HG2	3:A:51:SER:CB	2.38	0.53
20:R:96:LYS:HG2	20:R:98:ILE:HG23	1.89	0.53
1:X:420:C:H2'	1:X:421:G:C8	2.42	0.53
1:X:2607:C:H1'	1:X:2761:A:H2'	1.90	0.53
1:X:2707:G:H2'	1:X:2708:U:C6	2.43	0.53
9:G:90:LEU:HD23	9:G:93:LYS:NZ	2.23	0.53
11:I:41:SER:O	11:I:41:SER:OG	2.23	0.53
23:U:50:ALA:HB3	23:U:62:LEU:HB2	1.91	0.53
1:X:1781:C:H4'	3:A:209:ALA:HB2	1.90	0.53
32:X:3316:MPD:H53	32:X:3316:MPD:H12	1.91	0.53
5:C:45:THR:HG22	5:C:82:VAL:HG11	1.89	0.53
18:P:14:ARG:HA	18:P:17:GLN:HG2	1.91	0.53
1:X:754:G:H2'	1:X:755:C:H6	1.74	0.53
1:X:2062:U:H2'	1:X:2063:A:C8	2.43	0.53
1:X:2170:C:H3'	1:X:2171:U:H5"	1.90	0.53
9:G:119:LEU:HD13	9:G:122:HIS:CE1	2.43	0.53
1:X:595:A:N1	1:X:822:G:O2'	2.36	0.53
1:X:1801:C:N4	23:U:49:LYS:HB3	2.24	0.53
2:Y:39:C:H5"	2:Y:40:C:C5	2.44	0.53
4:B:10:GLY:O	4:B:25:VAL:N	2.33	0.53
7:E:154:PRO:HA	7:E:160:LYS:O	2.09	0.53
14:L:90:ASP:OD1	14:L:91:ARG:N	2.38	0.53
22:T:32:LYS:H	22:T:35:ASN:ND2	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:250:C:H2'	1:X:251:C:H5"	1.91	0.53
1:X:1441:A:H4'	1:X:1442:C:O5'	2.08	0.53
1:X:1451:C:H2'	1:X:1452:U:H6	1.73	0.53
5:C:59:TYR:OH	5:C:67:ALA:O	2.15	0.53
9:G:30:LYS:HE3	17:O:4:ILE:HG23	1.90	0.53
21:S:8:ARG:NE	21:S:8:ARG:O	2.41	0.53
1:X:652:C:H42	1:X:657:A:H61	1.57	0.53
1:X:1134:C:H2'	1:X:1135:C:H6	1.74	0.53
1:X:2005:U:O2'	1:X:2596:C:H5'	2.09	0.53
2:Y:17:A:H1'	2:Y:112:A:C8	2.44	0.53
14:L:43:ILE:HG23	14:L:50:THR:HG23	1.90	0.53
20:R:80:LYS:NZ	20:R:81:VAL:O	2.30	0.53
20:R:81:VAL:HG22	20:R:82:ALA:H	1.73	0.53
28:2:38:GLY:O	28:2:40:HIS:N	2.36	0.53
1:X:1668:G:H5'	13:K:39:THR:OG1	2.09	0.53
2:Y:64:C:H2'	2:Y:65:A:H8	1.73	0.53
3:A:43:ARG:HG2	3:A:51:SER:HB3	1.91	0.53
11:I:73:GLU:HB2	11:I:106:VAL:HG22	1.89	0.53
1:X:116:A:N3	1:X:155:G:H1'	2.24	0.53
6:D:172:SER:O	6:D:174:GLY:N	2.41	0.53
13:K:99:ARG:HG2	13:K:99:ARG:HH11	1.75	0.53
1:X:1279:G:O5'	18:P:36:ARG:NH2	2.42	0.52
6:D:10:ASP:O	6:D:14:PRO:HD3	2.08	0.52
1:X:642:A:O2'	11:I:65:PHE:HB2	2.10	0.52
1:X:1716:G:O2'	1:X:1718[B]:A:OP1	2.27	0.52
1:X:1865:C:H3'	1:X:1866:G:H8	1.74	0.52
1:X:120:G:H1	1:X:127:C:H42	1.57	0.52
1:X:742:G:OP2	3:A:13:ARG:NH1	2.42	0.52
1:X:1250:A:H2'	1:X:1251:G:O4'	2.09	0.52
1:X:2656:G:H1	1:X:2710:C:H42	1.56	0.52
6:D:134:GLU:HG2	6:D:136:LEU:H	1.74	0.52
9:G:116:ARG:HG3	9:G:118:ALA:HB3	1.90	0.52
1:X:98:U:O2	1:X:100:G:N1	2.42	0.52
1:X:624:A:O2'	1:X:626:A:OP2	2.22	0.52
1:X:1074:G:H1	1:X:1086:C:H42	1.56	0.52
10:H:1:MET:N	10:H:1:MET:SD	2.83	0.52
16:N:47:TYR:CE2	17:O:73:LYS:HE2	2.44	0.52
27:1:14:SER:HB3	27:1:23:THR:HB	1.91	0.52
1:X:5:A:H2'	1:X:6:A:H8	1.73	0.52
1:X:1054:C:H42	1:X:1123:G:H1	1.57	0.52
1:X:1443:G:H2'	1:X:1444:C:C6	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2339:A:H1'	11:I:59:ARG:HH11	1.75	0.52
12:J:67:ILE:HG12	12:J:105:PHE:HD1	1.74	0.52
1:X:946:U:H2'	1:X:947:C:C6	2.44	0.52
1:X:2282:G:H4'	6:D:122:PHE:HA	1.91	0.52
19:Q:20:MET:HG3	19:Q:25:TYR:CE1	2.45	0.52
1:X:250:C:N3	1:X:270:G:N2	2.58	0.52
1:X:656:U:O2'	1:X:657:A:O5'	2.27	0.52
1:X:1706:A:H2'	1:X:1707:A:C8	2.45	0.52
3:A:69:ARG:NH2	3:A:192:THR:OG1	2.43	0.52
1:X:559:C:O2	17:O:67:LYS:HB2	2.09	0.52
1:X:830:C:O2'	1:X:852:U:H5"	2.09	0.52
1:X:1685:A:H5"	10:H:5:GLN:HG2	1.90	0.52
1:X:1989:C:O2'	1:X:2798:A:N3	2.43	0.52
6:D:70:ALA:O	6:D:71:LYS:HB3	2.09	0.52
7:E:94:PHE:CG	7:E:107:ILE:HG22	2.45	0.52
18:P:39:ARG:HH11	18:P:39:ARG:HB2	1.74	0.52
20:R:92:THR:O	20:R:92:THR:OG1	2.26	0.52
1:X:542:A:C5'	16:N:28:ARG:HH21	2.23	0.52
1:X:1817:U:H2'	1:X:1818:G:C8	2.45	0.52
1:X:2324:G:N3	1:X:2360:C:H2'	2.24	0.52
6:D:171:GLN:HA	6:D:175:LEU:HD13	1.92	0.52
10:H:9:ASP:O	10:H:96:ALA:N	2.33	0.52
1:X:1417:C:H2'	1:X:1418:C:H6	1.75	0.52
1:X:2479:U:O2	32:X:3316:MPD:O2	2.27	0.52
4:B:26:VAL:HG11	4:B:198:LEU:HD11	1.92	0.52
5:C:5:ASN:ND2	5:C:10:ASN:HB2	2.25	0.52
16:N:59:ARG:O	16:N:63:GLN:HB2	2.10	0.52
28:2:34:ARG:NH1	28:2:42:LEU:HB2	2.25	0.52
1:X:1333:G:N7	1:X:1342:U:H5'	2.25	0.51
1:X:1422:C:H2'	1:X:1423:A:H8	1.76	0.51
1:X:1834:G:H2'	1:X:1835:C:C6	2.45	0.51
1:X:1984:A:P	13:K:2:ARG:HH22	2.33	0.51
9:G:84:ASN:HA	9:G:153:GLY:H	1.74	0.51
13:K:73:LYS:O	13:K:76:VAL:HG12	2.09	0.51
14:L:29:LEU:O	14:L:90:ASP:HB3	2.10	0.51
1:X:946:U:H2'	1:X:947:C:H6	1.76	0.51
1:X:1332:G:C6	1:X:1333:G:N1	2.78	0.51
3:A:246:PRO:O	3:A:247:VAL:HG13	2.10	0.51
11:I:88:PHE:HB2	11:I:90:ARG:NH2	2.25	0.51
12:J:110:VAL:HB	12:J:114:GLN:HB3	1.92	0.51
20:R:58:VAL:HG12	20:R:60:PRO:HD2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1079:G:N2	1:X:1106:A:O2'	2.43	0.51
1:X:1147:G:H2'	1:X:1148:G:H8	1.75	0.51
1:X:1406:A:H62	19:Q:15:LYS:HD3	1.75	0.51
1:X:2713:A:N1	4:B:203:LYS:HG3	2.24	0.51
5:C:23:ASN:O	5:C:27:LEU:HB2	2.11	0.51
5:C:56:ARG:HG2	5:C:57:LYS:N	2.26	0.51
12:J:45:SER:O	12:J:49:GLU:HB2	2.10	0.51
21:S:152:ILE:HD11	21:S:168:VAL:HG21	1.92	0.51
1:X:227:G:H2'	1:X:228:A:C8	2.46	0.51
1:X:705:C:C5'	3:A:41:GLY:HA2	2.41	0.51
1:X:1291:G:OP1	13:K:36:THR:OG1	2.18	0.51
1:X:2015:G:N2	4:B:146:THR:OG1	2.39	0.51
1:X:2545:A:H61	10:H:40:GLY:HA3	1.76	0.51
16:N:7:GLY:O	16:N:8:ILE:HG12	2.10	0.51
1:X:7:G:H2'	1:X:8:A:C8	2.45	0.51
1:X:826:U:H2'	1:X:827:C:C6	2.46	0.51
1:X:865:A:H2'	1:X:866:U:C6	2.46	0.51
3:A:251:GLY:O	3:A:252:LYS:HB2	2.10	0.51
5:C:28:HIS:HA	5:C:31:VAL:HG22	1.92	0.51
7:E:9:ILE:HG12	7:E:69:ARG:HE	1.75	0.51
14:L:38:ILE:HD11	14:L:40:ALA:HB2	1.92	0.51
15:M:27:PHE:HB3	15:M:93:ILE:HD12	1.92	0.51
18:P:32:ARG:NH1	18:P:119:LYS:HE2	2.26	0.51
1:X:69:G:H1'	1:X:72:A:H1'	1.93	0.51
1:X:1128:G:H3'	1:X:1129:A:H5"	1.92	0.51
1:X:2006:G:H5'	1:X:2596:C:H4'	1.92	0.51
1:X:2312:A:H4'	1:X:2313:G:O5'	2.11	0.51
1:X:2557:G:H2'	1:X:2558:C:C6	2.45	0.51
5:C:152:THR:HB	5:C:189:ASP:HB3	1.93	0.51
14:L:27:LEU:O	14:L:88:VAL:HA	2.11	0.51
15:M:32:THR:H	15:M:94:VAL:H	1.57	0.51
18:P:114:ALA:O	18:P:115:ASN:ND2	2.44	0.51
26:Z:35:GLN:HG3	26:Z:51:TYR:CD2	2.45	0.51
1:X:421:G:H2'	1:X:422:C:H6	1.76	0.51
1:X:1325:U:H4'	1:X:1326:U:O5'	2.10	0.51
1:X:2432:A:C2	32:X:3316:MPD:HM1	2.46	0.51
1:X:2787:A:H2'	1:X:2788:C:H6	1.75	0.51
1:X:2787:A:H2'	1:X:2788:C:C6	2.46	0.51
14:L:87:VAL:HA	14:L:108:ARG:HH21	1.76	0.51
1:X:163:A:H2'	1:X:164:G:H8	1.75	0.51
1:X:542:A:H5'	16:N:28:ARG:HH21	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:875:G:H2'	1:X:876:A:O4'	2.11	0.51
1:X:2363:G:OP2	22:T:55:ARG:NH1	2.44	0.51
2:Y:45:C:O2	6:D:92:ARG:NH2	2.44	0.51
23:U:17:SER:OG	23:U:45:ASN:N	2.44	0.51
1:X:635:C:O2'	1:X:670:U:OP1	2.26	0.51
1:X:877:G:H1	1:X:924:C:H42	1.59	0.51
1:X:1147:G:H2'	1:X:1148:G:C8	2.46	0.51
1:X:2432:A:H2	32:X:3316:MPD:HM1	1.76	0.51
11:I:62:LYS:CB	29:3:12:ARG:HA	2.41	0.51
14:L:27:LEU:C	14:L:88:VAL:HG13	2.31	0.51
29:3:52:LYS:NZ	29:3:56:ALA:HB2	2.26	0.51
1:X:121:G:H2'	1:X:122:G:O4'	2.11	0.51
1:X:1086:C:H3'	1:X:1087:C:H5"	1.93	0.51
1:X:1142:G:H4'	9:G:111:LYS:HE2	1.93	0.51
1:X:2352:A:H2'	1:X:2353:G:H8	1.75	0.51
1:X:2441:U:H1'	1:X:2470:U:O4	2.11	0.51
3:A:268:ARG:NH1	3:A:268:ARG:HA	2.25	0.51
1:X:2270:U:O2'	1:X:2353:G:N3	2.43	0.50
1:X:2343:C:H4'	22:T:56:ASP:OD1	2.10	0.50
1:X:2528:G:H2'	1:X:2529:G:C8	2.45	0.50
1:X:2674:C:H2'	1:X:2675:U:H6	1.74	0.50
4:B:143:GLN:HB2	4:B:147:PRO:HG3	1.93	0.50
4:B:152:LYS:HB3	9:G:106:TYR:HA	1.93	0.50
12:J:117:GLU:OE2	12:J:120:ARG:NH2	2.44	0.50
1:X:421:G:H2'	1:X:422:C:C6	2.47	0.50
1:X:1401:G:H1	1:X:1412:C:N4	2.09	0.50
1:X:1952:A:O2'	1:X:1955:G:N3	2.38	0.50
9:G:113:GLU:CD	9:G:113:GLU:H	2.14	0.50
21:S:96:VAL:HG12	21:S:134:LEU:HB2	1.92	0.50
1:X:2845:C:H2'	1:X:2846:G:H5'	1.92	0.50
9:G:61:ARG:NH1	9:G:66:HIS:HB2	2.26	0.50
10:H:4:PRO:O	10:H:5:GLN:HB2	2.10	0.50
11:I:21:ARG:HE	11:I:22:GLY:N	2.08	0.50
16:N:13:ARG:O	16:N:16:LYS:HB3	2.12	0.50
23:U:11:LYS:HG2	23:U:12:ASN:N	2.26	0.50
1:X:115:G:OP2	1:X:117:A:O2'	2.27	0.50
1:X:652:C:H42	1:X:657:A:N6	2.09	0.50
1:X:1021:A:O2'	1:X:1163:C:O2	2.29	0.50
1:X:1173:G:H2'	1:X:1174:G:H8	1.76	0.50
1:X:1919:A:H2	1:X:1926:U:H3	1.60	0.50
1:X:2827:G:H2'	1:X:2828:C:O4'	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Q:34:THR:O	19:Q:38:ILE:HG12	2.12	0.50
27:1:33:ALA:C	27:1:35:LEU:H	2.15	0.50
28:2:38:GLY:C	28:2:40:HIS:N	2.63	0.50
1:X:705:C:H5'	3:A:41:GLY:HA2	1.94	0.50
1:X:1785:A:H2'	1:X:1786:C:C6	2.47	0.50
1:X:2708:U:H2'	1:X:2709:C:C6	2.47	0.50
7:E:38:ASN:ND2	7:E:40:GLU:OE2	2.37	0.50
13:K:39:THR:O	13:K:42:LYS:N	2.44	0.50
1:X:760:U:HO2'	1:X:761:G:P	2.33	0.50
1:X:1810:U:OP2	3:A:157:ARG:HD2	2.11	0.50
1:X:2314:A:O2'	1:X:2315:A:H2'	2.11	0.50
1:X:2382:C:N4	1:X:2393:G:H1	2.09	0.50
9:G:160:ALA:O	9:G:161:GLN:NE2	2.45	0.50
1:X:1016:C:H1'	1:X:1023:U:N3	2.27	0.50
1:X:2797:G:OP2	4:B:111:LYS:HG3	2.12	0.50
3:A:231:HIS:NE2	3:A:248:THR:HB	2.26	0.50
4:B:99:GLY:N	4:B:172:VAL:O	2.42	0.50
5:C:48:ARG:O	5:C:51:VAL:N	2.43	0.50
5:C:192:ALA:C	5:C:194:GLU:H	2.15	0.50
9:G:113:GLU:O	9:G:114:THR:HB	2.12	0.50
11:I:88:PHE:O	11:I:90:ARG:NH2	2.42	0.50
14:L:15:ARG:HA	14:L:15:ARG:HH11	1.76	0.50
16:N:83:LEU:HD11	16:N:109:LEU:HD13	1.94	0.50
29:3:44:LYS:O	29:3:44:LYS:HE3	2.12	0.50
1:X:2493:U:H2'	1:X:2494:C:C6	2.46	0.50
9:G:84:ASN:HD21	9:G:154:GLU:HG2	1.76	0.50
10:H:76:ARG:NH1	10:H:113:PRO:O	2.41	0.50
18:P:59:PHE:CE2	26:Z:30:LEU:HD21	2.46	0.50
23:U:51:ILE:HG13	23:U:59:THR:HG23	1.93	0.50
23:U:65:ASN:HA	23:U:68:ARG:HD3	1.93	0.50
26:Z:51:TYR:HE1	26:Z:55:ARG:HD2	1.77	0.50
1:X:586:G:H2'	1:X:587:A:C8	2.47	0.50
1:X:1203:A:OP1	11:I:35:LYS:NZ	2.33	0.50
1:X:1407:G:H4'	1:X:1619:A:H4'	1.94	0.50
6:D:63:GLN:NE2	6:D:90:THR:O	2.30	0.50
7:E:9:ILE:HA	7:E:69:ARG:HH11	1.76	0.50
14:L:104:ALA:O	14:L:108:ARG:N	2.45	0.50
1:X:691:C:H2'	1:X:692:C:C6	2.47	0.49
1:X:1751:A:H2'	1:X:1752:U:C6	2.47	0.49
1:X:1830:C:N4	1:X:1882:G:OP2	2.43	0.49
1:X:2664:G:O2'	1:X:2665:G:H5'	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:X:3319:MPD:O4	32:X:3319:MPD:O2	2.17	0.49
20:R:29:HIS:CG	20:R:51:VAL:HG22	2.47	0.49
1:X:546:A:H2'	1:X:547:U:C6	2.47	0.49
1:X:613:A:N3	1:X:613:A:H2'	2.27	0.49
1:X:1482:U:OP2	1:X:1562:G:O2'	2.29	0.49
1:X:1752:U:H3'	1:X:1753:A:H5"	1.93	0.49
1:X:2432:A:C2	32:X:3316:MPD:H32	2.45	0.49
6:D:132:ILE:HG13	6:D:154:ILE:HD13	1.93	0.49
11:I:78:SER:HB3	11:I:112:GLY:HA3	1.94	0.49
1:X:659:G:H2'	1:X:660:G:C8	2.47	0.49
1:X:757:U:H2'	1:X:758:G:O4'	2.13	0.49
1:X:1504:G:N2	1:X:1517:C:O2	2.45	0.49
1:X:2546:G:H2'	1:X:2547:C:C6	2.47	0.49
3:A:168:LYS:HB3	3:A:173:VAL:HG13	1.94	0.49
14:L:42:ILE:O	14:L:50:THR:HG22	2.12	0.49
1:X:46:C:H2'	1:X:47:G:H8	1.77	0.49
1:X:810:U:OP2	5:C:56:ARG:HG3	2.11	0.49
1:X:1275:A:OP1	18:P:120:ARG:NH1	2.46	0.49
1:X:1584:G:P	3:A:63:ARG:HH22	2.35	0.49
1:X:1679:U:H2'	1:X:1680:U:O4'	2.11	0.49
1:X:2824:C:OP1	15:M:100:ARG:NH1	2.45	0.49
8:F:108:ALA:HB2	8:F:127:VAL:HG21	1.93	0.49
25:W:2:LYS:HG3	25:W:4:LYS:HZ1	1.76	0.49
26:Z:51:TYR:CE1	26:Z:55:ARG:HD2	2.48	0.49
1:X:699:G:N2	28:2:7:PRO:O	2.46	0.49
1:X:1301:U:O2'	1:X:1664:G:N2	2.45	0.49
1:X:2038:C:C2	32:X:3316:MPD:H13	2.47	0.49
1:X:2222:U:H2'	1:X:2223:U:C6	2.48	0.49
2:Y:51:G:H2'	2:Y:52:G:C8	2.42	0.49
4:B:117:MET:HE3	4:B:122:PHE:O	2.13	0.49
26:Z:32:GLU:HA	26:Z:39:LYS:HA	1.95	0.49
1:X:171:G:H2'	1:X:172:A:O4'	2.13	0.49
1:X:387:A:N6	1:X:414:A:O4'	2.46	0.49
1:X:494:A:HO2'	20:R:68:GLY:H	1.53	0.49
1:X:554:U:H5"	1:X:556:A:C2	2.48	0.49
1:X:1005:U:H1'	17:O:21:ARG:HH22	1.78	0.49
1:X:2768:C:O2'	1:X:2784:A:N3	2.41	0.49
1:X:2797:G:N7	4:B:111:LYS:HE3	2.27	0.49
1:X:2860:C:H2'	1:X:2861:A:O4'	2.12	0.49
2:Y:21:C:N4	2:Y:66:G:H1	2.11	0.49
5:C:33:TRP:HD1	5:C:93:TYR:CZ	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:62:ILE:O	9:G:77:GLY:HA3	2.13	0.49
1:X:812:G:OP1	5:C:50:GLN:NE2	2.43	0.49
1:X:1448:A:N6	1:X:1574:A:H61	2.10	0.49
1:X:2546:G:H2'	1:X:2547:C:H6	1.78	0.49
4:B:4:ILE:HG12	4:B:5:LEU:N	2.26	0.49
4:B:144:ARG:HG3	4:B:145:LYS:H	1.78	0.49
14:L:27:LEU:HD13	14:L:42:ILE:HD11	1.95	0.49
1:X:1406:A:N6	19:Q:15:LYS:HD3	2.27	0.49
1:X:1918:G:H1'	1:X:1947:G:N2	2.27	0.49
1:X:1949:A:H1'	1:X:2572:U:H5'	1.93	0.49
1:X:2314:A:HO2'	1:X:2315:A:H8	1.59	0.49
5:C:36:ALA:O	5:C:39:ARG:HB3	2.12	0.49
13:K:9:LYS:HG2	13:K:11:ASN:H	1.78	0.49
16:N:66:ASN:HD22	16:N:70:ARG:NH2	2.09	0.49
25:W:5:LEU:HB2	25:W:25:LEU:HD13	1.94	0.49
1:X:540:G:C6	1:X:2005:U:H5"	2.48	0.49
1:X:971:A:H61	12:J:83:ARG:HH22	1.59	0.49
1:X:1515:U:H2'	1:X:1516:A:H8	1.78	0.49
1:X:2204:A:H4'	1:X:2205:C:O5'	2.13	0.49
4:B:6:GLY:HA3	4:B:27:LEU:O	2.13	0.49
7:E:89:LEU:HB2	7:E:129:THR:HB	1.93	0.49
25:W:26:ARG:NE	25:W:26:ARG:HA	2.28	0.49
27:1:12:MET:HB3	27:1:27:ASN:ND2	2.28	0.49
29:3:49:VAL:HG22	29:3:51:ALA:H	1.78	0.49
1:X:1164:C:H2'	1:X:1165:G:O4'	2.12	0.49
1:X:1267:A:H5"	1:X:1268:U:H5"	1.94	0.49
1:X:1623:C:H4'	1:X:1624:A:O5'	2.13	0.49
1:X:1727:C:H2'	1:X:1728:A:C8	2.48	0.49
1:X:1949:A:O2'	1:X:2571:G:O3'	2.31	0.49
2:Y:9:G:H5'	14:L:32:TYR:CE1	2.47	0.49
2:Y:39:C:N4	2:Y:51:G:O4'	2.46	0.49
3:A:231:HIS:HE2	3:A:248:THR:HB	1.76	0.49
3:A:252:LYS:HG3	3:A:253:PRO:HD2	1.95	0.49
6:D:70:ALA:O	6:D:71:LYS:NZ	2.39	0.49
12:J:82:THR:OG1	12:J:83:ARG:N	2.44	0.49
1:X:66:U:H2'	1:X:67:G:C8	2.48	0.48
1:X:591:G:H1	1:X:1271:C:H42	1.61	0.48
1:X:732:G:H2'	1:X:733:G:C8	2.48	0.48
1:X:814:G:OP2	5:C:49:ALA:HB3	2.13	0.48
1:X:859:U:H1'	1:X:860:U:C5	2.48	0.48
1:X:2309:G:H2'	1:X:2310:G:O4'	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2604:G:H2'	1:X:2605:C:C6	2.48	0.48
6:D:135:GLN:HB3	6:D:151:GLY:HA2	1.95	0.48
7:E:33:LEU:HD22	7:E:136:ILE:HG22	1.94	0.48
9:G:161:GLN:HE21	9:G:161:GLN:HA	1.78	0.48
10:H:116:ARG:HD3	15:M:40:ARG:HE	1.77	0.48
21:S:113:VAL:HA	21:S:171:VAL:HG22	1.95	0.48
23:U:33:LYS:HD2	23:U:34:THR:H	1.77	0.48
1:X:682:G:H3'	1:X:683:A:C8	2.48	0.48
1:X:1204:G:H2'	1:X:1205:G:H8	1.77	0.48
1:X:1805:G:O2'	3:A:43:ARG:HG3	2.13	0.48
1:X:1831:G:H2'	1:X:1832:G:C8	2.43	0.48
1:X:2301:A:H2'	1:X:2302:G:O4'	2.13	0.48
1:X:2691:C:H2'	1:X:2694:G:H5"	1.94	0.48
2:Y:17:A:H5'	2:Y:18:G:C8	2.48	0.48
27:1:12:MET:HE3	27:1:13:GLU:HG2	1.94	0.48
1:X:2197:U:H5'	1:X:2198:U:OP1	2.14	0.48
4:B:132:LYS:N	4:B:132:LYS:HD2	2.28	0.48
21:S:91:PRO:HG3	21:S:127:PRO:HG3	1.95	0.48
1:X:755:C:H2'	1:X:756:C:O4'	2.13	0.48
1:X:795:A:N7	3:A:221:GLN:HG2	2.29	0.48
1:X:1181:C:N4	1:X:1182:U:O4	2.47	0.48
1:X:2281:C:N4	1:X:2293:G:H1	2.11	0.48
6:D:114:PHE:CZ	6:D:116:GLY:HA2	2.48	0.48
16:N:50:ARG:HA	16:N:53:LYS:HE3	1.96	0.48
1:X:1601:U:O2'	1:X:1602:G:N7	2.42	0.48
1:X:2441:U:H2'	1:X:2442:C:C6	2.47	0.48
2:Y:42:U:H3'	2:Y:43:G:H5'	1.94	0.48
3:A:244:ARG:HH11	3:A:246:PRO:HG2	1.78	0.48
5:C:119:ALA:HB3	5:C:189:ASP:HA	1.96	0.48
12:J:71:PRO:HA	12:J:96:SER:HB2	1.95	0.48
13:K:60:LEU:HD11	13:K:64:ARG:NE	2.27	0.48
13:K:87:TYR:HE1	13:K:94:TYR:HD2	1.59	0.48
17:O:26:GLN:HB2	17:O:63:HIS:CE1	2.48	0.48
23:U:16:ASN:O	23:U:17:SER:OG	2.19	0.48
27:1:9:ILE:HB	27:1:27:ASN:O	2.12	0.48
1:X:334:G:C8	5:C:164:VAL:HA	2.49	0.48
1:X:689:A:H8	1:X:2052:G:H21	1.60	0.48
1:X:736:G:H2'	1:X:737:C:O4'	2.14	0.48
1:X:757:U:H3	1:X:766:A:H61	1.61	0.48
1:X:1296:G:N2	1:X:1299:A:H5'	2.29	0.48
1:X:2441:U:H2'	1:X:2442:C:H6	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2679:G:H2'	1:X:2680:U:C6	2.48	0.48
3:A:13:ARG:NH1	3:A:16:MET:SD	2.87	0.48
4:B:176:ARG:HH22	15:M:16:ILE:HA	1.77	0.48
16:N:84:LYS:HA	16:N:92:ARG:HH22	1.79	0.48
20:R:84:VAL:HG12	20:R:90:LYS:O	2.13	0.48
1:X:1151:U:OP1	9:G:53:ARG:NH2	2.47	0.48
1:X:1782:A:O2'	3:A:207:GLY:O	2.27	0.48
3:A:166:GLN:HB3	3:A:174:ILE:HB	1.94	0.48
1:X:691:C:H2'	1:X:692:C:H6	1.78	0.48
1:X:859:U:O2'	1:X:860:U:H6	1.95	0.48
5:C:128:ALA:C	5:C:130:THR:H	2.17	0.48
6:D:133:LYS:O	6:D:151:GLY:HA3	2.12	0.48
1:X:279:A:N6	1:X:280:C:H41	2.12	0.48
1:X:545:C:H2'	1:X:546:A:C8	2.49	0.48
1:X:859:U:H1'	1:X:860:U:H5	1.77	0.48
1:X:1412:C:O2'	1:X:1413:U:O5'	2.32	0.48
1:X:1514:C:H4'	1:X:1592:U:O2'	2.13	0.48
1:X:1563:U:H2'	1:X:1564:U:C6	2.49	0.48
1:X:2039:G:C2	1:X:2040:A:C8	3.02	0.48
1:X:2039:G:O2'	26:Z:8:LYS:HE2	2.14	0.48
1:X:2591:C:O2'	1:X:2592:U:OP1	2.30	0.48
1:X:2821:G:H2'	1:X:2822:U:O4'	2.14	0.48
2:Y:19:C:H2'	2:Y:20:A:C8	2.48	0.48
3:A:145:LEU:HD21	3:A:185:VAL:HG21	1.95	0.48
10:H:76:ARG:HB2	10:H:95:ALA:HB3	1.94	0.48
13:K:9:LYS:HD2	13:K:11:ASN:N	2.27	0.48
15:M:113:LYS:HA	15:M:113:LYS:HE2	1.96	0.48
19:Q:89:GLU:HB3	19:Q:90:ALA:H	1.51	0.48
1:X:513:A:H5"	1:X:514:G:H5'	1.96	0.48
1:X:1974:U:H2'	1:X:1975:G:H5"	1.95	0.48
4:B:113:THR:HA	4:B:159:HIS:HA	1.96	0.48
11:I:97:ARG:HD3	11:I:99:VAL:HG22	1.96	0.48
11:I:120:VAL:HB	11:I:140:VAL:HG22	1.96	0.48
12:J:38:MET:SD	12:J:131:LYS:HE3	2.54	0.48
13:K:13:ASN:HB2	13:K:16:ALA:H	1.78	0.48
14:L:29:LEU:HD12	14:L:42:ILE:HB	1.96	0.48
1:X:165:G:H1	1:X:185:C:H42	1.60	0.47
1:X:825:C:O2'	1:X:1239:A:O2'	2.30	0.47
1:X:1500:U:H3	1:X:1520:G:H1	1.62	0.47
5:C:97:ARG:O	5:C:101:GLN:HG2	2.14	0.47
6:D:36:VAL:HG13	6:D:154:ILE:HG13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:128:GLU:HG3	9:G:150:VAL:HG21	1.97	0.47
23:U:17:SER:CB	23:U:44:ALA:HA	2.44	0.47
1:X:313:U:H2'	1:X:314:G:C8	2.47	0.47
1:X:529:U:H2'	1:X:530:G:C8	2.49	0.47
1:X:1004:A:H2	17:O:21:ARG:HH21	1.60	0.47
1:X:1026:U:H2'	1:X:1027:C:C6	2.49	0.47
1:X:1427:G:H2'	1:X:1428:G:H4'	1.95	0.47
1:X:2015:G:N7	32:X:3316:MPD:H11	2.30	0.47
1:X:2040:A:H2'	1:X:2041:A:C8	2.50	0.47
1:X:2809:A:H8	1:X:2858:A:N6	2.06	0.47
3:A:163:VAL:HG22	3:A:177:LEU:HA	1.95	0.47
5:C:149:LEU:HD23	5:C:180:ILE:HG22	1.96	0.47
11:I:63:ARG:O	29:3:11:LYS:HB3	2.14	0.47
13:K:81:ASP:O	13:K:85:PRO:HG2	2.14	0.47
16:N:76:TYR:CZ	16:N:80:ILE:HG13	2.49	0.47
17:O:20:ILE:HD12	17:O:21:ARG:HG2	1.96	0.47
18:P:60:ILE:HA	18:P:61:PRO:HD3	1.47	0.47
1:X:196:A:N6	1:X:441:A:OP1	2.47	0.47
1:X:572:G:H5'	1:X:581:A:H4'	1.96	0.47
1:X:1116:U:H2'	1:X:1117:G:C8	2.46	0.47
1:X:2727:G:O6	1:X:2735:C:H5"	2.14	0.47
5:C:56:ARG:CG	5:C:57:LYS:H	2.23	0.47
18:P:9:ARG:HH11	18:P:10:ASN:HD21	1.61	0.47
1:X:477:A:H5'	28:2:21:ARG:NH2	2.29	0.47
1:X:502:A:H2'	1:X:503:G:O4'	2.15	0.47
1:X:794:A:H2	1:X:1767:G:N3	2.12	0.47
1:X:1909:U:H4'	1:X:1910:A:OP1	2.15	0.47
3:A:132:PRO:HD3	3:A:190:TYR:CE1	2.49	0.47
13:K:99:ARG:NH1	26:Z:43:HIS:O	2.43	0.47
1:X:240:U:H2'	1:X:241:C:O4'	2.14	0.47
1:X:537:C:H2'	1:X:538:A:C2	2.49	0.47
1:X:2844:G:H2'	1:X:2845:C:O4'	2.15	0.47
4:B:105:THR:HG21	4:B:199:ARG:HH11	1.80	0.47
9:G:61:ARG:HA	9:G:61:ARG:HE	1.79	0.47
12:J:43:ILE:HG21	12:J:48:ILE:HG23	1.96	0.47
20:R:17:LYS:HG2	20:R:18:LYS:H	1.79	0.47
1:X:1729:C:H2'	1:X:1730:G:C8	2.50	0.47
1:X:2367:A:N7	1:X:2368:G:C6	2.83	0.47
1:X:2557:G:N7	4:B:140:SER:HB2	2.29	0.47
3:A:91:ARG:CZ	3:A:198:ASN:H	2.28	0.47
18:P:22:LYS:HA	18:P:23:PRO:HD3	1.59	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:59:G:H1'	1:X:73:A:C2	2.50	0.47
1:X:202:A:C2	1:X:203:G:H1'	2.50	0.47
1:X:490:A:HO2'	1:X:492:G:H8	1.63	0.47
1:X:512:A:OP1	18:P:16:GLN:HB3	2.15	0.47
1:X:571:U:HO2'	1:X:581:A:H8	1.61	0.47
1:X:1070:G:N2	8:F:130:THR:OG1	2.47	0.47
1:X:1560:A:C6	1:X:1561:A:C6	3.03	0.47
1:X:2478:C:N3	32:X:3316:MPD:H52	2.29	0.47
1:X:2616:U:H5'	4:B:44:TYR:CE2	2.50	0.47
3:A:8:PRO:HB3	3:A:14:ARG:HB3	1.96	0.47
3:A:160:GLY:H	3:A:196:VAL:HB	1.80	0.47
4:B:14:ILE:HA	15:M:20:HIS:CD2	2.49	0.47
5:C:22:VAL:HG13	5:C:106:MET:HB3	1.97	0.47
5:C:148:VAL:HG12	5:C:166:TRP:CD1	2.49	0.47
5:C:158:ARG:HD2	5:C:169:VAL:HG13	1.97	0.47
6:D:74:ILE:HG23	6:D:75:SER:H	1.79	0.47
17:O:50:ASP:O	17:O:53:LYS:HB3	2.14	0.47
21:S:69:VAL:HG13	21:S:81:VAL:HG22	1.97	0.47
29:3:14:ILE:HG21	29:3:56:ALA:HB1	1.96	0.47
1:X:655:A:C2'	1:X:656:U:H5'	2.45	0.47
1:X:790:A:O2'	3:A:48:ARG:NH2	2.47	0.47
1:X:810:U:H2'	1:X:811:G:O4'	2.14	0.47
1:X:825:C:H2'	1:X:826:U:H6	1.80	0.47
1:X:1003:C:H2'	1:X:1004:A:H8	1.78	0.47
1:X:2245:A:H4'	1:X:2246:A:N3	2.29	0.47
4:B:132:LYS:HA	4:B:132:LYS:HZ2	1.79	0.47
10:H:20:MET:HG2	10:H:21:CYS:N	2.29	0.47
14:L:39:TYR:N	14:L:39:TYR:CD1	2.83	0.47
16:N:66:ASN:OD1	16:N:66:ASN:N	2.48	0.47
1:X:597:U:H2'	1:X:598:U:C6	2.49	0.47
1:X:1573:G:O6	1:X:1574:A:N6	2.47	0.47
1:X:2000:U:H4'	26:Z:8:LYS:O	2.15	0.47
1:X:2370:G:O6	1:X:2406:C:H1'	2.15	0.47
1:X:2511:G:N2	1:X:2642:G:O2'	2.48	0.47
2:Y:32:C:H1'	2:Y:59:A:N6	2.29	0.47
3:A:231:HIS:CE1	3:A:247:VAL:HG12	2.50	0.47
4:B:5:LEU:HB3	4:B:197:VAL:HG22	1.97	0.47
4:B:26:VAL:HG12	4:B:182:ILE:HG23	1.96	0.47
5:C:33:TRP:CE3	5:C:95:LEU:HD12	2.49	0.47
6:D:174:GLY:O	6:D:176:PRO:HD3	2.15	0.47
1:X:426:C:HO2'	1:X:1863:U:HO2'	1.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1554:G:H2'	1:X:1555:A:H8	1.80	0.47
1:X:2543:A:C2	1:X:2626:U:H4'	2.50	0.47
17:O:36:LYS:HZ1	17:O:56:VAL:HG13	1.80	0.47
27:1:24:THR:O	27:1:24:THR:OG1	2.27	0.47
1:X:1336:G:H2'	1:X:1337:G:H5'	1.97	0.46
1:X:1582:A:O4'	3:A:214:TRP:HB3	2.15	0.46
5:C:179:ASP:HA	5:C:182:ARG:HD3	1.97	0.46
8:F:77:LEU:O	8:F:103:GLN:NE2	2.48	0.46
13:K:66:VAL:HG12	13:K:76:VAL:HG23	1.95	0.46
15:M:104:LEU:HD23	15:M:104:LEU:HA	1.65	0.46
27:1:53:LYS:HG2	27:1:54:LYS:H	1.80	0.46
1:X:768:U:C4	1:X:769:C:C4	3.03	0.46
1:X:941:U:H2'	1:X:942:U:O4'	2.16	0.46
1:X:2270:U:H2'	1:X:2271:C:C6	2.51	0.46
2:Y:89:G:N2	2:Y:92:G:OP2	2.34	0.46
3:A:18:THR:OG1	3:A:19:ALA:N	2.47	0.46
5:C:149:LEU:HD11	5:C:170:LEU:HB2	1.98	0.46
15:M:60:SER:O	15:M:63:ARG:NH1	2.48	0.46
16:N:79:PHE:CE1	16:N:110:VAL:HA	2.48	0.46
19:Q:7:LEU:HD13	19:Q:7:LEU:H	1.80	0.46
1:X:884:C:H4'	12:J:70:PHE:CE1	2.50	0.46
1:X:1257:U:OP1	11:I:16:ARG:NH1	2.48	0.46
1:X:1710:U:O2'	3:A:14:ARG:NH2	2.49	0.46
1:X:2058:U:C4	1:X:2217:G:C6	3.03	0.46
1:X:2448:A:H4'	12:J:57:ARG:HD2	1.97	0.46
1:X:2557:G:C5	4:B:140:SER:HB2	2.51	0.46
5:C:129:LYS:C	5:C:131:LYS:H	2.18	0.46
9:G:114:THR:O	9:G:119:LEU:HG	2.16	0.46
9:G:156:HIS:HB2	9:G:157:PRO:HD3	1.97	0.46
11:I:93:LEU:HD12	11:I:97:ARG:HB2	1.97	0.46
14:L:26:ARG:NE	14:L:87:VAL:HG22	2.30	0.46
19:Q:26:SER:HB3	19:Q:79:ILE:HG12	1.97	0.46
22:T:29:GLU:O	22:T:67:VAL:HG12	2.15	0.46
1:X:123:A:C5	28:2:10:ARG:HB2	2.50	0.46
1:X:1812:U:N3	3:A:200:GLU:OE1	2.48	0.46
1:X:2241:U:OP1	22:T:19:LYS:HG3	2.16	0.46
4:B:132:LYS:NZ	4:B:132:LYS:HA	2.30	0.46
4:B:193:GLY:O	15:M:2:GLN:N	2.49	0.46
16:N:47:TYR:O	16:N:51:ARG:NH1	2.45	0.46
21:S:72:ASP:HB2	21:S:79:ILE:HG23	1.97	0.46
22:T:15:ASP:OD1	22:T:16:SER:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:29:U:C5	32:X:3315:MPD:H51	2.50	0.46
1:X:533:C:O2	1:X:563:U:O2'	2.34	0.46
1:X:663:G:H8	1:X:664:C:H4'	1.79	0.46
1:X:2186:G:H2'	1:X:2187:A:C8	2.50	0.46
1:X:2772:U:H2'	1:X:2773:G:C8	2.50	0.46
2:Y:39:C:H5'	2:Y:40:C:OP2	2.16	0.46
4:B:31:CYS:HB2	4:B:90:SER:HB3	1.98	0.46
7:E:61:HIS:C	7:E:63:ALA:H	2.18	0.46
14:L:43:ILE:HA	14:L:50:THR:HA	1.98	0.46
1:X:717:G:N3	1:X:739:G:C2	2.84	0.46
1:X:1149:G:O2'	1:X:1154:A:N1	2.44	0.46
1:X:1586:A:H2'	1:X:1587:A:C8	2.50	0.46
1:X:1599:G:H2'	1:X:1600:U:H4'	1.97	0.46
1:X:1670:G:C6	13:K:9:LYS:HG3	2.50	0.46
1:X:1725:C:H42	1:X:1741:G:H1	1.62	0.46
1:X:1781:C:H2'	1:X:1782:A:C5	2.51	0.46
1:X:1845:A:N3	1:X:2212:U:O2'	2.36	0.46
1:X:2210:C:OP1	23:U:45:ASN:HA	2.14	0.46
1:X:2672:U:H2'	1:X:2673:G:C8	2.41	0.46
5:C:104:LEU:HA	5:C:107:ALA:HB3	1.97	0.46
12:J:20:GLY:H	12:J:99:LYS:NZ	2.14	0.46
1:X:646:C:H2'	1:X:647:G:O4'	2.16	0.46
1:X:1361:G:H1	1:X:1614:C:H42	1.63	0.46
1:X:2447:G:O2'	1:X:2448:A:H8	1.97	0.46
3:A:247:VAL:N	3:A:250:TRP:O	2.49	0.46
5:C:163:ASN:OD1	5:C:164:VAL:N	2.41	0.46
6:D:38:GLU:O	6:D:87:ILE:HG12	2.16	0.46
10:H:51:ILE:HG12	10:H:52:VAL:N	2.31	0.46
18:P:55:ASP:CG	26:Z:39:LYS:HG3	2.36	0.46
27:1:13:GLU:HB2	27:1:24:THR:HG22	1.98	0.46
1:X:227:G:H5'	29:3:8:LYS:HD3	1.96	0.46
1:X:308:C:H5"	20:R:95:ARG:HD3	1.98	0.46
1:X:554:U:H5"	1:X:556:A:N3	2.31	0.46
1:X:1991:C:H2'	1:X:1992:G:H8	1.80	0.46
1:X:2226:A:H2'	1:X:2227:C:C6	2.51	0.46
1:X:2428:U:H4'	1:X:2429:A:OP1	2.15	0.46
1:X:2552:C:H5"	1:X:2553:G:H5"	1.98	0.46
1:X:2725:C:H2'	1:X:2726:U:C6	2.51	0.46
1:X:2790:C:H2'	1:X:2791:C:C6	2.51	0.46
4:B:60:ASN:O	4:B:64:GLN:HG3	2.16	0.46
16:N:6:THR:HG21	16:N:10:ARG:NH2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:S:25:ASN:HB3	21:S:85:MET:HG3	1.98	0.46
21:S:116:VAL:N	21:S:168:VAL:O	2.44	0.46
1:X:104:C:H2'	1:X:105:G:H8	1.80	0.46
1:X:224:G:H4'	1:X:399:G:C4	2.50	0.46
1:X:500:G:H8	1:X:500:G:OP1	1.99	0.46
1:X:540:G:C5	1:X:2005:U:H5"	2.51	0.46
1:X:1437:A:H2'	1:X:1438:G:C8	2.50	0.46
1:X:2842:C:H6	1:X:2842:C:H2'	1.57	0.46
7:E:147:ASN:O	7:E:150:LYS:HB2	2.16	0.46
15:M:13:LEU:HD12	15:M:13:LEU:HA	1.66	0.46
18:P:17:GLN:HG3	18:P:18:VAL:HG23	1.98	0.46
1:X:26:G:C6	1:X:27:G:N1	2.84	0.46
1:X:139:A:H2'	1:X:140:G:H8	1.80	0.46
1:X:420:C:H2'	1:X:421:G:H8	1.81	0.46
1:X:1336:G:O6	1:X:1337:G:C6	2.69	0.46
1:X:1623:C:H5"	1:X:1624:A:H5'	1.98	0.46
1:X:2078:G:H1	1:X:2177:U:H3	1.62	0.46
1:X:2171:U:H4'	1:X:2171:U:OP1	2.14	0.46
6:D:40:LEU:HD11	6:D:53:ALA:HB3	1.97	0.46
6:D:104:ILE:HA	6:D:108:LEU:HD12	1.98	0.46
9:G:70:PHE:HB3	16:N:64:ARG:HG2	1.97	0.46
9:G:103:TYR:CG	9:G:104:THR:N	2.83	0.46
16:N:81:ASN:O	16:N:85:ARG:N	2.40	0.46
1:X:172:A:H61	1:X:175:C:H3'	1.81	0.45
1:X:1124:U:H2'	1:X:1125:G:H8	1.81	0.45
1:X:1310:C:H2'	1:X:1311:C:H6	1.80	0.45
1:X:1706:A:H2'	1:X:1707:A:H8	1.80	0.45
1:X:1806:G:O5'	3:A:43:ARG:NE	2.48	0.45
2:Y:28:A:H8	2:Y:29:C:C2	2.34	0.45
3:A:71:ASP:N	3:A:71:ASP:OD1	2.49	0.45
19:Q:25:TYR:OH	19:Q:87:SER:HA	2.16	0.45
1:X:219:G:H4'	1:X:220:U:O5'	2.15	0.45
1:X:1268:U:C5	5:C:67:ALA:HA	2.51	0.45
1:X:2240:C:OP1	22:T:17:ASN:ND2	2.49	0.45
3:A:170:SER:OG	3:A:171:ASP:N	2.48	0.45
4:B:111:LYS:HB3	13:K:1:MET:HE2	1.97	0.45
6:D:33:LYS:HD3	6:D:92:ARG:NH1	2.30	0.45
7:E:27:LYS:HG2	7:E:32:GLU:HB3	1.98	0.45
11:I:123:ASP:OD1	11:I:123:ASP:N	2.50	0.45
16:N:3:ARG:HH21	16:N:5:LYS:HB3	1.81	0.45
18:P:9:ARG:HD2	18:P:10:ASN:ND2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:U:22:GLY:HA3	23:U:39:LYS:CB	2.47	0.45
23:U:47:HIS:CG	23:U:48:LYS:N	2.84	0.45
23:U:55:GLY:O	23:U:56:GLN:HB3	2.16	0.45
1:X:36:G:N3	1:X:462:G:O2'	2.48	0.45
1:X:116:A:OP2	1:X:117:A:H2'	2.17	0.45
1:X:1016:C:C2	1:X:1154:A:C5	3.04	0.45
1:X:2411:A:C6	1:X:2412:A:C6	3.04	0.45
26:Z:25:LEU:HD12	26:Z:25:LEU:HA	1.83	0.45
28:2:34:ARG:HD3	28:2:42:LEU:HD13	1.98	0.45
1:X:32:C:O2'	1:X:33:C:H5'	2.16	0.45
1:X:58:C:H1'	1:X:72:A:H2'	1.98	0.45
1:X:503:G:H2'	1:X:504:G:O4'	2.16	0.45
1:X:1278:A:H2	1:X:1997:A:H62	1.63	0.45
1:X:1493:A:H2'	1:X:1494:G:O4'	2.15	0.45
1:X:1542:G:H22	1:X:1562:G:N2	2.15	0.45
1:X:1715:A:O4'	1:X:1717:A:H4'	2.16	0.45
1:X:1973:C:H2'	1:X:1974:U:O4'	2.16	0.45
1:X:2328:G:OP2	29:3:42:ARG:HG3	2.16	0.45
6:D:4:LEU:C	6:D:6:THR:H	2.20	0.45
6:D:135:GLN:N	6:D:150:ARG:O	2.41	0.45
9:G:70:PHE:O	16:N:64:ARG:NH1	2.48	0.45
12:J:62:GLY:HA3	12:J:64:LYS:HD2	1.98	0.45
1:X:250:C:C2'	1:X:251:C:H5"	2.46	0.45
1:X:396:U:O4	1:X:398:C:H2'	2.16	0.45
1:X:1432:G:H21	1:X:1596:A:H62	1.63	0.45
1:X:1672:A:C2	1:X:1673:C:H1'	2.51	0.45
3:A:33:LEU:O	3:A:64:ILE:HB	2.17	0.45
3:A:36:ALA:HB3	3:A:61:LEU:HD22	1.97	0.45
3:A:86:PRO:O	3:A:87:ASN:ND2	2.50	0.45
4:B:84:PHE:CD1	4:B:86:PRO:HD3	2.51	0.45
14:L:38:ILE:HG22	14:L:99:ARG:HH21	1.80	0.45
18:P:31:VAL:HG22	18:P:122:SER:O	2.17	0.45
18:P:32:ARG:NH1	18:P:119:LYS:HB3	2.32	0.45
28:2:10:ARG:HA	28:2:13:ALA:HB3	1.99	0.45
1:X:784:U:H2'	1:X:785:U:C6	2.52	0.45
1:X:1074:G:H1	1:X:1086:C:N4	2.15	0.45
1:X:1891:C:H2'	1:X:1892:C:O4'	2.17	0.45
1:X:1997:A:H2'	1:X:1998:A:C8	2.51	0.45
1:X:2033:C:N4	1:X:2034:A:N1	2.65	0.45
1:X:2048:C:O2	1:X:2428:U:N3	2.39	0.45
2:Y:7:C:H2'	2:Y:8:C:C6	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:J:48:ILE:HG21	12:J:69:ILE:HD12	1.98	0.45
21:S:149:ALA:HB1	21:S:160:LEU:HD11	1.97	0.45
27:1:43:VAL:HG23	27:1:44:ALA:H	1.81	0.45
29:3:51:ALA:O	29:3:55:TRP:HZ3	2.00	0.45
1:X:26:G:H1'	1:X:525:A:H61	1.82	0.45
1:X:79:G:H2'	1:X:80:A:C8	2.52	0.45
1:X:347:C:H4'	20:R:15:HIS:CD2	2.52	0.45
1:X:780:U:O2'	1:X:781:G:OP2	2.32	0.45
1:X:1289:A:C2	1:X:1290:A:C8	3.04	0.45
1:X:1811:A:OP2	3:A:156:ALA:HA	2.16	0.45
1:X:2034:A:H4'	4:B:141:ILE:HG12	1.99	0.45
1:X:2076:G:N3	1:X:2181:A:N6	2.62	0.45
1:X:2660:C:C2	1:X:2704:U:O4	2.70	0.45
3:A:76:ASN:OD1	3:A:118:ASN:ND2	2.46	0.45
9:G:162:LYS:N	9:G:163:PRO:HD2	2.32	0.45
14:L:42:ILE:HG23	14:L:52:ALA:H	1.82	0.45
21:S:3:LEU:HD11	21:S:6:LYS:HD3	1.99	0.45
1:X:1893:G:H4'	1:X:1908:C:C6	2.52	0.45
1:X:1999:U:O2	26:Z:7:PRO:HG2	2.16	0.45
1:X:2661:G:N3	4:B:22:PRO:HB3	2.31	0.45
2:Y:26:G:N7	2:Y:58:G:O2'	2.31	0.45
5:C:6:VAL:HG21	5:C:136:TRP:CZ2	2.52	0.45
5:C:17:LEU:HG	5:C:109:ALA:HB1	1.99	0.45
6:D:65:PRO:HA	6:D:89:VAL:HG13	1.99	0.45
14:L:51:LEU:HD11	14:L:82:LYS:HG2	1.99	0.45
18:P:37:LYS:O	18:P:40:LEU:HB2	2.17	0.45
27:1:27:ASN:N	27:1:27:ASN:OD1	2.50	0.45
29:3:15:LYS:HB2	29:3:23:MET:HB2	1.98	0.45
1:X:18:U:O2'	1:X:563:U:OP1	2.34	0.45
1:X:538:A:HO2'	1:X:539:A:P	2.36	0.45
1:X:1134:C:H2'	1:X:1135:C:C6	2.50	0.45
1:X:1882:G:H21	1:X:1885:C:H41	1.62	0.45
1:X:2543:A:OP1	1:X:2627:G:O2'	2.21	0.45
1:X:2556:A:H5"	1:X:2557:G:H5'	1.99	0.45
7:E:103:LEU:HD21	7:E:131:ILE:HD13	1.98	0.45
9:G:89:ALA:O	9:G:90:LEU:HD12	2.17	0.45
12:J:47:GLN:O	12:J:50:ALA:N	2.50	0.45
18:P:91:PHE:CD1	18:P:131:LYS:HD3	2.52	0.45
22:T:46:LYS:HB3	22:T:78:PHE:CE1	2.52	0.45
1:X:609:U:H4'	11:I:18:ARG:NH2	2.31	0.45
1:X:687:G:O2'	5:C:61:GLN:NE2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:836:G:H2'	1:X:837:U:H6	1.81	0.45
1:X:1182:U:O2'	1:X:1183:C:H5"	2.16	0.45
1:X:1398:G:O2'	1:X:1399:C:O4'	2.27	0.45
1:X:2523:G:H2'	1:X:2524:G:O4'	2.17	0.45
1:X:2541:U:O2'	10:H:23:ARG:NH2	2.47	0.45
1:X:2596:C:H2'	1:X:2597:G:C8	2.50	0.45
2:Y:94:G:H5"	21:S:74:ARG:HH22	1.82	0.45
3:A:67:PHE:HB3	3:A:153:ALA:H	1.81	0.45
9:G:97:ASP:O	9:G:99:VAL:HG13	2.17	0.45
11:I:42:GLY:HA2	11:I:45:LYS:NZ	2.32	0.45
22:T:24:LYS:HB2	22:T:36:ILE:O	2.17	0.45
1:X:832:A:OP2	1:X:1201:G:N2	2.42	0.44
1:X:1173:G:H2'	1:X:1174:G:C8	2.52	0.44
1:X:1727:C:H2'	1:X:1728:A:H8	1.82	0.44
1:X:2067:U:H2'	1:X:2068:C:C6	2.52	0.44
1:X:2255:G:C2	1:X:2256:G:C8	3.05	0.44
6:D:10:ASP:HB3	6:D:11:GLN:H	1.63	0.44
20:R:23:ILE:HB	20:R:81:VAL:HG11	1.98	0.44
21:S:91:PRO:HG3	21:S:127:PRO:CG	2.47	0.44
29:3:15:LYS:HA	29:3:15:LYS:HD3	1.56	0.44
1:X:79:G:H2'	1:X:80:A:H8	1.81	0.44
1:X:427:C:H1'	1:X:1856:U:H1'	1.99	0.44
1:X:545:C:O3'	16:N:53:LYS:NZ	2.34	0.44
1:X:1212:U:H2'	1:X:1213:U:H6	1.81	0.44
1:X:1419:G:H2'	1:X:1420:A:C8	2.52	0.44
1:X:1469:U:H1'	13:K:60:LEU:CD1	2.44	0.44
1:X:1682:A:O2'	10:H:1:MET:N	2.31	0.44
1:X:2043:A:O2'	1:X:2481:G:O4'	2.35	0.44
1:X:2551:A:N7	4:B:145:LYS:HB3	2.32	0.44
2:Y:10:U:OP1	14:L:12:ARG:NH2	2.50	0.44
11:I:11:GLY:HA3	11:I:14:LYS:HD2	2.00	0.44
17:O:19:VAL:HG13	17:O:90:PHE:CD2	2.53	0.44
17:O:38:LEU:HD13	17:O:39:PHE:N	2.32	0.44
20:R:46:VAL:HG21	20:R:80:LYS:HE3	1.98	0.44
21:S:70:GLN:HB3	21:S:80:HIS:CB	2.45	0.44
1:X:573:C:HO2'	1:X:1266:G:H1	1.66	0.44
1:X:742:G:O6	3:A:208:LYS:HB3	2.17	0.44
1:X:1921:A:O2'	1:X:1922:U:H5"	2.18	0.44
1:X:2241:U:H2'	1:X:2242:C:H6	1.82	0.44
1:X:2684:A:O5'	1:X:2684:A:H8	2.01	0.44
1:X:2825:A:C2	1:X:2826:C:C2	3.06	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2827:G:C6	1:X:2828:C:N3	2.85	0.44
4:B:105:THR:HG21	4:B:199:ARG:NH1	2.32	0.44
6:D:34:ILE:HD13	6:D:156:ILE:HA	1.99	0.44
6:D:84:PRO:O	6:D:85:VAL:HG22	2.18	0.44
16:N:50:ARG:O	16:N:53:LYS:HG2	2.18	0.44
19:Q:43:GLN:HG2	19:Q:48:VAL:O	2.17	0.44
1:X:123:A:H2'	28:2:13:ALA:HB1	1.99	0.44
1:X:334:G:C6	5:C:164:VAL:HG22	2.52	0.44
1:X:699:G:C6	28:2:12:ARG:HA	2.53	0.44
1:X:761:G:C8	1:X:763:A:C8	3.06	0.44
1:X:1433:A:OP2	1:X:1593:C:N4	2.50	0.44
1:X:1919:A:N6	1:X:1946:U:H3	2.14	0.44
1:X:2020:G:H2'	1:X:2021:G:C8	2.52	0.44
1:X:2197:U:H2'	1:X:2198:U:C2	2.52	0.44
1:X:2629:U:H2'	1:X:2630:C:C6	2.52	0.44
33:X:3321:SPD:H31	9:G:110:LEU:HD11	1.98	0.44
3:A:6:TYR:HB2	3:A:13:ARG:O	2.18	0.44
10:H:83:ARG:HH22	15:M:38:LYS:NZ	2.15	0.44
14:L:33:ARG:HG3	14:L:99:ARG:NH2	2.33	0.44
16:N:66:ASN:HA	16:N:69:ALA:HB3	1.99	0.44
16:N:68:GLY:O	16:N:71:LEU:HB3	2.17	0.44
21:S:138:VAL:O	21:S:141:MET:HG2	2.18	0.44
1:X:28:A:H1'	1:X:523:A:C2	2.52	0.44
1:X:192:G:H4'	1:X:193:A:H4'	1.99	0.44
1:X:219:G:H1'	1:X:220:U:OP2	2.17	0.44
1:X:865:A:H2'	1:X:866:U:H6	1.83	0.44
1:X:939:C:OP2	1:X:940:G:H8	2.01	0.44
1:X:1061:A:N1	1:X:2731:G:C6	2.86	0.44
1:X:1599:G:C2	1:X:1600:U:H1'	2.52	0.44
1:X:1662:G:H5"	1:X:1663:C:H5'	1.98	0.44
1:X:2487:G:C2	1:X:2561:G:C6	3.06	0.44
7:E:111:HIS:HA	7:E:112:PRO:HD2	1.76	0.44
14:L:11:LEU:HD22	14:L:93:SER:HA	1.99	0.44
16:N:7:GLY:O	16:N:9:VAL:HG23	2.18	0.44
1:X:38:G:H1	1:X:453:U:H3	1.64	0.44
1:X:252:G:H4'	1:X:252:G:OP1	2.17	0.44
1:X:573:C:H2'	1:X:574:C:O4'	2.18	0.44
1:X:1255:A:H2'	1:X:1256:C:C6	2.52	0.44
1:X:1811:A:O2'	1:X:1812:U:OP2	2.26	0.44
1:X:2195:C:H2'	1:X:2196:U:C5	2.53	0.44
1:X:2811:G:H2'	1:X:2812:A:C8	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:39:C:N4	2:Y:50:U:O2'	2.51	0.44
18:P:46:ARG:NE	18:P:95:ALA:O	2.51	0.44
19:Q:71:GLN:HG2	19:Q:72:ARG:HB2	1.99	0.44
1:X:334:G:N7	5:C:164:VAL:HA	2.33	0.44
1:X:636:G:O2'	1:X:669:G:H4'	2.18	0.44
1:X:1201:G:H5"	17:O:80:TYR:CE1	2.52	0.44
1:X:1585:A:H2'	1:X:1586:A:C8	2.53	0.44
1:X:1998:A:N3	26:Z:6:VAL:HG12	2.33	0.44
1:X:2196:U:H3'	1:X:2197:U:C4'	2.48	0.44
12:J:76:THR:HB	12:J:88:LYS:O	2.18	0.44
18:P:28:ALA:O	18:P:123:HIS:HA	2.17	0.44
20:R:15:HIS:O	20:R:16:PHE:CG	2.71	0.44
25:W:16:GLN:O	25:W:20:VAL:HG23	2.18	0.44
1:X:998:C:H2'	1:X:999:A:O4'	2.18	0.44
1:X:1313:U:H4'	1:X:1314:A:C5'	2.46	0.44
1:X:1769:U:C4	1:X:1775:A:C8	3.05	0.44
1:X:2297:G:O2'	1:X:2300:G:O6	2.22	0.44
1:X:2362:G:H21	1:X:2363:G:H1'	1.83	0.44
4:B:203:LYS:HA	4:B:203:LYS:HD2	1.53	0.44
5:C:176:ASN:OD1	5:C:178:TYR:HB3	2.18	0.44
9:G:93:LYS:HZ3	9:G:93:LYS:HG2	1.34	0.44
15:M:29:PRO:O	15:M:96:ARG:NH1	2.50	0.44
1:X:79:G:H1	1:X:104:C:H42	1.65	0.44
1:X:356:A:H2'	1:X:357:A:C8	2.53	0.44
1:X:712:A:H2'	1:X:713:G:O4'	2.18	0.44
1:X:939:C:OP2	1:X:940:G:C8	2.71	0.44
1:X:1021:A:H1'	1:X:1164:C:H1'	1.99	0.44
1:X:1094:C:O2	1:X:1096:A:H2'	2.18	0.44
1:X:1987:G:C5	1:X:1988:A:C8	3.06	0.44
1:X:2653:A:O3'	10:H:42:LYS:HA	2.18	0.44
2:Y:25:G:H1	2:Y:62:C:H42	1.66	0.44
3:A:3:VAL:HG13	3:A:17:THR:HG23	1.98	0.44
5:C:1:MET:HA	5:C:14:THR:HA	2.00	0.44
6:D:13:ARG:NH1	6:D:14:PRO:HG3	2.33	0.44
19:Q:60:GLY:HA3	19:Q:74:ASP:H	1.83	0.44
1:X:945:G:H2'	1:X:946:U:H6	1.82	0.43
1:X:1072:U:O4'	1:X:1081:A:H1'	2.17	0.43
1:X:2364:C:H2'	1:X:2365:U:C6	2.53	0.43
2:Y:28:A:C8	2:Y:29:C:C2	3.06	0.43
4:B:10:GLY:O	4:B:25:VAL:HG23	2.18	0.43
10:H:28:GLY:CA	10:H:50:ILE:HD11	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L:28:ARG:O	14:L:43:ILE:HD12	2.17	0.43
16:N:22:LYS:C	16:N:24:PHE:H	2.21	0.43
21:S:48:THR:HG22	21:S:66:VAL:O	2.18	0.43
29:3:9:MET:HA	29:3:12:ARG:HB3	1.99	0.43
1:X:1194:U:O2'	1:X:1195:U:O4'	2.37	0.43
1:X:1655:C:H5"	1:X:2689:C:O2'	2.19	0.43
3:A:61:LEU:HB2	3:A:63:ARG:HH12	1.84	0.43
4:B:14:ILE:HG12	15:M:20:HIS:NE2	2.33	0.43
4:B:55:ALA:HB3	4:B:58:LYS:HE2	2.01	0.43
6:D:135:GLN:HG3	6:D:136:LEU:HD23	2.01	0.43
11:I:42:GLY:HA2	11:I:45:LYS:HZ1	1.82	0.43
14:L:96:TYR:O	14:L:97:HIS:ND1	2.38	0.43
21:S:84:TYR:CG	21:S:85:MET:N	2.86	0.43
21:S:122:ILE:O	21:S:123:VAL:HB	2.18	0.43
1:X:13:A:N3	1:X:15:G:C6	2.86	0.43
1:X:564:U:H2'	1:X:565:A:C8	2.54	0.43
1:X:1374:G:N2	1:X:1384:G:H1'	2.33	0.43
1:X:2023:C:H2'	1:X:2024:U:C6	2.53	0.43
3:A:128:GLY:HA2	3:A:192:THR:HG23	2.00	0.43
5:C:116:LYS:HZ2	5:C:116:LYS:HA	1.84	0.43
5:C:147:LYS:H	5:C:184:ASP:CG	2.21	0.43
12:J:15:ARG:HD2	12:J:73:LYS:HG3	2.00	0.43
17:O:10:LYS:CG	17:O:11:GLN:HG2	2.48	0.43
18:P:21:ARG:HD3	18:P:83:ASP:OD1	2.18	0.43
18:P:40:LEU:HD12	26:Z:25:LEU:HD13	1.99	0.43
20:R:88:THR:HG22	20:R:89:GLY:H	1.83	0.43
24:V:17:GLU:O	24:V:21:ARG:HD3	2.18	0.43
1:X:205:A:H2'	1:X:206:U:H5'	2.00	0.43
1:X:538:A:H2'	1:X:538:A:N3	2.33	0.43
1:X:636:G:N7	11:I:101:ARG:NH1	2.63	0.43
1:X:1173:G:H4'	17:O:22:VAL:HG22	1.99	0.43
1:X:1310:C:C2	1:X:1311:C:C5	3.06	0.43
1:X:1418:C:H2'	1:X:1419:G:C8	2.54	0.43
1:X:2287:G:O2'	1:X:2288:A:P	2.76	0.43
1:X:2621:G:OP1	9:G:110:LEU:HD13	2.18	0.43
1:X:2871:U:H2'	1:X:2872:U:C6	2.54	0.43
2:Y:53:G:C6	14:L:36:LYS:HD2	2.52	0.43
3:A:27:LYS:HE2	3:A:27:LYS:HB2	1.88	0.43
5:C:47:THR:HB	5:C:48:ARG:H	1.46	0.43
17:O:30:GLY:O	17:O:60:VAL:HG23	2.18	0.43
1:X:70:A:H5"	1:X:71:A:H2'	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:387:A:H5'	1:X:435:A:H2	1.84	0.43
1:X:415:A:N6	1:X:416:U:O4	2.51	0.43
1:X:759:C:HO2'	1:X:2590:U:HO2'	1.64	0.43
1:X:1040:A:C8	1:X:1041:G:C8	3.06	0.43
1:X:1670:G:C6	13:K:9:LYS:HD3	2.53	0.43
1:X:2069:U:H2'	1:X:2070:G:C8	2.53	0.43
1:X:2262:C:C2	1:X:2368:G:C2	3.07	0.43
2:Y:34:C:H2'	2:Y:35:C:C6	2.54	0.43
4:B:79:ARG:HA	4:B:79:ARG:HD3	1.87	0.43
5:C:30:VAL:HA	5:C:95:LEU:HD11	2.01	0.43
6:D:148:LYS:HE3	6:D:150:ARG:HG3	1.99	0.43
9:G:63:ARG:HA	9:G:63:ARG:HD2	1.83	0.43
11:I:34:HIS:O	11:I:35:LYS:HE3	2.17	0.43
11:I:129:ALA:O	11:I:133:VAL:HG23	2.19	0.43
20:R:81:VAL:HG13	20:R:82:ALA:N	2.32	0.43
22:T:74:LYS:HB3	22:T:75:GLY:H	1.57	0.43
1:X:618:A:H2'	1:X:619:A:C8	2.53	0.43
1:X:1357:U:H4'	1:X:1397:A:C6	2.53	0.43
1:X:2476:A:N3	1:X:2477:C:N4	2.67	0.43
4:B:122:PHE:HE2	4:B:138:PRO:HA	1.83	0.43
5:C:144:GLY:HA2	5:C:166:TRP:CD2	2.53	0.43
16:N:70:ARG:HG2	16:N:74:MET:O	2.18	0.43
20:R:22:VAL:HG23	20:R:83:LEU:H	1.82	0.43
20:R:35:LYS:HE2	20:R:35:LYS:HB3	1.88	0.43
23:U:8:THR:HA	23:U:14:VAL:HG22	1.99	0.43
1:X:389:G:H2'	1:X:390:U:C6	2.54	0.43
1:X:458:G:H4'	1:X:459:A:H5'	2.01	0.43
1:X:755:C:H2'	1:X:756:C:C6	2.49	0.43
1:X:836:G:H2'	1:X:837:U:C6	2.53	0.43
1:X:854:G:N2	1:X:948:C:N3	2.56	0.43
1:X:914:C:H2'	1:X:915:C:C6	2.54	0.43
3:A:45:ASN:CG	3:A:46:ARG:H	2.22	0.43
4:B:6:GLY:HA2	4:B:51:TYR:CZ	2.54	0.43
6:D:66:ILE:N	6:D:88:LYS:O	2.46	0.43
13:K:87:TYR:CE1	13:K:94:TYR:HD2	2.35	0.43
24:V:11:ALA:HA	24:V:14:PHE:HB2	2.01	0.43
1:X:479:G:C6	1:X:480:G:C4	3.07	0.43
1:X:1413:U:H2'	1:X:1414:G:H8	1.84	0.43
1:X:2201:G:H5"	3:A:186:HIS:NE2	2.33	0.43
5:C:144:GLY:HA2	5:C:166:TRP:CE2	2.54	0.43
20:R:77:HIS:HB3	20:R:79:SER:H	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:U:34:THR:OG1	23:U:35:THR:N	2.52	0.43
28:2:10:ARG:O	28:2:14:LYS:HB2	2.19	0.43
1:X:8:A:H2'	1:X:9:U:C6	2.53	0.43
1:X:759:C:H1'	18:P:111:ARG:HH22	1.84	0.43
1:X:787:A:H2	1:X:800:U:O2'	1.99	0.43
1:X:2263:C:H3'	27:1:28:ARG:HH12	1.82	0.43
1:X:2279:G:H8	1:X:2279:G:O5'	2.02	0.43
1:X:2474:G:H4'	12:J:82:THR:HA	1.99	0.43
29:3:22:VAL:HG21	29:3:53:ALA:HB1	2.01	0.43
1:X:170:U:N3	1:X:180:C:O2	2.51	0.43
1:X:338:G:H5'	20:R:9:HIS:CE1	2.54	0.43
1:X:504:G:H4'	18:P:27:VAL:CG1	2.47	0.43
1:X:1194:U:O2'	1:X:1195:U:H6	2.02	0.43
1:X:1596:A:H2'	1:X:1597:A:O4'	2.18	0.43
1:X:2237:C:H3'	1:X:2238:G:H8	1.83	0.43
1:X:2260:C:O2'	1:X:2261:G:H5'	2.19	0.43
1:X:2314:A:O2'	1:X:2315:A:H8	2.02	0.43
1:X:2628:C:H2'	1:X:2629:U:H6	1.83	0.43
1:X:2845:C:C2'	1:X:2846:G:H5'	2.48	0.43
3:A:33:LEU:HD12	3:A:104:TYR:HD2	1.84	0.43
6:D:40:LEU:H	6:D:86:GLY:HA2	1.83	0.43
9:G:67:ARG:HB2	9:G:70:PHE:H	1.84	0.43
10:H:89:ILE:HG12	15:M:79:ARG:HD3	2.00	0.43
11:I:62:LYS:HD3	11:I:63:ARG:N	2.33	0.43
16:N:109:LEU:HD22	16:N:109:LEU:HA	1.84	0.43
22:T:33:ALA:HB2	22:T:64:ASP:OD1	2.19	0.43
23:U:20:ARG:HD2	23:U:43:ARG:NE	2.34	0.43
23:U:65:ASN:O	23:U:68:ARG:HB2	2.18	0.43
1:X:393:U:H2'	1:X:394:U:C6	2.54	0.42
1:X:1383:C:H3'	1:X:1384:G:H8	1.83	0.42
1:X:2043:A:H1'	1:X:2481:G:C1'	2.49	0.42
1:X:2234:G:H2'	1:X:2235:G:O4'	2.18	0.42
1:X:2310:G:H4'	22:T:43:THR:H	1.84	0.42
1:X:2631:C:H2'	1:X:2632:U:O4'	2.19	0.42
3:A:128:GLY:HA2	3:A:192:THR:CG2	2.49	0.42
5:C:31:VAL:HA	5:C:34:GLN:HB2	2.00	0.42
9:G:116:ARG:HB2	9:G:118:ALA:H	1.84	0.42
10:H:76:ARG:NE	15:M:75:GLU:OE1	2.45	0.42
13:K:2:ARG:O	13:K:5:LYS:NZ	2.47	0.42
15:M:103:LYS:HA	15:M:103:LYS:HD2	1.73	0.42
21:S:72:ASP:OD2	21:S:75:LYS:HD3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:175:C:H2'	1:X:176:A:H5"	2.01	0.42
1:X:430:C:H1'	1:X:2386:G:N2	2.35	0.42
1:X:761:G:O5'	18:P:110:ALA:HB2	2.19	0.42
1:X:1999:U:O2'	26:Z:7:PRO:O	2.31	0.42
1:X:2362:G:N2	1:X:2363:G:H1'	2.34	0.42
4:B:110:GLY:HA3	4:B:161:GLY:HA3	2.00	0.42
11:I:62:LYS:HE2	11:I:64:GLY:N	2.34	0.42
12:J:15:ARG:HB2	12:J:15:ARG:NH1	2.31	0.42
1:X:95:G:H2'	1:X:96:C:C6	2.54	0.42
1:X:224:G:H4'	1:X:399:G:C5	2.53	0.42
1:X:640:C:H4'	1:X:660:G:H21	1.83	0.42
1:X:705:C:H5"	3:A:40:THR:O	2.19	0.42
1:X:1469:U:O2'	1:X:1470:G:O5'	2.31	0.42
1:X:1515:U:H2'	1:X:1516:A:C8	2.54	0.42
1:X:2026:C:H2'	1:X:2027:C:H6	1.85	0.42
1:X:2269:G:N2	1:X:2322:U:H1'	2.34	0.42
1:X:2442:C:H2'	1:X:2443:C:H6	1.84	0.42
4:B:6:GLY:HA3	4:B:28:ALA:HA	2.01	0.42
5:C:22:VAL:CG1	5:C:106:MET:HB3	2.49	0.42
5:C:116:LYS:NZ	5:C:186:LEU:O	2.48	0.42
13:K:29:LEU:HA	13:K:29:LEU:HD23	1.81	0.42
21:S:97:PRO:HA	21:S:119:ASN:H	1.83	0.42
24:V:14:PHE:O	24:V:18:ILE:HG13	2.19	0.42
1:X:591:G:H2'	1:X:592:G:C8	2.54	0.42
1:X:938:G:HO2'	1:X:939:C:P	2.42	0.42
1:X:1278:A:N6	1:X:1996:A:H5"	2.34	0.42
1:X:1699:A:H2'	1:X:1700:C:C6	2.54	0.42
1:X:2532:G:C2	1:X:2533:U:H1'	2.55	0.42
1:X:2695:C:C2	1:X:2696:A:C8	3.08	0.42
2:Y:30:C:OP1	14:L:37:HIS:CE1	2.72	0.42
3:A:37:LEU:H	3:A:37:LEU:HD22	1.85	0.42
4:B:133:LYS:O	4:B:134:TRP:C	2.57	0.42
5:C:158:ARG:O	5:C:161:ALA:HB2	2.19	0.42
9:G:70:PHE:HB3	16:N:64:ARG:NE	2.34	0.42
10:H:28:GLY:O	10:H:29:ILE:HG13	2.20	0.42
11:I:91:ASP:HB3	11:I:121:HIS:CD2	2.54	0.42
11:I:93:LEU:HD22	11:I:93:LEU:HA	1.71	0.42
14:L:87:VAL:HA	14:L:108:ARG:NH2	2.34	0.42
20:R:92:THR:HA	20:R:108:VAL:HB	2.00	0.42
21:S:46:GLN:O	21:S:49:THR:OG1	2.31	0.42
1:X:182:G:HO2'	1:X:183:U:P	2.43	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:383:G:H4'	1:X:384:A:OP2	2.19	0.42
1:X:1361:G:H1	1:X:1614:C:N4	2.17	0.42
1:X:1448:A:H61	1:X:1574:A:N6	2.15	0.42
1:X:1842:G:H1	1:X:1875:C:H42	1.67	0.42
1:X:2044:G:H2'	1:X:2480:C:O2'	2.19	0.42
1:X:2442:C:H2'	1:X:2443:C:C6	2.54	0.42
1:X:2708:U:H2'	1:X:2709:C:H6	1.85	0.42
3:A:21:PHE:O	3:A:22:SER:HB3	2.20	0.42
9:G:30:LYS:NZ	17:O:13:ARG:HH22	2.18	0.42
12:J:55:MET:HG2	12:J:118:ALA:O	2.19	0.42
12:J:135:ARG:H	12:J:135:ARG:HG3	1.66	0.42
14:L:8:ARG:HE	14:L:9:ARG:HG3	1.84	0.42
17:O:27:GLY:H	17:O:60:VAL:HG21	1.84	0.42
20:R:88:THR:HB	20:R:90:LYS:HG3	2.02	0.42
22:T:19:LYS:HD3	22:T:19:LYS:HA	1.84	0.42
29:3:50:LEU:HA	29:3:53:ALA:HB3	2.01	0.42
1:X:1332:G:C2	1:X:1333:G:C2	3.08	0.42
1:X:1479:G:H2'	1:X:1480:G:H8	1.84	0.42
1:X:1908:C:O2'	1:X:1909:U:OP1	2.37	0.42
1:X:2756:A:H3'	1:X:2756:A:OP1	2.19	0.42
33:X:3322:SPD:H51	33:X:3322:SPD:H82	1.85	0.42
5:C:33:TRP:HB2	5:C:93:TYR:OH	2.19	0.42
6:D:107:GLY:HA2	6:D:139:PRO:HD3	2.01	0.42
11:I:13:ARG:HD3	11:I:14:LYS:HG3	2.01	0.42
16:N:97:ASP:OD1	16:N:101:ARG:NH1	2.53	0.42
18:P:101:PRO:O	18:P:121:THR:OG1	2.27	0.42
19:Q:28:TRP:CZ3	19:Q:75:ARG:HG3	2.54	0.42
21:S:93:GLU:HG2	21:S:123:VAL:HB	2.01	0.42
1:X:39:C:H2'	1:X:40:U:C6	2.54	0.42
1:X:597:U:O4	1:X:683:A:H1'	2.19	0.42
1:X:1386:A:H5"	1:X:2191:A:N6	2.35	0.42
1:X:1815:G:H2'	1:X:1816:G:H8	1.85	0.42
1:X:2226:A:H2'	1:X:2227:C:H6	1.84	0.42
1:X:2329:C:H2'	1:X:2330:G:O4'	2.20	0.42
1:X:2628:C:H2'	1:X:2629:U:C6	2.55	0.42
2:Y:116:C:H4'	14:L:49:GLN:HG2	2.00	0.42
5:C:143:ASP:HB2	5:C:145:THR:H	1.85	0.42
12:J:73:LYS:HA	12:J:74:PRO:HD2	1.96	0.42
15:M:55:ILE:O	15:M:104:LEU:HB2	2.20	0.42
19:Q:17:TYR:O	19:Q:20:MET:HB3	2.20	0.42
19:Q:82:LEU:HD11	19:Q:88:ILE:HG23	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:1:51:ARG:HH11	27:1:53:LYS:HG2	1.85	0.42
1:X:64:C:OP1	19:Q:71:GLN:HB2	2.20	0.42
1:X:2007:G:C2	1:X:2023:C:C2	3.07	0.42
1:X:2398:U:OP1	29:3:41:ILE:HG21	2.20	0.42
1:X:2794:G:O2'	1:X:2795:A:H5"	2.20	0.42
5:C:30:VAL:HG11	5:C:177:VAL:HG21	2.01	0.42
5:C:99:VAL:O	5:C:103:GLY:N	2.52	0.42
9:G:85:ALA:HB3	9:G:152:ALA:HA	2.02	0.42
9:G:124:GLU:OE2	9:G:152:ALA:N	2.52	0.42
14:L:15:ARG:HA	14:L:15:ARG:HD3	1.72	0.42
14:L:26:ARG:CZ	14:L:87:VAL:HG22	2.50	0.42
14:L:42:ILE:HG13	14:L:88:VAL:HG11	2.01	0.42
15:M:85:SER:HA	15:M:86:PRO:HD3	1.83	0.42
18:P:25:PHE:HA	18:P:127:ILE:HG12	2.02	0.42
18:P:46:ARG:HH11	18:P:46:ARG:HG2	1.84	0.42
20:R:38:LEU:HB3	20:R:47:VAL:CG2	2.49	0.42
28:2:15:THR:O	28:2:17:GLY:N	2.53	0.42
1:X:640:C:H1'	1:X:650:U:H1'	2.02	0.42
1:X:1217:U:O2	11:I:13:ARG:HB3	2.19	0.42
1:X:1996:A:H4'	18:P:117:ILE:HD13	2.02	0.42
3:A:89:SER:O	3:A:159:ALA:HB2	2.19	0.42
3:A:142:VAL:HG12	3:A:193:ILE:HA	2.01	0.42
3:A:267:ASP:O	3:A:268:ARG:HD2	2.20	0.42
4:B:15:TRP:NE1	4:B:20:ALA:HB2	2.35	0.42
7:E:21:ASP:HB3	7:E:22:GLY:H	1.63	0.42
14:L:35:SER:OG	14:L:36:LYS:N	2.52	0.42
19:Q:12:ILE:H	19:Q:12:ILE:HG13	1.72	0.42
22:T:45:PHE:CE1	22:T:69:PHE:HE2	2.37	0.42
23:U:61:TRP:O	23:U:62:LEU:HD12	2.20	0.42
29:3:6:THR:CG2	29:3:59:LYS:HG3	2.49	0.42
1:X:88:G:C8	1:X:89:A:H2'	2.55	0.42
1:X:321:A:C6	1:X:323:G:C4	3.07	0.42
1:X:958:G:H2'	1:X:959:C:C6	2.54	0.42
1:X:960:U:H2'	1:X:961:G:C8	2.55	0.42
1:X:1007:A:O3'	16:N:93:LYS:HB3	2.19	0.42
1:X:1377:G:O5'	23:U:7:LEU:HD21	2.20	0.42
1:X:1411:C:N4	1:X:1412:C:H41	2.18	0.42
1:X:1625:A:H4'	1:X:1626:A:OP1	2.18	0.42
1:X:2796:A:P	4:B:111:LYS:HZ3	2.43	0.42
13:K:76:VAL:O	13:K:79:VAL:HG22	2.20	0.42
17:O:34:GLU:HB2	17:O:56:VAL:HG23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:585:U:H4'	1:X:2481:G:C8	2.55	0.41
1:X:1330:G:H2'	1:X:1331:G:O4'	2.20	0.41
1:X:1370:U:H3'	1:X:1371:G:H8	1.83	0.41
1:X:1391:A:O2'	1:X:1393:G:N7	2.42	0.41
1:X:1539:U:H2'	1:X:1540:C:C6	2.55	0.41
1:X:1703:C:H2'	1:X:1704:G:O4'	2.19	0.41
1:X:2510:A:C8	7:E:175:LYS:HB2	2.54	0.41
6:D:171:GLN:HA	6:D:175:LEU:HD22	2.01	0.41
16:N:40:LEU:HD12	17:O:74:TYR:CE1	2.55	0.41
16:N:61:TRP:O	16:N:65:ILE:HG13	2.20	0.41
19:Q:11:VAL:HG23	19:Q:27:PHE:HA	2.01	0.41
20:R:44:GLN:HB3	20:R:45:LYS:H	1.65	0.41
1:X:839:U:OP1	1:X:2407:G:H3'	2.21	0.41
1:X:1693:A:H2	1:X:1976:U:H5'	1.84	0.41
1:X:2170:C:H3'	1:X:2171:U:C5'	2.50	0.41
2:Y:70:C:H2'	2:Y:71:G:O4'	2.20	0.41
3:A:80:ALA:N	3:A:95:LEU:HA	2.34	0.41
5:C:46:ARG:HD2	5:C:46:ARG:HA	1.75	0.41
5:C:48:ARG:O	5:C:50:GLN:N	2.53	0.41
5:C:58:MET:HG2	5:C:59:TYR:H	1.85	0.41
6:D:36:VAL:HG11	6:D:57:LEU:HD21	2.02	0.41
9:G:169:GLN:HG3	9:G:171:LEU:N	2.35	0.41
10:H:28:GLY:O	10:H:34:LEU:HA	2.20	0.41
14:L:28:ARG:CG	14:L:90:ASP:HB2	2.50	0.41
25:W:4:LYS:HE2	25:W:4:LYS:HB3	1.88	0.41
25:W:12:ARG:HD2	25:W:13:PRO:HD2	2.02	0.41
1:X:17:G:H2'	1:X:18:U:C6	2.55	0.41
1:X:334:G:OP1	1:X:349:G:N2	2.53	0.41
1:X:812:G:H2'	1:X:813:A:C8	2.56	0.41
1:X:1060:C:H1'	1:X:1124:U:O2'	2.19	0.41
1:X:1310:C:H2'	1:X:1311:C:C6	2.55	0.41
1:X:1793:A:H2'	1:X:1794:A:C8	2.55	0.41
1:X:1979:C:H4'	1:X:1980:A:OP1	2.20	0.41
1:X:2042:A:O3'	5:C:63:GLY:HA2	2.20	0.41
1:X:2293:G:H2'	1:X:2294:U:C6	2.55	0.41
1:X:2870:C:H2'	1:X:2871:U:H6	1.84	0.41
2:Y:98:C:H2'	2:Y:99:G:C8	2.55	0.41
20:R:56:LYS:H	20:R:56:LYS:HD3	1.85	0.41
26:Z:35:GLN:HE21	26:Z:51:TYR:HD2	1.67	0.41
1:X:494:A:O4'	20:R:56:LYS:HB2	2.20	0.41
1:X:1745:C:OP1	15:M:101:ARG:NH2	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1817:U:H5"	3:A:247:VAL:HG11	2.02	0.41
1:X:2504:G:C2	1:X:2518:C:C2	3.08	0.41
1:X:2771:C:H2'	1:X:2772:U:O4'	2.21	0.41
5:C:137:ALA:HB1	5:C:142:LEU:HB2	2.03	0.41
9:G:51:LEU:HD13	9:G:88:VAL:HG21	2.03	0.41
9:G:67:ARG:CD	9:G:70:PHE:HA	2.45	0.41
9:G:69:ASP:OD2	9:G:76:GLN:HB3	2.21	0.41
9:G:75:ILE:HG13	9:G:75:ILE:O	2.20	0.41
10:H:70:VAL:HG22	10:H:71:LYS:N	2.36	0.41
11:I:93:LEU:HB3	11:I:97:ARG:HB2	2.01	0.41
12:J:83:ARG:HD3	12:J:83:ARG:HA	1.89	0.41
21:S:99:HIS:CD2	21:S:133:GLU:HB2	2.55	0.41
21:S:137:ASP:O	21:S:140:LYS:HE2	2.21	0.41
26:Z:49:CYS:SG	26:Z:51:TYR:HB2	2.61	0.41
1:X:186:C:H2'	1:X:187:U:C6	2.56	0.41
1:X:1429:A:H62	1:X:1600:U:H4'	1.85	0.41
1:X:1463:A:H2'	1:X:1464:A:H8	1.83	0.41
1:X:1693:A:H2'	1:X:1694:A:O4'	2.20	0.41
1:X:1718[A]:A:H2'	1:X:1718[A]:A:P	2.61	0.41
1:X:1750:A:H4'	1:X:2695:C:O4'	2.20	0.41
1:X:2287:G:HO2'	1:X:2288:A:P	2.43	0.41
3:A:33:LEU:HD22	3:A:33:LEU:HA	1.86	0.41
3:A:164:GLN:NE2	3:A:166:GLN:OE1	2.35	0.41
5:C:9:GLN:OE1	5:C:12:GLY:HA2	2.21	0.41
5:C:57:LYS:CG	5:C:58:MET:H	2.34	0.41
6:D:45:GLU:HB3	6:D:49:ALA:H	1.84	0.41
17:O:49:GLU:O	17:O:52:GLY:N	2.53	0.41
1:X:451:A:H2'	1:X:452:G:C8	2.55	0.41
1:X:871:U:O2	1:X:2247:A:H2'	2.21	0.41
1:X:1054:C:N4	1:X:1123:G:H1	2.19	0.41
1:X:2195:C:H5'	1:X:2196:U:OP1	2.21	0.41
1:X:2433:G:H1'	32:X:3316:MPD:C4	2.51	0.41
3:A:12:SER:HG	3:A:13:ARG:H	1.67	0.41
3:A:37:LEU:HB2	3:A:39:LYS:NZ	2.34	0.41
3:A:85:ASP:HA	3:A:86:PRO:HD2	1.82	0.41
4:B:95:ILE:HD13	4:B:95:ILE:HA	1.87	0.41
6:D:170:LEU:O	6:D:175:LEU:HB3	2.20	0.41
13:K:99:ARG:HG2	13:K:99:ARG:NH1	2.35	0.41
15:M:37:THR:O	15:M:87:LEU:HD13	2.21	0.41
1:X:500:G:C2	1:X:501:G:H1'	2.56	0.41
1:X:854:G:H1	1:X:948:C:N4	2.15	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:874:A:H2'	1:X:875:G:O4'	2.19	0.41
1:X:1161:U:H2'	1:X:1162:A:C8	2.56	0.41
1:X:1301:U:C2	1:X:1340:C:O2	2.74	0.41
1:X:1333:G:N2	1:X:1344:C:H41	2.18	0.41
1:X:1815:G:H2'	1:X:1816:G:C8	2.55	0.41
1:X:1943:A:H5'	1:X:1944:C:OP2	2.21	0.41
1:X:2044:G:N2	1:X:2046:C:C2	2.89	0.41
1:X:2433:G:C4	1:X:2434:G:C8	3.09	0.41
1:X:2705:A:O2'	1:X:2706:U:C6	2.73	0.41
2:Y:42:U:H2'	2:Y:45:C:H5	1.86	0.41
2:Y:44:C:O2	6:D:90:THR:N	2.36	0.41
2:Y:56:G:H21	6:D:26:MET:HG3	1.85	0.41
3:A:252:LYS:HB2	3:A:255:LYS:NZ	2.36	0.41
4:B:99:GLY:O	4:B:171:GLU:HG3	2.21	0.41
4:B:194:GLY:HA2	15:M:2:GLN:HB3	2.03	0.41
5:C:6:VAL:HG21	5:C:136:TRP:HZ2	1.85	0.41
14:L:12:ARG:HD2	14:L:92:GLY:HA2	2.02	0.41
14:L:29:LEU:HB2	14:L:88:VAL:HG12	2.01	0.41
14:L:55:SER:O	14:L:71:VAL:HB	2.21	0.41
23:U:52:ARG:HG2	23:U:79:GLU:OE1	2.21	0.41
27:1:9:ILE:O	27:1:10:VAL:HB	2.21	0.41
1:X:613:A:H5"	1:X:668:A:H61	1.86	0.41
1:X:670:U:H2'	1:X:671:A:C8	2.55	0.41
1:X:1142:G:O4'	9:G:111:LYS:HD3	2.21	0.41
1:X:1631:C:C2	18:P:108:PRO:HG3	2.56	0.41
1:X:1981:A:O2'	1:X:2704:U:O2'	2.22	0.41
1:X:2262:C:H2'	1:X:2263:C:O4'	2.20	0.41
6:D:44:LYS:HD2	6:D:44:LYS:HA	1.90	0.41
12:J:70:PHE:HA	12:J:71:PRO:HD3	1.81	0.41
25:W:4:LYS:HZ1	25:W:54:GLN:HB2	1.85	0.41
29:3:16:ILE:HB	29:3:64:ARG:HA	2.03	0.41
1:X:89:A:H4'	1:X:90:G:H5'	2.03	0.41
1:X:322:A:H3'	1:X:323:G:C8	2.56	0.41
1:X:328:A:H2'	1:X:329:C:C6	2.56	0.41
1:X:953:G:H5"	11:I:38:LYS:HA	2.02	0.41
1:X:1050:G:H1	1:X:1127:C:H42	1.67	0.41
1:X:1172:U:O2'	17:O:21:ARG:HG3	2.20	0.41
1:X:1488:G:HO2'	1:X:1489:C:H5	1.66	0.41
1:X:1584:G:OP2	3:A:63:ARG:NH2	2.53	0.41
1:X:1684:G:O2'	1:X:1974:U:O4	2.32	0.41
1:X:2021:G:C6	1:X:2022:C:C4	3.08	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2262:C:C5	1:X:2368:G:H2'	2.56	0.41
1:X:2290:A:N7	1:X:2291:U:C4	2.89	0.41
1:X:2557:G:OP1	1:X:2593:A:N6	2.53	0.41
1:X:2817:A:H2'	1:X:2818:G:O4'	2.21	0.41
2:Y:37:C:H2'	2:Y:38:C:O4'	2.21	0.41
3:A:79:VAL:HA	3:A:95:LEU:HB3	2.03	0.41
5:C:128:ALA:O	5:C:130:THR:N	2.51	0.41
6:D:66:ILE:HG23	6:D:88:LYS:HB3	2.02	0.41
6:D:175:LEU:H	6:D:175:LEU:HD23	1.86	0.41
9:G:32:TYR:CE2	9:G:34:PRO:HG3	2.56	0.41
10:H:113:PRO:HD3	15:M:73:PHE:HB2	2.03	0.41
12:J:59:PHE:C	12:J:61:ARG:H	2.24	0.41
13:K:59:ASP:OD1	13:K:59:ASP:N	2.54	0.41
14:L:51:LEU:HD22	14:L:84:ILE:HG21	2.02	0.41
20:R:23:ILE:H	20:R:81:VAL:HG12	1.86	0.41
20:R:72:ARG:HB3	20:R:73:GLU:H	1.62	0.41
21:S:62:PHE:HB2	21:S:85:MET:CE	2.51	0.41
1:X:474:G:N2	1:X:477:A:OP2	2.37	0.41
1:X:1020:A:OP1	9:G:65:LYS:NZ	2.45	0.41
1:X:1296:G:H4'	33:X:3322:SPD:HN6	1.86	0.41
1:X:1954:A:HO2'	1:X:1955:G:P	2.40	0.41
1:X:2204:A:H1'	1:X:2205:C:OP2	2.21	0.41
1:X:2271:C:P	14:L:18:ARG:HH22	2.43	0.41
1:X:2812:A:H2'	1:X:2813:G:H8	1.84	0.41
2:Y:78:A:H2'	2:Y:79:U:O4'	2.20	0.41
3:A:69:ARG:NH1	3:A:130:ALA:HB2	2.36	0.41
5:C:95:LEU:HD23	5:C:96:PRO:HD2	2.03	0.41
5:C:148:VAL:N	5:C:166:TRP:O	2.47	0.41
8:F:98:LYS:HE2	8:F:98:LYS:HB3	1.81	0.41
9:G:65:LYS:HD2	9:G:65:LYS:HA	1.82	0.41
12:J:124:HIS:O	12:J:125:LYS:HB2	2.21	0.41
15:M:32:THR:HG23	15:M:91:VAL:HG13	2.02	0.41
17:O:12:TYR:CB	17:O:40:VAL:HG22	2.51	0.41
20:R:15:HIS:ND1	20:R:82:ALA:HB2	2.36	0.41
23:U:15:VAL:HG13	23:U:45:ASN:O	2.21	0.41
27:1:38:LYS:O	27:1:49:VAL:HG23	2.21	0.41
29:3:28:GLY:HA2	29:3:29:LYS:HA	1.62	0.41
1:X:331:U:H4'	1:X:333:A:C8	2.56	0.40
1:X:485:G:C6	1:X:520:C:N4	2.88	0.40
1:X:492:G:O2'	1:X:516:G:N2	2.54	0.40
1:X:652:C:N4	1:X:657:A:H61	2.18	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1065:A:N6	1:X:1117:G:O6	2.54	0.40
1:X:2576:G:C5	1:X:2577:A:C6	3.08	0.40
3:A:38:PRO:HG3	3:A:60:ARG:O	2.20	0.40
9:G:101:THR:HA	9:G:112:THR:O	2.21	0.40
13:K:102:THR:H	13:K:102:THR:HG23	1.63	0.40
16:N:45:TYR:O	16:N:49:ASP:HB2	2.21	0.40
1:X:571:U:C2	1:X:581:A:C8	3.09	0.40
1:X:649:G:C6	1:X:662:G:N2	2.89	0.40
1:X:796:A:H8	1:X:797:A:H4'	1.85	0.40
1:X:1006:C:N3	9:G:31:THR:HG23	2.37	0.40
1:X:1156:U:H2'	1:X:1157:G:C8	2.56	0.40
1:X:1753:A:OP1	1:X:1753:A:H4'	2.21	0.40
1:X:2340:C:OP2	29:3:26:LYS:HE2	2.21	0.40
1:X:2481:G:H5"	1:X:2482:A:H5"	2.03	0.40
3:A:36:ALA:HB1	3:A:62:TYR:N	2.35	0.40
9:G:98:LYS:O	9:G:115:ALA:HB1	2.22	0.40
14:L:97:HIS:CG	14:L:98:GLY:H	2.37	0.40
18:P:11:LYS:HG3	18:P:14:ARG:NH2	2.36	0.40
18:P:32:ARG:O	18:P:33:MET:HG2	2.21	0.40
18:P:62:ARG:H	18:P:62:ARG:HG2	1.60	0.40
27:1:48:VAL:HG12	27:1:50:PHE:HE1	1.86	0.40
1:X:104:C:O2'	1:X:105:G:OP1	2.24	0.40
1:X:251:C:N4	1:X:269:G:N3	2.69	0.40
1:X:609:U:O2'	11:I:18:ARG:NH1	2.42	0.40
1:X:1231:A:H2'	1:X:1232:U:C6	2.56	0.40
1:X:1735:G:H2'	1:X:1736:C:C6	2.57	0.40
1:X:1835:C:H2'	1:X:1836:C:C6	2.56	0.40
1:X:2571:G:C6	1:X:2572:U:N3	2.90	0.40
2:Y:22:U:H1'	2:Y:66:G:H22	1.86	0.40
4:B:30:PRO:HB3	4:B:91:VAL:HG22	2.03	0.40
4:B:105:THR:HB	4:B:166:THR:HA	2.04	0.40
4:B:132:LYS:HZ2	4:B:132:LYS:HG3	1.60	0.40
6:D:65:PRO:HB3	6:D:89:VAL:HG22	2.02	0.40
9:G:85:ALA:HB3	9:G:152:ALA:CA	2.51	0.40
11:I:93:LEU:HB3	11:I:97:ARG:CB	2.51	0.40
14:L:90:ASP:CG	14:L:91:ARG:N	2.74	0.40
20:R:16:PHE:HE2	20:R:80:LYS:HZ1	1.69	0.40
21:S:5:ALA:O	21:S:33:ALA:HB3	2.21	0.40
21:S:168:VAL:HG12	21:S:169:VAL:HG23	2.03	0.40
23:U:10:LYS:HD2	23:U:10:LYS:HA	1.97	0.40
1:X:14:A:H5"	1:X:15:G:OP2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:59:G:O6	1:X:62:U:C2	2.75	0.40
1:X:63:A:H1'	19:Q:65:VAL:HB	2.04	0.40
1:X:388:G:H2'	1:X:389:G:O4'	2.21	0.40
1:X:626:A:H5'	5:C:38:ARG:NE	2.37	0.40
1:X:650:U:H2'	1:X:651:C:C6	2.56	0.40
1:X:1175:A:C2	1:X:1176:U:C2	3.10	0.40
1:X:1922:U:OP1	1:X:2583:U:O2'	2.39	0.40
1:X:2031:A:H2'	1:X:2032:G:O4'	2.21	0.40
2:Y:17:A:H1'	2:Y:112:A:C4	2.57	0.40
3:A:268:ARG:HA	3:A:268:ARG:CZ	2.52	0.40
5:C:7:ILE:HD12	5:C:7:ILE:HA	1.80	0.40
6:D:172:SER:N	6:D:175:LEU:HD22	2.37	0.40
10:H:97:VAL:HG21	10:H:126:ILE:HD11	2.04	0.40
11:I:93:LEU:H	11:I:97:ARG:NH1	2.19	0.40
13:K:10:LEU:O	13:K:12:ARG:HG2	2.22	0.40
14:L:70:ALA:O	14:L:74:ALA:N	2.50	0.40
17:O:36:LYS:HZ2	17:O:54:TYR:HB3	1.86	0.40
20:R:77:HIS:CG	20:R:78:ALA:H	2.39	0.40
25:W:47:VAL:HB	25:W:50:LEU:HD12	2.02	0.40
1:X:30:G:C6	1:X:31:C:C4	3.10	0.40
1:X:332:C:H5"	5:C:130:THR:OG1	2.22	0.40
1:X:387:A:H2	1:X:413:G:H21	1.70	0.40
1:X:661:C:N3	1:X:662:G:C2	2.90	0.40
1:X:844:G:C6	1:X:845:U:C4	3.09	0.40
1:X:1152:C:O2'	1:X:1153:A:OP1	2.33	0.40
1:X:1321:A:N6	1:X:1322:G:C2	2.90	0.40
1:X:1704:G:N2	1:X:1718[B]:A:H2	2.18	0.40
1:X:1800:A:HO2'	1:X:1802:A:H8	1.65	0.40
1:X:2293:G:H5'	6:D:35:VAL:HG11	2.03	0.40
1:X:2375:G:C2	1:X:2400:G:C2	3.10	0.40
3:A:245:VAL:O	3:A:253:PRO:HD2	2.21	0.40
9:G:61:ARG:HA	9:G:61:ARG:NE	2.36	0.40
13:K:29:LEU:HD13	13:K:79:VAL:CG1	2.51	0.40
18:P:10:ASN:OD1	18:P:12:LYS:HB3	2.22	0.40
18:P:29:LYS:HB3	18:P:30:TYR:CD2	2.56	0.40
21:S:130:ILE:H	21:S:130:ILE:HG13	1.52	0.40
23:U:48:LYS:HD3	23:U:48:LYS:HA	1.72	0.40
27:1:37:LEU:HA	27:1:51:ARG:HA	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	270/275 (98%)	226 (84%)	44 (16%)	0	100	100
4	B	203/211 (96%)	189 (93%)	13 (6%)	1 (0%)	29	65
5	C	193/205 (94%)	163 (84%)	27 (14%)	3 (2%)	9	41
6	D	175/180 (97%)	145 (83%)	27 (15%)	3 (2%)	9	40
7	E	169/185 (91%)	160 (95%)	8 (5%)	1 (1%)	25	61
8	F	61/144 (42%)	54 (88%)	6 (10%)	1 (2%)	9	41
9	G	140/174 (80%)	120 (86%)	16 (11%)	4 (3%)	4	29
10	H	132/134 (98%)	125 (95%)	7 (5%)	0	100	100
11	I	132/156 (85%)	103 (78%)	27 (20%)	2 (2%)	10	42
12	J	134/141 (95%)	111 (83%)	23 (17%)	0	100	100
13	K	113/116 (97%)	103 (91%)	10 (9%)	0	100	100
14	L	102/114 (90%)	79 (78%)	20 (20%)	3 (3%)	4	29
15	M	117/166 (70%)	109 (93%)	6 (5%)	2 (2%)	9	40
16	N	115/118 (98%)	105 (91%)	9 (8%)	1 (1%)	17	53
17	O	95/100 (95%)	83 (87%)	12 (13%)	0	100	100
18	P	126/134 (94%)	120 (95%)	6 (5%)	0	100	100
19	Q	91/95 (96%)	74 (81%)	15 (16%)	2 (2%)	6	35
20	R	108/115 (94%)	87 (81%)	20 (18%)	1 (1%)	17	53
21	S	178/237 (75%)	153 (86%)	21 (12%)	4 (2%)	6	35
22	T	72/91 (79%)	62 (86%)	10 (14%)	0	100	100
23	U	72/81 (89%)	52 (72%)	15 (21%)	5 (7%)	1	11
24	V	63/67 (94%)	59 (94%)	4 (6%)	0	100	100
25	W	53/55 (96%)	51 (96%)	2 (4%)	0	100	100
26	Z	55/60 (92%)	52 (94%)	3 (6%)	0	100	100
27	1	51/55 (93%)	33 (65%)	15 (29%)	3 (6%)	1	14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
28	2	44/47 (94%)	36 (82%)	7 (16%)	1 (2%)	6 34
29	3	57/66 (86%)	42 (74%)	13 (23%)	2 (4%)	3 25
All	All	3121/3522 (89%)	2696 (86%)	386 (12%)	39 (1%)	13 46

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	D	85	VAL
6	D	173	MET
9	G	85	ALA
28	2	39	ARG
29	3	40	GLU
5	C	22	VAL
9	G	103	TYR
9	G	114	THR
21	S	123	VAL
27	1	9	ILE
27	1	10	VAL
29	3	39	ASP
14	L	60	LYS
19	Q	6	ILE
19	Q	69	ILE
21	S	122	ILE
23	U	40	ARG
23	U	60	VAL
5	C	15	ILE
7	E	165	VAL
8	F	120	VAL
14	L	88	VAL
20	R	99	VAL
23	U	15	VAL
23	U	17	SER
23	U	32	ARG
4	B	40	GLN
6	D	172	SER
14	L	59	LEU
15	M	28	ARG
15	M	29	PRO
16	N	8	ILE
27	1	49	VAL
9	G	163	PRO

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Mol	Chain	Res	Type
21	S	81	VAL
11	I	68	VAL
5	C	18	PRO
11	I	19	VAL
21	S	125	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	A	212/216 (98%)	175 (82%)	37 (18%)	2 9
4	B	155/157 (99%)	134 (86%)	21 (14%)	4 19
5	C	155/163 (95%)	134 (86%)	21 (14%)	4 19
6	D	143/156 (92%)	126 (88%)	17 (12%)	5 23
7	E	136/144 (94%)	129 (95%)	7 (5%)	24 57
8	F	46/107 (43%)	44 (96%)	2 (4%)	29 62
9	G	118/146 (81%)	100 (85%)	18 (15%)	2 15
10	H	103/103 (100%)	84 (82%)	19 (18%)	1 7
11	I	96/121 (79%)	74 (77%)	22 (23%)	1 3
12	J	104/115 (90%)	81 (78%)	23 (22%)	1 3
13	K	92/93 (99%)	80 (87%)	12 (13%)	4 20
14	L	74/82 (90%)	49 (66%)	25 (34%)	0 1
15	M	99/134 (74%)	86 (87%)	13 (13%)	4 20
16	N	96/97 (99%)	87 (91%)	9 (9%)	8 34
17	O	76/79 (96%)	64 (84%)	12 (16%)	2 13
18	P	108/115 (94%)	95 (88%)	13 (12%)	5 23
19	Q	75/76 (99%)	64 (85%)	11 (15%)	3 16
20	R	88/96 (92%)	72 (82%)	16 (18%)	1 7
21	S	149/192 (78%)	130 (87%)	19 (13%)	4 20
22	T	55/67 (82%)	50 (91%)	5 (9%)	9 35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
23	U	55/66 (83%)	45 (82%)	10 (18%)	1 7
24	V	53/55 (96%)	50 (94%)	3 (6%)	20 53
25	W	48/48 (100%)	40 (83%)	8 (17%)	2 10
26	Z	49/53 (92%)	39 (80%)	10 (20%)	1 5
27	1	45/48 (94%)	34 (76%)	11 (24%)	0 3
28	2	39/40 (98%)	30 (77%)	9 (23%)	1 3
29	3	44/52 (85%)	28 (64%)	16 (36%)	0 1
All	All	2513/2821 (89%)	2124 (84%)	389 (16%)	2 14

All (389) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	3	VAL
3	A	13	ARG
3	A	15	GLN
3	A	26	LYS
3	A	27	LYS
3	A	28	ARG
3	A	33	LEU
3	A	37	LEU
3	A	39	LYS
3	A	40	THR
3	A	43	ARG
3	A	46	ARG
3	A	51	SER
3	A	63	ARG
3	A	87	ASN
3	A	88	ARG
3	A	106	LEU
3	A	111	LEU
3	A	138	VAL
3	A	143	HIS
3	A	148	VAL
3	A	151	LYS
3	A	186	HIS
3	A	200	GLU
3	A	206	LEU
3	A	208	LYS
3	A	212	SER
3	A	213	ARG

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Mol	Chain	Res	Type
3	A	214	TRP
3	A	218	LYS
3	A	220	HIS
3	A	245	VAL
3	A	247	VAL
3	A	248	THR
3	A	250	TRP
3	A	254	THR
3	A	260	ARG
4	B	4	ILE
4	B	5	LEU
4	B	26	VAL
4	B	59	VAL
4	B	60	ASN
4	B	84	PHE
4	B	105	THR
4	B	111	LYS
4	B	116	VAL
4	B	122	PHE
4	B	132	LYS
4	B	133	LYS
4	B	134	TRP
4	B	136	ARG
4	B	137	ARG
4	B	144	ARG
4	B	159	HIS
4	B	162	MET
4	B	182	ILE
4	B	188	ILE
4	B	203	LYS
5	C	5	ASN
5	C	7	ILE
5	C	16	GLU
5	C	21	GLU
5	C	28	HIS
5	C	34	GLN
5	C	45	THR
5	C	47	THR
5	C	94	THR
5	C	95	LEU
5	C	98	GLN
5	C	116	LYS

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Mol	Chain	Res	Type
5	C	145	THR
5	C	153	ASP
5	C	157	THR
5	C	162	ARG
5	C	166	TRP
5	C	169	VAL
5	C	175	VAL
5	C	186	LEU
5	C	188	ILE
6	D	37	ASN
6	D	45	GLU
6	D	51	ASP
6	D	52	LYS
6	D	57	LEU
6	D	66	ILE
6	D	67	ILE
6	D	71	LYS
6	D	83	MET
6	D	85	VAL
6	D	89	VAL
6	D	117	ILE
6	D	130	LEU
6	D	146	VAL
6	D	158	THR
6	D	175	LEU
6	D	177	PHE
7	E	34	THR
7	E	43	VAL
7	E	84	THR
7	E	125	VAL
7	E	129	THR
7	E	165	VAL
7	E	171	LEU
8	F	84	ILE
8	F	103	GLN
9	G	30	LYS
9	G	33	ILE
9	G	42	VAL
9	G	43	VAL
9	G	53	ARG
9	G	54	LEU
9	G	69	ASP

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Mol	Chain	Res	Type
9	G	71	THR
9	G	76	GLN
9	G	93	LYS
9	G	95	LEU
9	G	99	VAL
9	G	112	THR
9	G	119	LEU
9	G	151	TYR
9	G	161	GLN
9	G	168	THR
9	G	169	GLN
10	H	1	MET
10	H	5	GLN
10	H	7	ARG
10	H	9	ASP
10	H	10	VAL
10	H	19	ILE
10	H	35	THR
10	H	41	ASN
10	H	47	VAL
10	H	50	ILE
10	H	51	ILE
10	H	78	SER
10	H	81	ILE
10	H	102	GLN
10	H	106	ARG
10	H	120	ASP
10	H	126	ILE
10	H	127	VAL
10	H	133	VAL
11	I	12	SER
11	I	13	ARG
11	I	18	ARG
11	I	21	ARG
11	I	28	LYS
11	I	45	LYS
11	I	56	LEU
11	I	62	LYS
11	I	63	ARG
11	I	65	PHE
11	I	67	ASN
11	I	87	THR

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Mol	Chain	Res	Type
11	I	93	LEU
11	I	97	ARG
11	I	98	LEU
11	I	99	VAL
11	I	100	ARG
11	I	103	ASN
11	I	113	GLU
11	I	118	VAL
11	I	121	HIS
11	I	123	ASP
12	J	7	ARG
12	J	26	ASP
12	J	28	VAL
12	J	32	ASP
12	J	38	MET
12	J	64	LYS
12	J	68	ARG
12	J	69	ILE
12	J	72	ASP
12	J	84	MET
12	J	88	LYS
12	J	94	TRP
12	J	98	VAL
12	J	102	ARG
12	J	111	THR
12	J	114	GLN
12	J	125	LYS
12	J	128	ILE
12	J	133	VAL
12	J	134	LYS
12	J	135	ARG
12	J	136	GLU
12	J	137	VAL
13	K	1	MET
13	K	9	LYS
13	K	37	THR
13	K	45	ARG
13	K	51	LEU
13	K	73	LYS
13	K	76	VAL
13	K	94	TYR
13	K	95	THR

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Mol	Chain	Res	Type
13	K	98	LEU
13	K	99	ARG
13	K	109	THR
14	L	8	ARG
14	L	11	LEU
14	L	13	THR
14	L	15	ARG
14	L	26	ARG
14	L	31	VAL
14	L	32	TYR
14	L	34	SER
14	L	37	HIS
14	L	38	ILE
14	L	39	TYR
14	L	42	ILE
14	L	43	ILE
14	L	50	THR
14	L	65	THR
14	L	67	THR
14	L	71	VAL
14	L	75	LEU
14	L	82	LYS
14	L	91	ARG
14	L	93	SER
14	L	94	TYR
14	L	97	HIS
14	L	100	VAL
14	L	108	ARG
15	M	3	THR
15	M	6	LYS
15	M	13	LEU
15	M	23	GLN
15	M	31	ASP
15	M	32	THR
15	M	38	LYS
15	M	57	ILE
15	M	72	SER
15	M	90	GLN
15	M	95	GLU
15	M	103	LYS
15	M	116	ARG
16	N	11	ARG

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Mol	Chain	Res	Type
16	N	22	LYS
16	N	51	ARG
16	N	58	ARG
16	N	78	THR
16	N	87	ASN
16	N	90	LEU
16	N	91	ASN
16	N	109	LEU
17	O	2	PHE
17	O	20	ILE
17	O	21	ARG
17	O	22	VAL
17	O	28	GLU
17	O	31	ASP
17	O	43	GLU
17	O	46	VAL
17	O	63	HIS
17	O	81	ARG
17	O	91	THR
17	O	93	ILE
18	P	9	ARG
18	P	32	ARG
18	P	39	ARG
18	P	40	LEU
18	P	44	VAL
18	P	46	ARG
18	P	49	SER
18	P	62	ARG
18	P	109	ARG
18	P	113	SER
18	P	115	ASN
18	P	125	THR
18	P	126	ILE
19	Q	7	LEU
19	Q	15	LYS
19	Q	26	SER
19	Q	27	PHE
19	Q	34	THR
19	Q	56	MET
19	Q	58	VAL
19	Q	74	ASP
19	Q	84	GLU

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Mol	Chain	Res	Type
19	Q	86	GLN
19	Q	91	LEU
20	R	8	SER
20	R	11	ASN
20	R	21	THR
20	R	44	GLN
20	R	48	VAL
20	R	55	THR
20	R	56	LYS
20	R	58	VAL
20	R	80	LYS
20	R	81	VAL
20	R	83	LEU
20	R	88	THR
20	R	95	ARG
20	R	104	VAL
20	R	106	VAL
20	R	113	THR
21	S	2	GLU
21	S	8	ARG
21	S	22	VAL
21	S	25	ASN
21	S	26	LYS
21	S	32	PHE
21	S	34	LEU
21	S	40	ASP
21	S	60	GLU
21	S	85	MET
21	S	88	TYR
21	S	118	HIS
21	S	120	LEU
21	S	128	ARG
21	S	130	ILE
21	S	151	ASP
21	S	154	LEU
21	S	160	LEU
21	S	175	ARG
22	T	21	LEU
22	T	38	VAL
22	T	43	THR
22	T	64	ASP
22	T	81	ILE

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Mol	Chain	Res	Type
23	U	6	TYR
23	U	11	LYS
23	U	12	ASN
23	U	23	LYS
23	U	25	ARG
23	U	42	GLN
23	U	46	LEU
23	U	48	LYS
23	U	52	ARG
23	U	62	LEU
24	V	6	MET
24	V	14	PHE
24	V	29	ARG
25	W	3	ILE
25	W	4	LYS
25	W	6	VAL
25	W	9	VAL
25	W	26	ARG
25	W	34	VAL
25	W	37	THR
25	W	46	THR
26	Z	4	HIS
26	Z	11	THR
26	Z	18	MET
26	Z	25	LEU
26	Z	26	THR
26	Z	36	CYS
26	Z	37	HIS
26	Z	42	SER
26	Z	53	ASP
26	Z	57	VAL
27	1	8	ILE
27	1	20	PHE
27	1	27	ASN
27	1	28	ARG
27	1	30	ASN
27	1	35	LEU
27	1	40	TYR
27	1	41	ASP
27	1	43	VAL
27	1	51	ARG
27	1	52	GLU

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Mol	Chain	Res	Type
28	2	10	ARG
28	2	11	LYS
28	2	14	LYS
28	2	24	THR
28	2	31	LEU
28	2	40	HIS
28	2	41	GLN
28	2	42	LEU
28	2	45	SER
29	3	8	LYS
29	3	19	THR
29	3	26	LYS
29	3	27	SER
29	3	30	ARG
29	3	31	HIS
29	3	33	ASN
29	3	34	THR
29	3	42	ARG
29	3	44	LYS
29	3	46	LYS
29	3	52	LYS
29	3	58	MET
29	3	59	LYS
29	3	60	LEU
29	3	61	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
7	E	139	GLN
8	F	103	GLN
13	K	3	HIS
18	P	10	ASN
19	Q	43	GLN
24	V	54	ASN
26	Z	35	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	X	2700/2877 (93%)	584 (21%)	42 (1%)
2	Y	119/124 (95%)	25 (21%)	1 (0%)
All	All	2819/3001 (93%)	609 (21%)	43 (1%)

All (609) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	X	4	C
1	X	14	A
1	X	15	G
1	X	23	G
1	X	34	U
1	X	45	C
1	X	50	G
1	X	51	A
1	X	54	G
1	X	59	G
1	X	60	A
1	X	63	A
1	X	73	A
1	X	74	G
1	X	87	G
1	X	89	A
1	X	90	G
1	X	95	G
1	X	98	U
1	X	100	G
1	X	104	C
1	X	105	G
1	X	108	G
1	X	112	U
1	X	116	A
1	X	118	U
1	X	123	A
1	X	124	A
1	X	126	C
1	X	129	A
1	X	134	G
1	X	136	A
1	X	138	G
1	X	143	A
1	X	146	C
1	X	147	G

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Mol	Chain	Res	Type
1	X	158	A
1	X	173	A
1	X	176	A
1	X	180	C
1	X	181	A
1	X	192	G
1	X	193	A
1	X	199	A
1	X	203	G
1	X	205	A
1	X	206	U
1	X	207	U
1	X	210	A
1	X	219	G
1	X	220	U
1	X	222	G
1	X	225	G
1	X	229	G
1	X	241	C
1	X	242	A
1	X	243	G
1	X	245	C
1	X	249	A
1	X	250	C
1	X	251	C
1	X	252	G
1	X	253	A
1	X	255	A
1	X	256	C
1	X	257	G
1	X	258	C
1	X	259	U
1	X	260	U
1	X	261	G
1	X	262	C
1	X	263	G
1	X	264	U
1	X	266	U
1	X	268	G
1	X	272	U
1	X	273	U
1	X	274	G

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Mol	Chain	Res	Type
1	X	275	U
1	X	276	A
1	X	279	A
1	X	280	C
1	X	282	A
1	X	305	A
1	X	310	A
1	X	312	G
1	X	321	A
1	X	327	C
1	X	332	C
1	X	335	A
1	X	340	G
1	X	341	A
1	X	343	A
1	X	344	G
1	X	359	G
1	X	361	G
1	X	384	A
1	X	385	G
1	X	386	U
1	X	387	A
1	X	388	G
1	X	396	U
1	X	399	G
1	X	400	U
1	X	408	U
1	X	412	U
1	X	414	A
1	X	417	C
1	X	418	C
1	X	419	G
1	X	421	G
1	X	424	G
1	X	431	G
1	X	441	A
1	X	447	U
1	X	448	C
1	X	456	C
1	X	463	C
1	X	467	U
1	X	469	G

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Mol	Chain	Res	Type
1	X	483	A
1	X	484	G
1	X	488	A
1	X	491	A
1	X	492	G
1	X	495	C
1	X	504	G
1	X	514	G
1	X	515	A
1	X	519	C
1	X	537	C
1	X	538	A
1	X	539	A
1	X	541	C
1	X	542	A
1	X	543	G
1	X	554	U
1	X	556	A
1	X	558	G
1	X	560	G
1	X	561	U
1	X	572	G
1	X	582	G
1	X	583	C
1	X	584	A
1	X	591	G
1	X	595	A
1	X	613	A
1	X	614	G
1	X	626	A
1	X	627	A
1	X	628	A
1	X	631	G
1	X	632	A
1	X	633	G
1	X	645	G
1	X	648	A
1	X	649	G
1	X	654	A
1	X	655	A
1	X	656	U
1	X	657	A

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Mol	Chain	Res	Type
1	X	664	C
1	X	665	A
1	X	666	U
1	X	667	U
1	X	668	A
1	X	682	G
1	X	683	A
1	X	684	C
1	X	690	A
1	X	699	G
1	X	713	G
1	X	743	A
1	X	753	U
1	X	761	G
1	X	766	A
1	X	781	G
1	X	789	G
1	X	790	A
1	X	795	A
1	X	797	A
1	X	798	G
1	X	801	A
1	X	804	C
1	X	805	G
1	X	806	A
1	X	814	G
1	X	818	G
1	X	825	C
1	X	832	A
1	X	839	U
1	X	840	U
1	X	859	U
1	X	860	U
1	X	869	C
1	X	872	G
1	X	879	A
1	X	922	A
1	X	926	C
1	X	938	G
1	X	939	C
1	X	940	G
1	X	944	A

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Mol	Chain	Res	Type
1	X	952	A
1	X	956	A
1	X	957	G
1	X	964	A
1	X	969	U
1	X	972	C
1	X	973	U
1	X	985	G
1	X	994	A
1	X	998	C
1	X	1000	G
1	X	1006	C
1	X	1007	A
1	X	1016	C
1	X	1019	U
1	X	1022	A
1	X	1023	U
1	X	1028	G
1	X	1032	A
1	X	1033	G
1	X	1034	U
1	X	1036	G
1	X	1037	U
1	X	1044	U
1	X	1049	C
1	X	1052	C
1	X	1053	G
1	X	1055	A
1	X	1056	U
1	X	1058	G
1	X	1061	A
1	X	1072	U
1	X	1077	U
1	X	1079	G
1	X	1081	A
1	X	1082	G
1	X	1086	C
1	X	1087	C
1	X	1090	C
1	X	1096	A
1	X	1097	A
1	X	1099	A

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Mol	Chain	Res	Type
1	X	1100	G
1	X	1101	U
1	X	1121	G
1	X	1123	G
1	X	1128	G
1	X	1129	A
1	X	1145	C
1	X	1146	G
1	X	1149	G
1	X	1152	C
1	X	1153	A
1	X	1154	A
1	X	1166	A
1	X	1167	A
1	X	1176	U
1	X	1183	C
1	X	1185	C
1	X	1192	A
1	X	1194	U
1	X	1195	U
1	X	1223	G
1	X	1225	G
1	X	1240	G
1	X	1247	U
1	X	1250	A
1	X	1266	G
1	X	1269	G
1	X	1284	G
1	X	1285	A
1	X	1289	A
1	X	1301	U
1	X	1313	U
1	X	1314	A
1	X	1325	U
1	X	1334	A
1	X	1337	G
1	X	1342	U
1	X	1345	G
1	X	1359	G
1	X	1370	U
1	X	1372	A
1	X	1378	A

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Mol	Chain	Res	Type
1	X	1379	A
1	X	1381	G
1	X	1391	A
1	X	1392	U
1	X	1398	G
1	X	1404	C
1	X	1409	U
1	X	1413	U
1	X	1428	G
1	X	1430	G
1	X	1432	G
1	X	1433	A
1	X	1434	U
1	X	1440	G
1	X	1442	C
1	X	1443	G
1	X	1460	G
1	X	1465	G
1	X	1467	U
1	X	1468	A
1	X	1469	U
1	X	1470	G
1	X	1482	U
1	X	1490	U
1	X	1497	C
1	X	1498	G
1	X	1505	U
1	X	1513	U
1	X	1528	C
1	X	1531	C
1	X	1551	U
1	X	1552	C
1	X	1553	G
1	X	1554	G
1	X	1562	G
1	X	1563	U
1	X	1569	A
1	X	1570	C
1	X	1571	G
1	X	1574	A
1	X	1575	C
1	X	1582	A

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Mol	Chain	Res	Type
1	X	1585	A
1	X	1594	U
1	X	1600	U
1	X	1601	U
1	X	1602	G
1	X	1603	A
1	X	1608	U
1	X	1624	A
1	X	1625	A
1	X	1626	A
1	X	1630	A
1	X	1631	C
1	X	1632	A
1	X	1634	A
1	X	1648	C
1	X	1656	U
1	X	1661	C
1	X	1665	C
1	X	1668	G
1	X	1671	A
1	X	1686	A
1	X	1691	G
1	X	1710	U
1	X	1711	C
1	X	1714	A
1	X	1717	A
1	X	1733	U
1	X	1734	C
1	X	1735	G
1	X	1747	G
1	X	1753	A
1	X	1754	G
1	X	1755	G
1	X	1760	G
1	X	1764	A
1	X	1772	C
1	X	1775	A
1	X	1780	A
1	X	1782	A
1	X	1790	G
1	X	1791	C
1	X	1792	C

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Mol	Chain	Res	Type
1	X	1793	A
1	X	1796	A
1	X	1799	A
1	X	1801	C
1	X	1802	A
1	X	1807	A
1	X	1808	C
1	X	1811	A
1	X	1812	U
1	X	1813	A
1	X	1821	A
1	X	1825	C
1	X	1830	C
1	X	1831	G
1	X	1838	G
1	X	1839	A
1	X	1845	A
1	X	1861	G
1	X	1865	C
1	X	1867	A
1	X	1868	A
1	X	1875	C
1	X	1882	G
1	X	1884	A
1	X	1886	G
1	X	1887	G
1	X	1889	G
1	X	1891	C
1	X	1892	C
1	X	1893	G
1	X	1909	U
1	X	1910	A
1	X	1912	G
1	X	1920	A
1	X	1921	A
1	X	1922	U
1	X	1923	U
1	X	1924	C
1	X	1930	C
1	X	1943	A
1	X	1944	C
1	X	1946	U

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Mol	Chain	Res	Type
1	X	1947	G
1	X	1948	C
1	X	1949	A
1	X	1950	C
1	X	1953	A
1	X	1954	A
1	X	1955	G
1	X	1965	U
1	X	1976	U
1	X	1979	C
1	X	1980	A
1	X	2004	U
1	X	2006	G
1	X	2010	G
1	X	2014	A
1	X	2015	G
1	X	2019	C
1	X	2026	C
1	X	2032	G
1	X	2038	C
1	X	2039	G
1	X	2043	A
1	X	2044	G
1	X	2045	A
1	X	2052	G
1	X	2063	A
1	X	2083	G
1	X	2171	U
1	X	2189	A
1	X	2190	A
1	X	2191	A
1	X	2192	U
1	X	2195	C
1	X	2196	U
1	X	2197	U
1	X	2198	U
1	X	2199	C
1	X	2204	A
1	X	2205	C
1	X	2217	G
1	X	2218	G
1	X	2247	A

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Mol	Chain	Res	Type
1	X	2252	A
1	X	2253	A
1	X	2254	C
1	X	2259	G
1	X	2262	C
1	X	2266	A
1	X	2272	A
1	X	2284	U
1	X	2285	U
1	X	2286	G
1	X	2287	G
1	X	2288	A
1	X	2290	A
1	X	2298	U
1	X	2299	A
1	X	2301	A
1	X	2306	A
1	X	2312	A
1	X	2313	G
1	X	2316	G
1	X	2323	U
1	X	2324	G
1	X	2326	C
1	X	2329	C
1	X	2351	G
1	X	2358	C
1	X	2362	G
1	X	2364	C
1	X	2367	A
1	X	2369	U
1	X	2371	A
1	X	2372	A
1	X	2379	G
1	X	2381	A
1	X	2382	C
1	X	2385	U
1	X	2386	G
1	X	2401	A
1	X	2402	U
1	X	2404	A
1	X	2406	C
1	X	2408	G

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Mol	Chain	Res	Type
1	X	2410	U
1	X	2413	A
1	X	2420	C
1	X	2427	A
1	X	2429	A
1	X	2447	G
1	X	2448	A
1	X	2452	U
1	X	2455	A
1	X	2457	A
1	X	2458	U
1	X	2463	G
1	X	2470	U
1	X	2473	G
1	X	2477	C
1	X	2480	C
1	X	2481	G
1	X	2484	G
1	X	2485	U
1	X	2497	A
1	X	2508	G
1	X	2541	U
1	X	2545	A
1	X	2546	G
1	X	2551	A
1	X	2553	G
1	X	2556	A
1	X	2564	U
1	X	2581	A
1	X	2588	U
1	X	2591	C
1	X	2592	U
1	X	2594	U
1	X	2608	A
1	X	2609	G
1	X	2613	A
1	X	2625	U
1	X	2633	A
1	X	2642	G
1	X	2650	G
1	X	2664	G
1	X	2668	U

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Mol	Chain	Res	Type
1	X	2688	G
1	X	2691	C
1	X	2692	A
1	X	2693	U
1	X	2698	G
1	X	2713	A
1	X	2730	A
1	X	2731	G
1	X	2732	C
1	X	2737	A
1	X	2738	A
1	X	2744	A
1	X	2745	A
1	X	2746	G
1	X	2757	G
1	X	2758	A
1	X	2759	U
1	X	2760	G
1	X	2761	A
1	X	2762	G
1	X	2769	C
1	X	2771	C
1	X	2782	G
1	X	2783	U
1	X	2793	G
1	X	2795	A
1	X	2796	A
1	X	2808	U
1	X	2809	A
1	X	2810	A
1	X	2811	G
1	X	2824	C
1	X	2825	A
1	X	2842	C
1	X	2843	A
1	X	2848	A
1	X	2851	G
1	X	2854	G
1	X	2855	C
1	X	2858	A
1	X	2861	A
1	X	2864	C

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Mol	Chain	Res	Type
1	X	2866	A
1	X	2868	G
2	Y	9	G
2	Y	15	A
2	Y	17	A
2	Y	18	G
2	Y	22	U
2	Y	26	G
2	Y	27	A
2	Y	28	A
2	Y	29	C
2	Y	30	C
2	Y	37	C
2	Y	39	C
2	Y	42	U
2	Y	43	G
2	Y	44	C
2	Y	46	G
2	Y	47	A
2	Y	60	A
2	Y	68	A
2	Y	69	G
2	Y	99	G
2	Y	102	A
2	Y	108	G
2	Y	110	U
2	Y	112	A

All (43) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	X	50	G
1	X	104	C
1	X	219	G
1	X	265	U
1	X	334	G
1	X	383	G
1	X	483	A
1	X	537	C
1	X	656	U
1	X	838	A
1	X	840	U

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Mol	Chain	Res	Type
1	X	859	U
1	X	938	G
1	X	939	C
1	X	1031	C
1	X	1071	U
1	X	1096	A
1	X	1182	U
1	X	1223	G
1	X	1313	U
1	X	1391	A
1	X	1441	A
1	X	1466	C
1	X	1496	G
1	X	1607	A
1	X	1625	A
1	X	1811	A
1	X	1908	C
1	X	1923	U
1	X	1975	G
1	X	2018	G
1	X	2043	A
1	X	2204	A
1	X	2252	A
1	X	2287	G
1	X	2312	A
1	X	2409	A
1	X	2591	C
1	X	2593	A
1	X	2736	U
1	X	2756	A
1	X	2824	C
2	Y	27	A

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 455 ligands modelled in this entry, 446 are monoatomic - leaving 9 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	$\#\|Z\| > 2$
33	SPD	X	3321	-	9,9,9	0.29	0	8,8,8	0.78	0
32	MPD	X	3315	-	7,7,7	0.20	0	9,10,10	0.49	0
33	SPD	X	3322	-	9,9,9	0.32	0	8,8,8	0.63	0
32	MPD	X	3318	-	7,7,7	0.31	0	9,10,10	0.31	0
32	MPD	X	3316	-	7,7,7	0.46	0	9,10,10	1.11	1 (11%)
32	MPD	X	3317	-	7,7,7	0.31	0	9,10,10	0.25	0
30	6NO	X	2901	-	101,105,105	1.52	14 (13%)	130,164,164	1.71	27 (20%)
33	SPD	X	3320	-	9,9,9	0.31	0	8,8,8	0.91	0
32	MPD	X	3319	-	7,7,7	0.30	0	9,10,10	0.17	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	SPD	X	3321	-	-	3/7/7/7	-
32	MPD	X	3315	-	-	3/5/5/5	-
33	SPD	X	3322	-	-	2/7/7/7	-
32	MPD	X	3318	-	-	3/5/5/5	-
32	MPD	X	3316	-	-	1/5/5/5	-
32	MPD	X	3317	-	-	1/5/5/5	-
30	6NO	X	2901	-	-	13/47/211/211	0/11/11/11
33	SPD	X	3320	-	-	1/7/7/7	-
32	MPD	X	3319	-	-	4/5/5/5	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	X	2901	6NO	C08-C05	-6.08	1.39	1.51
30	X	2901	6NO	O53-C49	5.70	1.47	1.40
30	X	2901	6NO	C04-C09	-4.19	1.40	1.50
30	X	2901	6NO	C51-C50	-3.99	1.47	1.54
30	X	2901	6NO	O25-C16	3.87	1.48	1.41
30	X	2901	6NO	O50-C54	3.60	1.47	1.41
30	X	2901	6NO	O51-C54	3.50	1.47	1.41
30	X	2901	6NO	O44-C36	2.64	1.49	1.41
30	X	2901	6NO	O48-C44	2.48	1.47	1.41
30	X	2901	6NO	O19-C10	2.23	1.47	1.41
30	X	2901	6NO	O44-C44	2.21	1.48	1.41
30	X	2901	6NO	O26-C22	2.19	1.47	1.42
30	X	2901	6NO	C52-C51	-2.06	1.51	1.54
30	X	2901	6NO	O20-C16	2.04	1.43	1.41

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	X	2901	6NO	C44-O44-C36	-5.77	104.11	114.42
30	X	2901	6NO	C01-C06-C05	-5.12	119.54	122.79
30	X	2901	6NO	O47-C47-C46	-4.17	96.54	103.49
30	X	2901	6NO	C06-C01-C02	4.13	121.94	117.81
30	X	2901	6NO	C24-C23-C22	-3.51	108.98	115.07
30	X	2901	6NO	O44-C36-O40	3.46	120.34	110.67
30	X	2901	6NO	C13-O13-C09	-3.39	111.78	117.21
30	X	2901	6NO	C16-O20-C20	-3.32	109.14	112.16
30	X	2901	6NO	O46-C46-C47	-3.24	98.90	103.47
30	X	2901	6NO	C41-O37-C37	-3.15	106.26	114.52
30	X	2901	6NO	C35-C33-C32	-2.98	108.87	113.41
30	X	2901	6NO	O24-C24-C25	-2.97	98.27	101.85
30	X	2901	6NO	O44-C44-O48	2.95	115.66	109.08
30	X	2901	6NO	C48-C47-C46	-2.75	106.91	112.49
30	X	2901	6NO	O50-C50-C51	-2.65	98.31	105.36
30	X	2901	6NO	O44-C44-C45	2.63	114.44	109.10
30	X	2901	6NO	O25-C25-C26	2.61	114.18	108.57
30	X	2901	6NO	O20-C20-C21	2.58	109.06	105.85
30	X	2901	6NO	O51-C51-C50	-2.38	99.02	105.36
30	X	2901	6NO	O25-C25-C24	-2.36	99.22	103.64
30	X	2901	6NO	C30-C31-C32	-2.23	106.56	111.66
30	X	2901	6NO	C01-C02-C03	-2.19	117.44	120.63
30	X	2901	6NO	O26-C26-C28	2.15	111.34	106.70
30	X	2901	6NO	C08-C05-C06	-2.12	117.34	121.28
32	X	3316	MPD	C5-C4-C3	2.11	121.62	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	X	2901	6NO	O24-C24-C27	2.06	112.58	108.61
30	X	2901	6NO	C03-C02-CL2	2.03	122.21	118.90
30	X	2901	6NO	C01-C02-CL2	2.03	120.35	118.08

There are no chirality outliers.

All (31) torsion outliers are listed below:

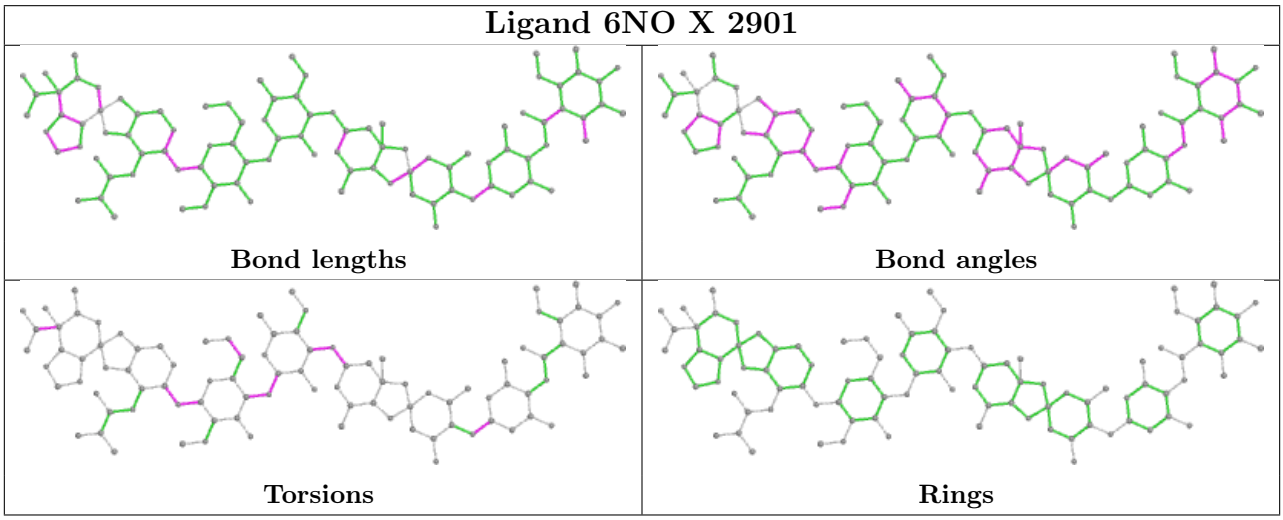
Mol	Chain	Res	Type	Atoms
30	X	2901	6NO	O33-C29-O39-C39
30	X	2901	6NO	C37-C36-O44-C44
30	X	2901	6NO	O40-C36-O44-C44
30	X	2901	6NO	O52-C52-C75-O75
32	X	3316	MPD	C2-C3-C4-C5
32	X	3317	MPD	C2-C3-C4-C5
32	X	3319	MPD	C2-C3-C4-O4
33	X	3321	SPD	C3-C4-C5-N6
30	X	2901	6NO	O14-C10-O19-C19
33	X	3322	SPD	C8-C7-N6-C5
30	X	2901	6NO	C40-C42-O42-C43
30	X	2901	6NO	C45-C44-O44-C36
33	X	3320	SPD	C7-C8-C9-N10
33	X	3321	SPD	N1-C2-C3-C4
30	X	2901	6NO	O48-C44-O44-C36
32	X	3318	MPD	O2-C2-C3-C4
32	X	3318	MPD	C2-C3-C4-C5
32	X	3319	MPD	C2-C3-C4-C5
30	X	2901	6NO	C38-C39-O39-C29
32	X	3315	MPD	CM-C2-C3-C4
32	X	3319	MPD	CM-C2-C3-C4
30	X	2901	6NO	O26-C22-O31-C31
30	X	2901	6NO	C40-C39-O39-C29
30	X	2901	6NO	C30-C31-O31-C22
33	X	3322	SPD	C2-C3-C4-C5
30	X	2901	6NO	C32-C31-O31-C22
32	X	3315	MPD	O2-C2-C3-C4
32	X	3319	MPD	O2-C2-C3-C4
33	X	3321	SPD	C4-C5-N6-C7
32	X	3315	MPD	C2-C3-C4-O4
32	X	3318	MPD	C2-C3-C4-O4

There are no ring outliers.

7 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	X	3321	SPD	3	0
32	X	3315	MPD	3	0
33	X	3322	SPD	3	0
32	X	3316	MPD	11	0
30	X	2901	6NO	2	0
33	X	3320	SPD	1	0
32	X	3319	MPD	1	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 then 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, 95^{th} 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	X	2710/2877 (94%)	-0.65	11 (0%) 92 91	35, 91, 200, 334	0
2	Y	120/124 (96%)	-0.72	1 (0%) 86 84	97, 137, 188, 213	0
3	A	272/275 (98%)	0.30	16 (5%) 22 24	53, 112, 177, 240	0
4	B	205/211 (97%)	-0.13	4 (1%) 65 64	28, 66, 136, 250	0
5	C	195/205 (95%)	0.12	11 (5%) 24 25	56, 103, 204, 281	0
6	D	177/180 (98%)	0.65	24 (13%) 3 4	120, 178, 253, 296	0
7	E	171/185 (92%)	0.18	6 (3%) 44 44	69, 137, 216, 268	0
8	F	63/144 (43%)	1.90	21 (33%) 0 0	142, 200, 295, 418	0
9	G	142/174 (81%)	0.29	10 (7%) 16 19	48, 89, 188, 342	0
10	H	134/134 (100%)	-0.37	0 100 100	29, 61, 104, 144	0
11	I	134/156 (85%)	0.61	17 (12%) 3 5	51, 120, 206, 280	0
12	J	136/141 (96%)	0.28	8 (5%) 22 24	58, 99, 176, 252	0
13	K	115/116 (99%)	-0.19	1 (0%) 84 83	25, 47, 100, 192	0
14	L	104/114 (91%)	1.06	21 (20%) 1 1	65, 124, 188, 298	0
15	M	119/166 (71%)	-0.20	5 (4%) 36 36	40, 62, 136, 200	0
16	N	117/118 (99%)	-0.20	1 (0%) 84 83	51, 82, 127, 243	0
17	O	97/100 (97%)	0.01	4 (4%) 37 37	63, 107, 193, 284	0
18	P	128/134 (95%)	-0.11	3 (2%) 60 59	17, 64, 110, 190	0
19	Q	93/95 (97%)	0.26	5 (5%) 25 27	57, 103, 159, 219	0
20	R	110/115 (95%)	0.69	12 (10%) 5 8	65, 110, 221, 253	0
21	S	180/237 (75%)	0.54	21 (11%) 4 7	95, 152, 223, 265	0
22	T	74/91 (81%)	0.90	12 (16%) 1 2	66, 101, 148, 193	0
23	U	74/81 (91%)	1.42	21 (28%) 0 0	62, 127, 214, 239	0
24	V	65/67 (97%)	0.40	7 (10%) 5 8	84, 131, 191, 271	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
25	W	55/55 (100%)	1.10	12 (21%) 0 1	57, 93, 139, 184	0
26	Z	57/60 (95%)	-0.46	0 100 100	28, 55, 117, 149	0
27	1	53/55 (96%)	1.22	13 (24%) 0 0	82, 147, 236, 292	0
28	2	46/47 (97%)	0.60	6 (13%) 3 5	56, 78, 116, 190	0
29	3	59/66 (89%)	1.05	12 (20%) 1 1	59, 106, 166, 333	0
All	All	6005/6523 (92%)	-0.13	285 (4%) 31 32	17, 100, 205, 418	0

All (285) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	G	155	THR	10.7
8	F	114	ASP	9.0
8	F	110	THR	8.6
8	F	127	VAL	7.8
8	F	113	PRO	7.8
14	L	52	ALA	7.6
1	X	1890	A	6.8
23	U	54	ASN	5.9
23	U	6	TYR	5.8
9	G	97	ASP	5.3
21	S	23	ALA	5.1
9	G	156	HIS	5.1
24	V	3	PRO	5.1
1	X	282	A	5.1
29	3	55	TRP	4.9
21	S	22	VAL	4.9
23	U	14	VAL	4.9
27	1	48	VAL	4.8
15	M	116	ARG	4.8
14	L	102	ALA	4.8
6	D	67	ILE	4.5
8	F	112	MET	4.5
5	C	50	GLN	4.5
14	L	40	ALA	4.5
14	L	53	ALA	4.4
8	F	120	VAL	4.4
6	D	81	GLN	4.4
8	F	119	SER	4.4
3	A	246	PRO	4.4
27	1	34	LYS	4.4

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Mol	Chain	Res	Type	RSRZ
23	U	8	THR	4.3
22	T	45	PHE	4.3
21	S	94	VAL	4.2
11	I	75	VAL	4.2
29	3	54	GLU	4.1
3	A	1	MET	4.1
14	L	51	LEU	4.0
25	W	6	VAL	4.0
14	L	56	SER	4.0
23	U	52	ARG	4.0
14	L	61	SER	4.0
23	U	51	ILE	3.9
29	3	63	PRO	3.8
15	M	115	ALA	3.8
21	S	20	ALA	3.8
5	C	20	PRO	3.8
21	S	83	PHE	3.8
3	A	44	ASN	3.8
22	T	71	ASN	3.8
1	X	1525	A	3.7
1	X	1839	A	3.7
24	V	4	SER	3.7
3	A	250	TRP	3.7
23	U	50	ALA	3.7
25	W	1	MET	3.6
8	F	107	ILE	3.6
9	G	159	SER	3.6
8	F	118	GLY	3.6
21	S	30	VAL	3.6
8	F	121	GLU	3.5
22	T	49	GLN	3.5
18	P	134	LYS	3.5
24	V	64	GLY	3.5
27	1	51	ARG	3.5
22	T	73	GLY	3.5
23	U	7	LEU	3.5
23	U	67	LEU	3.4
24	V	2	LYS	3.4
12	J	84	MET	3.4
25	W	25	LEU	3.4
3	A	242	ALA	3.4
23	U	70	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
6	D	145	MET	3.4
21	S	81	VAL	3.3
6	D	138	PHE	3.3
20	R	83	LEU	3.3
14	L	89	PHE	3.3
23	U	58	LYS	3.2
14	L	42	ILE	3.2
6	D	22	TYR	3.2
24	V	36	GLN	3.2
3	A	101	GLU	3.2
14	L	75	LEU	3.2
18	P	133	ASN	3.2
8	F	128	ALA	3.2
8	F	109	LYS	3.1
5	C	21	GLU	3.1
23	U	47	HIS	3.1
27	1	3	LYS	3.1
21	S	68	ALA	3.1
20	R	79	SER	3.1
29	3	9	MET	3.1
29	3	37	SER	3.1
7	E	43	VAL	3.1
25	W	54	GLN	3.1
22	T	77	ARG	3.1
29	3	10	ALA	3.1
5	C	49	ALA	3.1
3	A	241	GLY	3.0
28	2	46	ASP	3.0
11	I	70	THR	3.0
1	X	1889	G	3.0
6	D	142	THR	3.0
9	G	100	TYR	3.0
13	K	94	TYR	3.0
11	I	122	VAL	3.0
6	D	84	PRO	3.0
27	1	44	ALA	3.0
8	F	99	LEU	3.0
24	V	66	GLN	2.9
14	L	63	ASN	2.9
29	3	58	MET	2.9
12	J	79	PRO	2.9
3	A	72	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
25	W	26	ARG	2.8
6	D	76	ASN	2.8
27	1	45	LYS	2.8
9	G	158	HIS	2.8
23	U	60	VAL	2.8
8	F	93	LYS	2.8
21	S	11	LYS	2.8
25	W	5	LEU	2.8
21	S	165	GLU	2.8
21	S	12	GLN	2.8
22	T	79	ILE	2.8
20	R	46	VAL	2.8
6	D	36	VAL	2.8
27	1	38	LYS	2.7
27	1	2	ALA	2.7
23	U	45	ASN	2.7
28	2	37	LYS	2.7
15	M	117	ILE	2.7
23	U	62	LEU	2.7
6	D	144	ASP	2.7
5	C	148	VAL	2.7
8	F	103	GLN	2.7
23	U	61	TRP	2.7
22	T	69	PHE	2.7
21	S	113	VAL	2.7
7	E	115	ILE	2.7
19	Q	65	VAL	2.6
21	S	171	VAL	2.6
27	1	11	LYS	2.6
28	2	28	ARG	2.6
1	X	1734	C	2.6
3	A	103	ARG	2.6
6	D	80	ARG	2.6
6	D	169	LEU	2.6
11	I	79	GLN	2.6
27	1	14	SER	2.6
11	I	69	GLY	2.6
27	1	13	GLU	2.6
22	T	37	LEU	2.6
7	E	46	ASP	2.6
16	N	91	ASN	2.6
22	T	67	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
5	C	150	LEU	2.6
14	L	97	HIS	2.6
6	D	20	PHE	2.5
12	J	21	ASP	2.5
29	3	14	ILE	2.5
6	D	149	THR	2.5
20	R	81	VAL	2.5
11	I	123	ASP	2.5
11	I	27	ASP	2.5
21	S	82	ASP	2.5
6	D	147	ASP	2.5
8	F	76	TYR	2.5
12	J	140	GLU	2.5
21	S	92	VAL	2.5
5	C	166	TRP	2.5
12	J	105	PHE	2.5
1	X	281	C	2.5
3	A	33	LEU	2.5
19	Q	64	ARG	2.5
4	B	135	HIS	2.5
9	G	99	VAL	2.5
28	2	31	LEU	2.5
11	I	108	LEU	2.4
11	I	82	ASP	2.4
21	S	66	VAL	2.4
8	F	94	ALA	2.4
14	L	54	ALA	2.4
20	R	77	HIS	2.4
21	S	72	ASP	2.4
23	U	13	LEU	2.4
29	3	64	ARG	2.4
3	A	97	TYR	2.4
25	W	4	LYS	2.4
15	M	40	ARG	2.4
8	F	81	ALA	2.4
19	Q	89	GLU	2.4
3	A	102	LYS	2.4
20	R	60	PRO	2.4
12	J	27	TYR	2.4
17	O	18	ASP	2.4
22	T	40	GLN	2.4
25	W	17	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
17	O	28	GLU	2.4
21	S	76	ARG	2.4
11	I	76	LYS	2.4
17	O	74	TYR	2.4
7	E	37	TYR	2.3
5	C	163	ASN	2.3
19	Q	63	LYS	2.3
4	B	146	THR	2.3
11	I	66	ASN	2.3
11	I	74	VAL	2.3
25	W	53	VAL	2.3
29	3	60	LEU	2.3
12	J	22	ALA	2.3
11	I	54	SER	2.3
18	P	7	THR	2.3
14	L	60	LYS	2.3
15	M	114	ALA	2.3
25	W	9	VAL	2.3
25	W	51	LEU	2.3
5	C	19	LEU	2.3
14	L	59	LEU	2.3
5	C	180	ILE	2.3
14	L	31	VAL	2.3
11	I	39	SER	2.3
21	S	21	ALA	2.3
27	1	20	PHE	2.3
29	3	61	MET	2.2
5	C	91	TYR	2.2
17	O	71	ILE	2.2
6	D	156	ILE	2.2
1	X	302	U	2.2
3	A	251	GLY	2.2
11	I	36	GLY	2.2
19	Q	71	GLN	2.2
22	T	46	LYS	2.2
20	R	62	MET	2.2
6	D	165	GLU	2.2
3	A	267	ASP	2.2
27	1	49	VAL	2.2
1	X	1753	A	2.2
6	D	143	TYR	2.2
23	U	40	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
21	S	86	VAL	2.2
14	L	12	ARG	2.2
6	D	28	VAL	2.2
28	2	1	MET	2.2
23	U	25	ARG	2.2
12	J	91	VAL	2.1
25	W	20	VAL	2.1
4	B	3	GLY	2.1
22	T	59	LEU	2.1
23	U	16	ASN	2.1
7	E	53	GLU	2.1
20	R	41	PRO	2.1
7	E	41	LEU	2.1
3	A	269	PHE	2.1
14	L	57	ALA	2.1
14	L	58	ALA	2.1
29	3	23	MET	2.1
20	R	57	ASN	2.1
11	I	45	LYS	2.1
14	L	38	ILE	2.1
20	R	14	LEU	2.1
24	V	10	GLN	2.1
28	2	27	GLY	2.1
14	L	29	LEU	2.1
9	G	102	ARG	2.1
6	D	103	LEU	2.1
20	R	38	LEU	2.1
6	D	121	ALA	2.1
23	U	20	ARG	2.1
1	X	1551	U	2.1
9	G	168	THR	2.1
6	D	29	PRO	2.1
2	Y	14	C	2.1
6	D	62	LEU	2.0
20	R	21	THR	2.0
1	X	1037	U	2.0
8	F	132	ARG	2.0
6	D	87	ILE	2.0
4	B	205	SER	2.0
21	S	112	LEU	2.0
3	A	55	GLY	2.0
8	F	85	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
8	F	125	ASN	2.0
11	I	50	GLU	2.0
9	G	106	TYR	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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
31	MG	X	3239	1/1	0.19	0.78	84,84,84,84	0
31	MG	X	3252	1/1	0.30	0.42	111,111,111,111	0
31	MG	X	3000	1/1	0.42	1.83	82,82,82,82	0
31	MG	X	3266	1/1	0.42	0.76	56,56,56,56	0
31	MG	X	3261	1/1	0.46	0.60	78,78,78,78	0
31	MG	X	3144	1/1	0.46	0.28	76,76,76,76	0
31	MG	X	3245	1/1	0.47	0.39	98,98,98,98	0
31	MG	X	3169	1/1	0.49	0.19	77,77,77,77	0
31	MG	X	3074	1/1	0.53	0.39	61,61,61,61	0
31	MG	X	3248	1/1	0.57	0.53	87,87,87,87	0
31	MG	X	3089	1/1	0.59	0.48	79,79,79,79	0
31	MG	X	3234	1/1	0.61	0.55	83,83,83,83	0
31	MG	X	3273	1/1	0.61	0.28	70,70,70,70	0
31	MG	X	3301	1/1	0.62	1.14	80,80,80,80	0
31	MG	X	3072	1/1	0.64	0.65	73,73,73,73	0
31	MG	X	3180	1/1	0.64	0.40	115,115,115,115	0
31	MG	X	3225	1/1	0.64	0.55	79,79,79,79	0
31	MG	X	3170	1/1	0.67	0.60	105,105,105,105	0
31	MG	Y	209	1/1	0.67	0.40	81,81,81,81	0
31	MG	X	3300	1/1	0.68	0.65	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
31	MG	X	3103	1/1	0.70	0.43	84,84,84,84	0
31	MG	X	3160	1/1	0.71	0.46	92,92,92,92	0
31	MG	X	3102	1/1	0.71	0.54	46,46,46,46	0
31	MG	X	3064	1/1	0.71	1.11	76,76,76,76	0
31	MG	X	3060	1/1	0.71	0.21	47,47,47,47	0
31	MG	Y	218	1/1	0.71	0.13	83,83,83,83	0
31	MG	X	3087	1/1	0.72	0.37	54,54,54,54	0
31	MG	Y	216	1/1	0.72	0.37	70,70,70,70	0
31	MG	X	3054	1/1	0.72	0.53	72,72,72,72	0
31	MG	X	3073	1/1	0.73	0.79	94,94,94,94	0
31	MG	X	3039	1/1	0.73	0.54	51,51,51,51	0
31	MG	X	3314	1/1	0.73	0.87	62,62,62,62	0
31	MG	Y	219	1/1	0.73	0.34	81,81,81,81	0
31	MG	X	3176	1/1	0.74	0.21	47,47,47,47	0
31	MG	X	3229	1/1	0.74	0.40	71,71,71,71	0
31	MG	X	3250	1/1	0.74	0.79	73,73,73,73	0
31	MG	X	3305	1/1	0.74	0.05	125,125,125,125	0
31	MG	X	3309	1/1	0.74	0.30	87,87,87,87	0
31	MG	X	3189	1/1	0.74	0.46	61,61,61,61	0
31	MG	X	3219	1/1	0.74	0.47	85,85,85,85	0
31	MG	X	3262	1/1	0.74	0.28	113,113,113,113	0
31	MG	X	3241	1/1	0.74	0.32	85,85,85,85	0
31	MG	X	3271	1/1	0.74	0.12	78,78,78,78	0
31	MG	X	3091	1/1	0.75	0.40	49,49,49,49	0
31	MG	X	3255	1/1	0.75	0.16	69,69,69,69	0
31	MG	X	3104	1/1	0.75	0.93	70,70,70,70	0
31	MG	X	3231	1/1	0.75	1.07	96,96,96,96	0
31	MG	X	2958	1/1	0.76	0.54	38,38,38,38	0
31	MG	X	3215	1/1	0.76	0.40	54,54,54,54	0
31	MG	X	3033	1/1	0.76	0.46	75,75,75,75	0
31	MG	X	3069	1/1	0.76	0.27	49,49,49,49	0
31	MG	X	3132	1/1	0.77	0.40	70,70,70,70	0
31	MG	X	3177	1/1	0.78	0.29	75,75,75,75	0
31	MG	X	3080	1/1	0.78	0.38	29,29,29,29	0
31	MG	X	3049	1/1	0.78	0.38	70,70,70,70	0
31	MG	X	3010	1/1	0.78	0.89	72,72,72,72	0
31	MG	X	3126	1/1	0.78	0.26	42,42,42,42	0
31	MG	X	3059	1/1	0.78	0.33	51,51,51,51	0
31	MG	X	3004	1/1	0.79	0.28	43,43,43,43	0
31	MG	X	2904	1/1	0.79	0.41	64,64,64,64	0
31	MG	X	3191	1/1	0.79	0.31	32,32,32,32	0
31	MG	3	101	1/1	0.79	0.64	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
31	MG	X	3137	1/1	0.80	0.60	57,57,57,57	0
31	MG	X	3178	1/1	0.80	0.21	60,60,60,60	0
31	MG	X	3218	1/1	0.80	0.31	78,78,78,78	0
31	MG	X	3115	1/1	0.81	0.19	75,75,75,75	0
31	MG	Y	215	1/1	0.81	0.56	81,81,81,81	0
31	MG	X	3257	1/1	0.81	0.55	77,77,77,77	0
31	MG	X	3249	1/1	0.82	0.33	103,103,103,103	0
31	MG	Y	210	1/1	0.82	0.31	64,64,64,64	0
31	MG	X	3086	1/1	0.82	0.31	41,41,41,41	0
31	MG	X	2961	1/1	0.82	0.60	35,35,35,35	0
31	MG	X	3141	1/1	0.82	0.30	62,62,62,62	0
31	MG	X	3312	1/1	0.82	0.14	71,71,71,71	0
31	MG	X	3062	1/1	0.82	0.73	49,49,49,49	0
31	MG	X	3112	1/1	0.83	0.62	42,42,42,42	0
31	MG	X	3195	1/1	0.83	0.28	90,90,90,90	0
31	MG	X	3113	1/1	0.83	0.31	38,38,38,38	0
31	MG	X	2915	1/1	0.83	0.56	39,39,39,39	0
31	MG	X	3065	1/1	0.83	0.75	57,57,57,57	0
31	MG	X	3190	1/1	0.83	0.64	56,56,56,56	0
31	MG	Y	206	1/1	0.84	0.19	70,70,70,70	0
31	MG	X	3275	1/1	0.84	0.40	70,70,70,70	0
31	MG	X	3179	1/1	0.84	0.41	62,62,62,62	0
31	MG	X	3083	1/1	0.84	0.29	50,50,50,50	0
31	MG	X	3145	1/1	0.84	0.23	83,83,83,83	0
31	MG	X	3267	1/1	0.84	0.44	50,50,50,50	0
31	MG	X	3230	1/1	0.84	0.36	99,99,99,99	0
31	MG	K	201	1/1	0.84	0.54	48,48,48,48	0
31	MG	X	3153	1/1	0.84	0.62	58,58,58,58	0
31	MG	X	3156	1/1	0.85	0.31	72,72,72,72	0
31	MG	X	3224	1/1	0.85	0.21	32,32,32,32	0
31	MG	Y	213	1/1	0.85	0.40	83,83,83,83	0
31	MG	X	3082	1/1	0.85	0.29	51,51,51,51	0
31	MG	X	3105	1/1	0.85	0.29	80,80,80,80	0
31	MG	X	3207	1/1	0.85	0.29	75,75,75,75	0
31	MG	X	3152	1/1	0.85	0.20	74,74,74,74	0
31	MG	X	3251	1/1	0.85	0.29	85,85,85,85	0
31	MG	X	3093	1/1	0.85	0.67	44,44,44,44	0
31	MG	X	3202	1/1	0.86	0.22	64,64,64,64	0
31	MG	X	3056	1/1	0.86	0.32	66,66,66,66	0
31	MG	X	3212	1/1	0.86	0.29	53,53,53,53	0
31	MG	X	2990	1/1	0.86	0.36	60,60,60,60	0
31	MG	X	3182	1/1	0.86	0.31	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
31	MG	X	3016	1/1	0.86	0.44	60,60,60,60	0
31	MG	X	3111	1/1	0.86	0.60	49,49,49,49	0
31	MG	X	3133	1/1	0.86	0.30	73,73,73,73	0
31	MG	T	101	1/1	0.86	0.40	30,30,30,30	0
31	MG	X	3088	1/1	0.86	0.29	51,51,51,51	0
33	SPD	X	3322	10/10	0.86	0.23	90,90,90,90	0
31	MG	Y	212	1/1	0.87	0.41	78,78,78,78	0
31	MG	X	3221	1/1	0.87	0.29	49,49,49,49	0
31	MG	X	3181	1/1	0.87	0.44	51,51,51,51	0
31	MG	X	3034	1/1	0.87	0.46	35,35,35,35	0
31	MG	X	3268	1/1	0.87	0.11	115,115,115,115	0
31	MG	X	3095	1/1	0.88	0.65	65,65,65,65	0
31	MG	X	3173	1/1	0.88	0.46	82,82,82,82	0
31	MG	X	3254	1/1	0.88	0.63	19,19,19,19	0
31	MG	X	2981	1/1	0.88	0.41	52,52,52,52	0
31	MG	Y	203	1/1	0.88	0.45	30,30,30,30	0
31	MG	X	3198	1/1	0.88	0.21	66,66,66,66	0
31	MG	X	2937	1/1	0.88	0.22	31,31,31,31	0
31	MG	X	3120	1/1	0.88	0.39	56,56,56,56	0
31	MG	X	3265	1/1	0.88	0.27	74,74,74,74	0
31	MG	X	3238	1/1	0.88	0.28	50,50,50,50	0
31	MG	X	3208	1/1	0.88	0.23	61,61,61,61	0
31	MG	X	3240	1/1	0.88	0.51	82,82,82,82	0
31	MG	X	3012	1/1	0.88	0.53	49,49,49,49	0
31	MG	X	3046	1/1	0.88	0.13	64,64,64,64	0
31	MG	X	2956	1/1	0.88	0.40	31,31,31,31	0
31	MG	X	3283	1/1	0.88	0.39	50,50,50,50	0
31	MG	X	3135	1/1	0.88	0.27	67,67,67,67	0
31	MG	X	3136	1/1	0.88	0.10	43,43,43,43	0
31	MG	X	3149	1/1	0.89	0.27	24,24,24,24	0
31	MG	X	2996	1/1	0.89	0.27	41,41,41,41	0
31	MG	X	3067	1/1	0.89	0.41	60,60,60,60	0
31	MG	Y	202	1/1	0.89	0.28	52,52,52,52	0
31	MG	X	3155	1/1	0.89	0.25	68,68,68,68	0
31	MG	X	2962	1/1	0.89	0.31	84,84,84,84	0
31	MG	Y	208	1/1	0.89	0.20	72,72,72,72	0
31	MG	X	3159	1/1	0.89	0.66	31,31,31,31	0
31	MG	X	3187	1/1	0.89	0.25	57,57,57,57	0
31	MG	X	3114	1/1	0.89	0.27	70,70,70,70	0
31	MG	X	2979	1/1	0.89	0.17	37,37,37,37	0
31	MG	X	3279	1/1	0.89	0.28	50,50,50,50	0
31	MG	X	3281	1/1	0.89	0.61	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
31	MG	X	3045	1/1	0.89	0.61	30,30,30,30	0
31	MG	X	3298	1/1	0.89	0.39	20,20,20,20	0
31	MG	X	3106	1/1	0.89	0.26	57,57,57,57	0
31	MG	X	3175	1/1	0.89	0.25	72,72,72,72	0
31	MG	X	3303	1/1	0.89	0.23	67,67,67,67	0
32	MPD	X	3316	8/8	0.89	0.39	62,62,62,62	0
31	MG	X	3127	1/1	0.89	1.51	52,52,52,52	0
31	MG	X	2916	1/1	0.90	0.54	0,0,0,0	0
31	MG	X	2994	1/1	0.90	0.68	58,58,58,58	0
31	MG	X	3150	1/1	0.90	0.43	65,65,65,65	0
31	MG	X	3036	1/1	0.90	0.27	41,41,41,41	0
31	MG	X	3047	1/1	0.90	0.62	23,23,23,23	0
31	MG	X	3038	1/1	0.90	0.65	32,32,32,32	0
31	MG	X	3075	1/1	0.90	0.63	52,52,52,52	0
31	MG	X	3077	1/1	0.90	0.28	61,61,61,61	0
31	MG	X	3213	1/1	0.90	0.16	34,34,34,34	0
31	MG	X	3302	1/1	0.90	0.14	100,100,100,100	0
31	MG	X	3263	1/1	0.90	0.38	59,59,59,59	0
31	MG	X	3214	1/1	0.90	0.55	71,71,71,71	0
31	MG	A	301	1/1	0.90	0.40	46,46,46,46	0
31	MG	X	3051	1/1	0.90	0.24	29,29,29,29	0
31	MG	X	3311	1/1	0.90	0.27	59,59,59,59	0
31	MG	X	3053	1/1	0.90	0.19	64,64,64,64	0
31	MG	X	3119	1/1	0.90	0.38	62,62,62,62	0
32	MPD	X	3318	8/8	0.90	0.18	79,79,79,79	0
31	MG	X	3328	1/1	0.90	0.32	33,33,33,33	0
31	MG	X	3313	1/1	0.91	0.15	74,74,74,74	0
31	MG	X	3217	1/1	0.91	0.55	48,48,48,48	0
31	MG	X	3246	1/1	0.91	0.40	87,87,87,87	0
31	MG	X	2972	1/1	0.91	0.17	33,33,33,33	0
31	MG	X	3003	1/1	0.91	0.47	49,49,49,49	0
31	MG	Y	204	1/1	0.91	0.65	60,60,60,60	0
31	MG	Y	205	1/1	0.91	0.34	44,44,44,44	0
31	MG	X	3276	1/1	0.91	0.52	114,114,114,114	0
31	MG	X	3277	1/1	0.91	0.40	39,39,39,39	0
31	MG	X	3123	1/1	0.91	0.48	18,18,18,18	0
31	MG	X	3196	1/1	0.91	0.37	95,95,95,95	0
31	MG	Y	211	1/1	0.91	0.07	59,59,59,59	0
31	MG	X	3282	1/1	0.91	0.40	58,58,58,58	0
31	MG	X	3138	1/1	0.91	1.02	44,44,44,44	0
31	MG	X	3290	1/1	0.91	0.14	71,71,71,71	0
31	MG	X	3032	1/1	0.91	0.36	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
31	MG	X	3204	1/1	0.91	0.32	51,51,51,51	0
31	MG	X	2997	1/1	0.91	0.39	47,47,47,47	0
31	MG	X	3130	1/1	0.91	0.57	62,62,62,62	0
31	MG	X	3235	1/1	0.91	0.33	79,79,79,79	0
31	MG	X	3007	1/1	0.91	0.41	30,30,30,30	0
31	MG	X	3307	1/1	0.91	0.38	25,25,25,25	0
31	MG	X	3184	1/1	0.91	0.64	131,131,131,131	0
31	MG	X	3172	1/1	0.91	0.32	60,60,60,60	0
33	SPD	X	3321	10/10	0.91	0.27	88,88,88,88	0
31	MG	X	2999	1/1	0.91	0.30	29,29,29,29	0
31	MG	X	3210	1/1	0.92	0.15	62,62,62,62	0
31	MG	X	3325	1/1	0.92	0.65	104,104,104,104	0
31	MG	X	3327	1/1	0.92	0.20	66,66,66,66	0
31	MG	X	2973	1/1	0.92	0.33	23,23,23,23	0
31	MG	X	3329	1/1	0.92	0.56	95,95,95,95	0
31	MG	X	3134	1/1	0.92	0.58	25,25,25,25	0
31	MG	X	2974	1/1	0.92	0.41	45,45,45,45	0
31	MG	X	3011	1/1	0.92	0.35	33,33,33,33	0
31	MG	X	3278	1/1	0.92	0.16	50,50,50,50	0
31	MG	X	3216	1/1	0.92	0.14	70,70,70,70	0
31	MG	X	3094	1/1	0.92	0.38	76,76,76,76	0
31	MG	X	2965	1/1	0.92	0.42	52,52,52,52	0
31	MG	X	3101	1/1	0.92	0.22	52,52,52,52	0
31	MG	X	3289	1/1	0.92	0.28	74,74,74,74	0
31	MG	X	3220	1/1	0.92	0.16	66,66,66,66	0
31	MG	X	3292	1/1	0.92	0.37	28,28,28,28	0
31	MG	X	3143	1/1	0.92	0.46	56,56,56,56	0
31	MG	X	2933	1/1	0.92	0.74	32,32,32,32	0
31	MG	X	3055	1/1	0.92	0.28	49,49,49,49	0
31	MG	X	3258	1/1	0.92	0.64	56,56,56,56	0
31	MG	X	3228	1/1	0.92	0.83	85,85,85,85	0
31	MG	X	3200	1/1	0.92	0.29	64,64,64,64	0
31	MG	X	3306	1/1	0.92	0.09	116,116,116,116	0
31	MG	X	3201	1/1	0.92	0.56	69,69,69,69	0
31	MG	X	3070	1/1	0.92	0.20	39,39,39,39	0
31	MG	X	3028	1/1	0.92	0.19	3,3,3,3	0
31	MG	X	3005	1/1	0.92	0.45	45,45,45,45	0
31	MG	X	3110	1/1	0.92	0.26	55,55,55,55	0
31	MG	X	3244	1/1	0.93	0.07	61,61,61,61	0
31	MG	X	3174	1/1	0.93	0.41	52,52,52,52	0
31	MG	X	3129	1/1	0.93	0.15	21,21,21,21	0
31	MG	X	2976	1/1	0.93	0.23	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
31	MG	X	3096	1/1	0.93	0.23	50,50,50,50	0
31	MG	X	3014	1/1	0.93	0.55	28,28,28,28	0
31	MG	X	2967	1/1	0.93	0.28	14,14,14,14	0
31	MG	X	3017	1/1	0.93	0.33	30,30,30,30	0
31	MG	X	3118	1/1	0.93	0.16	113,113,113,113	0
31	MG	X	3209	1/1	0.93	0.32	52,52,52,52	0
31	MG	X	3076	1/1	0.93	0.54	90,90,90,90	0
31	MG	X	3323	1/1	0.93	0.20	22,22,22,22	0
31	MG	X	2917	1/1	0.93	0.44	6,6,6,6	0
31	MG	X	3285	1/1	0.93	0.23	84,84,84,84	0
31	MG	X	3168	1/1	0.93	0.52	76,76,76,76	0
31	MG	X	2925	1/1	0.93	0.51	9,9,9,9	0
31	MG	Y	201	1/1	0.93	0.41	57,57,57,57	0
31	MG	X	3142	1/1	0.93	0.44	57,57,57,57	0
32	MPD	X	3319	8/8	0.93	0.15	91,91,91,91	0
31	MG	X	3107	1/1	0.93	0.22	67,67,67,67	0
30	6NO	X	2901	95/95	0.93	0.19	114,114,114,114	0
31	MG	X	3023	1/1	0.94	0.30	50,50,50,50	0
31	MG	X	3024	1/1	0.94	0.25	27,27,27,27	0
31	MG	X	3025	1/1	0.94	0.19	33,33,33,33	0
31	MG	X	3206	1/1	0.94	0.22	57,57,57,57	0
31	MG	X	3310	1/1	0.94	0.29	63,63,63,63	0
31	MG	X	2988	1/1	0.94	0.50	48,48,48,48	0
31	MG	X	3031	1/1	0.94	0.22	64,64,64,64	0
31	MG	X	3057	1/1	0.94	0.33	36,36,36,36	0
31	MG	X	3165	1/1	0.94	0.32	8,8,8,8	0
31	MG	X	3122	1/1	0.94	0.31	52,52,52,52	0
31	MG	X	2923	1/1	0.94	0.47	13,13,13,13	0
31	MG	X	3326	1/1	0.94	0.44	55,55,55,55	0
31	MG	X	3124	1/1	0.94	0.20	47,47,47,47	0
31	MG	X	2993	1/1	0.94	0.64	26,26,26,26	0
31	MG	X	3061	1/1	0.94	0.26	38,38,38,38	0
31	MG	X	3092	1/1	0.94	0.16	53,53,53,53	0
31	MG	X	2924	1/1	0.94	0.22	26,26,26,26	0
31	MG	X	3131	1/1	0.94	0.21	36,36,36,36	0
31	MG	X	3270	1/1	0.94	0.16	85,85,85,85	0
31	MG	X	3063	1/1	0.94	0.27	52,52,52,52	0
31	MG	X	2939	1/1	0.94	0.42	24,24,24,24	0
31	MG	Y	207	1/1	0.94	0.49	93,93,93,93	0
31	MG	X	3274	1/1	0.94	0.23	74,74,74,74	0
31	MG	X	2975	1/1	0.94	0.50	38,38,38,38	0
31	MG	X	3097	1/1	0.94	0.76	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
31	MG	X	3066	1/1	0.94	0.41	48,48,48,48	0
31	MG	X	3013	1/1	0.94	0.10	42,42,42,42	0
31	MG	X	3068	1/1	0.94	0.65	48,48,48,48	0
31	MG	Y	214	1/1	0.94	0.37	64,64,64,64	0
31	MG	X	3185	1/1	0.94	0.20	87,87,87,87	0
31	MG	X	3040	1/1	0.94	0.70	70,70,70,70	0
31	MG	X	3042	1/1	0.94	0.22	42,42,42,42	0
31	MG	X	3237	1/1	0.94	0.34	88,88,88,88	0
31	MG	X	2949	1/1	0.94	0.41	16,16,16,16	0
31	MG	J	201	1/1	0.94	0.26	55,55,55,55	0
31	MG	X	2908	1/1	0.94	0.37	15,15,15,15	0
31	MG	X	3194	1/1	0.94	0.18	70,70,70,70	0
31	MG	X	3293	1/1	0.94	0.41	71,71,71,71	0
31	MG	X	2968	1/1	0.94	0.58	34,34,34,34	0
32	MPD	X	3317	8/8	0.94	0.36	73,73,73,73	0
31	MG	X	3146	1/1	0.94	0.36	46,46,46,46	0
31	MG	X	3048	1/1	0.94	0.42	0,0,0,0	0
33	SPD	X	3320	10/10	0.94	0.27	44,44,44,44	0
31	MG	X	3020	1/1	0.94	0.36	47,47,47,47	0
31	MG	X	3247	1/1	0.94	0.20	101,101,101,101	0
31	MG	X	3148	1/1	0.95	0.15	29,29,29,29	0
31	MG	X	3280	1/1	0.95	0.08	84,84,84,84	0
31	MG	X	3197	1/1	0.95	0.26	49,49,49,49	0
31	MG	X	2935	1/1	0.95	0.19	15,15,15,15	0
31	MG	X	3222	1/1	0.95	0.21	21,21,21,21	0
31	MG	X	3223	1/1	0.95	0.26	34,34,34,34	0
31	MG	X	3253	1/1	0.95	0.14	25,25,25,25	0
31	MG	X	3058	1/1	0.95	0.35	35,35,35,35	0
31	MG	X	3019	1/1	0.95	0.24	44,44,44,44	0
31	MG	X	2920	1/1	0.95	0.63	19,19,19,19	0
31	MG	X	3294	1/1	0.95	0.23	78,78,78,78	0
31	MG	X	3296	1/1	0.95	0.24	56,56,56,56	0
31	MG	X	3297	1/1	0.95	0.26	25,25,25,25	0
31	MG	X	2921	1/1	0.95	0.27	7,7,7,7	0
31	MG	X	2941	1/1	0.95	0.19	40,40,40,40	0
31	MG	X	3008	1/1	0.95	0.72	39,39,39,39	0
31	MG	X	3233	1/1	0.95	0.66	63,63,63,63	0
31	MG	X	3264	1/1	0.95	0.29	47,47,47,47	0
31	MG	X	3304	1/1	0.95	0.15	88,88,88,88	0
31	MG	X	2942	1/1	0.95	0.17	19,19,19,19	0
31	MG	X	2948	1/1	0.95	0.41	32,32,32,32	0
31	MG	X	3236	1/1	0.95	0.28	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
31	MG	X	2998	1/1	0.95	0.45	50,50,50,50	0
31	MG	N	201	1/1	0.95	0.20	44,44,44,44	0
31	MG	X	3211	1/1	0.95	0.22	32,32,32,32	0
31	MG	X	3188	1/1	0.95	0.23	68,68,68,68	0
31	MG	X	3272	1/1	0.95	0.13	105,105,105,105	0
31	MG	X	2934	1/1	0.95	0.20	64,64,64,64	0
31	MG	X	2985	1/1	0.95	0.41	29,29,29,29	0
31	MG	X	3015	1/1	0.95	0.28	46,46,46,46	0
31	MG	X	3193	1/1	0.95	0.08	63,63,63,63	0
31	MG	X	3128	1/1	0.95	0.25	73,73,73,73	0
31	MG	X	3001	1/1	0.95	0.54	57,57,57,57	0
31	MG	X	3116	1/1	0.96	0.21	61,61,61,61	0
31	MG	X	3324	1/1	0.96	0.53	26,26,26,26	0
31	MG	X	2955	1/1	0.96	0.36	14,14,14,14	0
31	MG	X	3002	1/1	0.96	0.24	34,34,34,34	0
31	MG	X	2971	1/1	0.96	0.79	38,38,38,38	0
31	MG	X	2902	1/1	0.96	0.31	27,27,27,27	0
31	MG	X	2928	1/1	0.96	0.26	10,10,10,10	0
31	MG	X	2930	1/1	0.96	0.38	26,26,26,26	0
31	MG	X	3021	1/1	0.96	0.46	48,48,48,48	0
31	MG	X	3183	1/1	0.96	0.17	40,40,40,40	0
31	MG	X	3284	1/1	0.96	0.07	56,56,56,56	0
31	MG	X	3151	1/1	0.96	0.14	79,79,79,79	0
31	MG	X	3286	1/1	0.96	0.15	47,47,47,47	0
31	MG	X	3288	1/1	0.96	0.18	54,54,54,54	0
31	MG	X	2910	1/1	0.96	0.19	25,25,25,25	0
31	MG	X	3186	1/1	0.96	0.10	45,45,45,45	0
31	MG	X	3291	1/1	0.96	0.09	116,116,116,116	0
31	MG	X	3078	1/1	0.96	0.47	82,82,82,82	0
31	MG	X	3154	1/1	0.96	0.26	70,70,70,70	0
31	MG	X	3043	1/1	0.96	0.29	33,33,33,33	0
31	MG	X	3044	1/1	0.96	0.12	10,10,10,10	0
31	MG	X	2963	1/1	0.96	0.29	29,29,29,29	0
31	MG	X	3259	1/1	0.96	0.47	69,69,69,69	0
31	MG	X	3260	1/1	0.96	0.19	63,63,63,63	0
31	MG	X	3084	1/1	0.96	0.17	37,37,37,37	0
31	MG	X	3161	1/1	0.96	0.33	25,25,25,25	0
31	MG	X	3109	1/1	0.96	0.24	74,74,74,74	0
31	MG	X	3166	1/1	0.96	0.35	18,18,18,18	0
31	MG	X	3085	1/1	0.96	0.35	45,45,45,45	0
31	MG	X	2911	1/1	0.96	0.34	11,11,11,11	0
31	MG	X	3232	1/1	0.96	0.33	8,8,8,8	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
31	MG	X	3308	1/1	0.96	0.18	46,46,46,46	0
31	MG	X	3026	1/1	0.96	0.53	35,35,35,35	0
31	MG	X	3171	1/1	0.96	0.25	39,39,39,39	0
31	MG	X	2919	1/1	0.96	0.49	40,40,40,40	0
31	MG	X	3029	1/1	0.96	0.22	48,48,48,48	0
31	MG	X	3205	1/1	0.96	0.15	55,55,55,55	0
31	MG	X	2984	1/1	0.96	0.24	22,22,22,22	0
31	MG	X	3090	1/1	0.97	0.20	11,11,11,11	0
31	MG	X	2947	1/1	0.97	0.09	33,33,33,33	0
31	MG	X	2931	1/1	0.97	0.45	25,25,25,25	0
31	MG	X	2932	1/1	0.97	0.46	31,31,31,31	0
31	MG	X	2952	1/1	0.97	0.22	31,31,31,31	0
31	MG	X	2954	1/1	0.97	0.23	36,36,36,36	0
31	MG	X	2978	1/1	0.97	0.52	42,42,42,42	0
31	MG	X	2905	1/1	0.97	0.36	13,13,13,13	0
31	MG	X	3100	1/1	0.97	0.29	69,69,69,69	0
31	MG	X	3269	1/1	0.97	0.13	62,62,62,62	0
31	MG	X	3006	1/1	0.97	0.17	29,29,29,29	0
31	MG	X	3037	1/1	0.97	0.52	60,60,60,60	0
31	MG	X	2907	1/1	0.97	0.47	18,18,18,18	0
31	MG	X	2982	1/1	0.97	0.46	40,40,40,40	0
31	MG	X	2913	1/1	0.97	0.51	0,0,0,0	0
31	MG	X	3041	1/1	0.97	0.27	30,30,30,30	0
31	MG	X	3071	1/1	0.97	0.16	46,46,46,46	0
31	MG	X	2926	1/1	0.97	0.63	23,23,23,23	0
31	MG	X	2986	1/1	0.97	0.48	42,42,42,42	0
31	MG	X	3192	1/1	0.97	0.51	55,55,55,55	0
31	MG	X	2987	1/1	0.97	0.62	32,32,32,32	0
31	MG	X	2927	1/1	0.97	0.31	9,9,9,9	0
31	MG	X	2989	1/1	0.97	0.20	45,45,45,45	0
31	MG	X	2940	1/1	0.97	0.26	32,32,32,32	0
31	MG	X	2991	1/1	0.97	0.20	22,22,22,22	0
31	MG	X	3079	1/1	0.97	0.12	62,62,62,62	0
31	MG	X	3242	1/1	0.97	0.25	72,72,72,72	0
31	MG	X	3243	1/1	0.97	0.15	83,83,83,83	0
31	MG	X	3199	1/1	0.97	0.18	53,53,53,53	0
31	MG	X	3157	1/1	0.97	0.14	77,77,77,77	0
31	MG	X	3158	1/1	0.97	0.19	118,118,118,118	0
31	MG	Y	217	1/1	0.97	0.06	65,65,65,65	0
31	MG	X	3117	1/1	0.97	0.15	64,64,64,64	0
31	MG	X	2914	1/1	0.97	0.38	4,4,4,4	0
31	MG	X	3081	1/1	0.97	0.09	16,16,16,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
31	MG	X	3295	1/1	0.97	0.16	59,59,59,59	0
31	MG	X	3164	1/1	0.97	0.48	16,16,16,16	0
31	MG	M	201	1/1	0.97	0.57	7,7,7,7	0
31	MG	X	3050	1/1	0.97	0.23	41,41,41,41	0
31	MG	X	2903	1/1	0.97	0.32	11,11,11,11	0
31	MG	X	3299	1/1	0.97	0.20	89,89,89,89	0
32	MPD	X	3315	8/8	0.97	0.14	62,62,62,62	0
31	MG	X	3052	1/1	0.97	0.13	21,21,21,21	0
31	MG	X	2995	1/1	0.97	0.40	41,41,41,41	0
31	MG	X	3022	1/1	0.97	0.16	53,53,53,53	0
31	MG	X	3256	1/1	0.97	0.23	48,48,48,48	0
31	MG	X	2943	1/1	0.97	0.22	35,35,35,35	0
31	MG	X	2970	1/1	0.97	0.53	30,30,30,30	0
31	MG	X	2946	1/1	0.97	0.28	11,11,11,11	0
31	MG	X	2969	1/1	0.98	0.23	8,8,8,8	0
31	MG	X	2944	1/1	0.98	0.25	1,1,1,1	0
31	MG	X	2945	1/1	0.98	0.19	32,32,32,32	0
31	MG	X	2909	1/1	0.98	0.21	24,24,24,24	0
31	MG	X	2957	1/1	0.98	0.25	26,26,26,26	0
31	MG	X	3121	1/1	0.98	0.18	30,30,30,30	0
31	MG	X	2992	1/1	0.98	0.15	25,25,25,25	0
31	MG	X	3098	1/1	0.98	0.38	23,23,23,23	0
31	MG	X	3035	1/1	0.98	0.11	31,31,31,31	0
31	MG	X	3125	1/1	0.98	0.31	37,37,37,37	0
31	MG	X	2918	1/1	0.98	0.39	6,6,6,6	0
31	MG	X	2960	1/1	0.98	0.56	30,30,30,30	0
31	MG	X	2922	1/1	0.98	0.24	12,12,12,12	0
31	MG	X	2977	1/1	0.98	0.21	33,33,33,33	0
31	MG	X	2936	1/1	0.98	0.43	21,21,21,21	0
31	MG	X	2950	1/1	0.98	0.56	31,31,31,31	0
31	MG	X	2980	1/1	0.98	0.13	23,23,23,23	0
31	MG	X	3108	1/1	0.98	0.07	74,74,74,74	0
31	MG	X	3162	1/1	0.98	0.31	20,20,20,20	0
31	MG	X	2964	1/1	0.98	0.33	9,9,9,9	0
31	MG	X	2951	1/1	0.98	0.21	15,15,15,15	0
31	MG	X	2983	1/1	0.98	0.20	27,27,27,27	0
31	MG	X	2966	1/1	0.98	0.38	32,32,32,32	0
31	MG	X	3226	1/1	0.98	0.20	145,145,145,145	0
31	MG	X	3287	1/1	0.98	0.41	65,65,65,65	0
31	MG	X	3227	1/1	0.98	0.13	44,44,44,44	0
31	MG	X	2912	1/1	0.98	0.38	3,3,3,3	0
31	MG	X	3139	1/1	0.98	0.34	29,29,29,29	0

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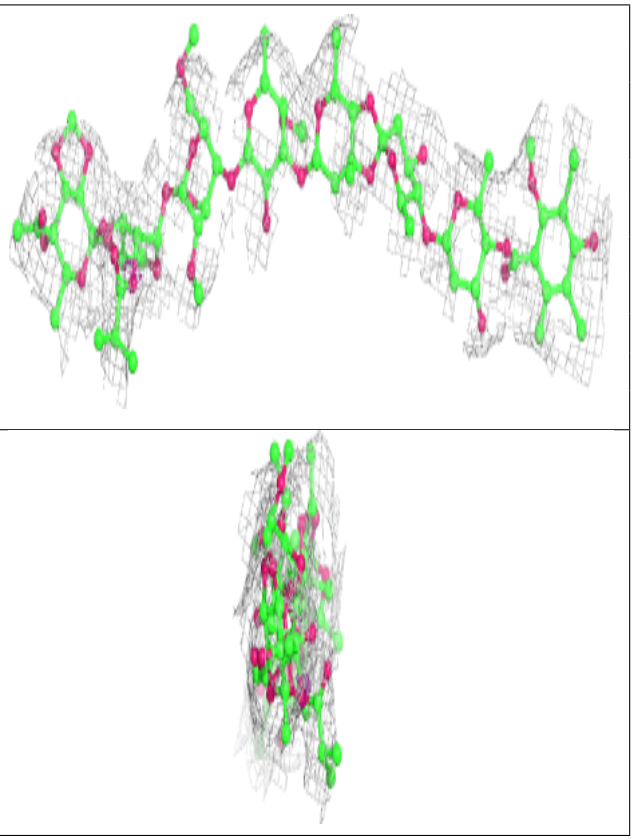
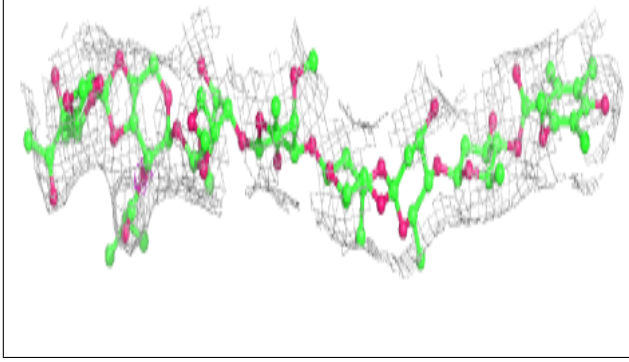
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
31	MG	X	3140	1/1	0.98	0.31	27,27,27,27	0
31	MG	X	2953	1/1	0.98	0.30	53,53,53,53	0
31	MG	X	3027	1/1	0.98	0.30	14,14,14,14	0
31	MG	X	3167	1/1	0.99	0.06	7,7,7,7	0
31	MG	X	3099	1/1	0.99	0.32	46,46,46,46	0
31	MG	X	2959	1/1	0.99	0.22	39,39,39,39	0
31	MG	X	3203	1/1	0.99	0.04	42,42,42,42	0
31	MG	X	3030	1/1	0.99	0.27	0,0,0,0	0
31	MG	X	3018	1/1	0.99	0.20	35,35,35,35	0
31	MG	X	2938	1/1	0.99	0.27	8,8,8,8	0
31	MG	X	3009	1/1	0.99	0.71	31,31,31,31	0
31	MG	X	3163	1/1	0.99	0.47	0,0,0,0	0
31	MG	X	2906	1/1	0.99	0.30	35,35,35,35	0
31	MG	X	2929	1/1	0.99	0.24	21,21,21,21	0
31	MG	X	3147	1/1	0.99	0.10	82,82,82,82	0

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

Electron density around 6NO X 2901:

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





6.5 Other polymers (i)

There are no such residues in this entry.