



# Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 02:34 pm BST

PDB ID : 4WT8  
Title : Crystal Structure of bactobolin A bound to 70S ribosome-tRNA complex  
Authors : Amunts, A.; Fiedorczuk, K.; Ramakrishnan, V.  
Deposited on : 2014-10-29  
Resolution : 3.40 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

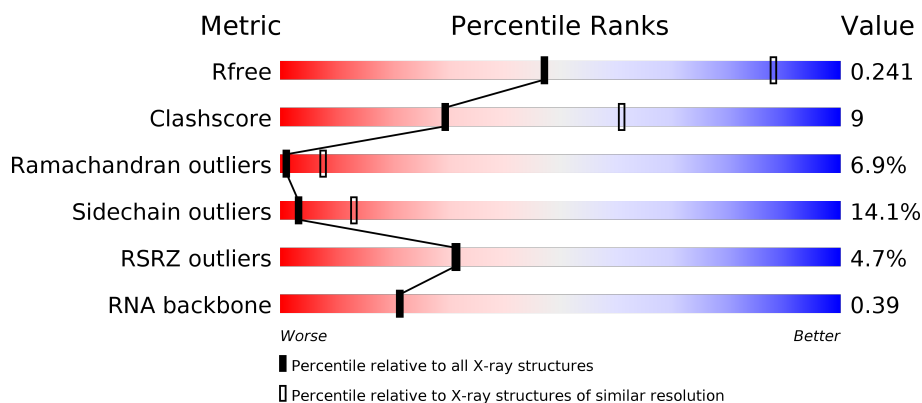
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.40 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.






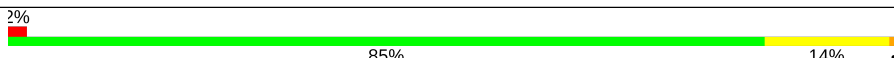
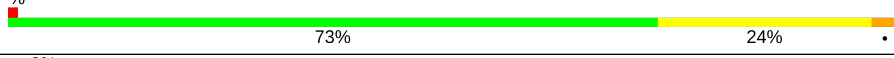

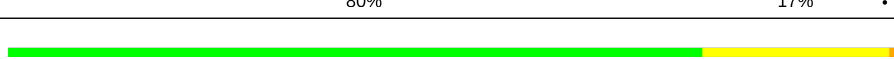



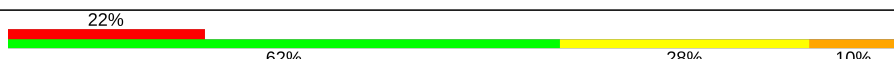



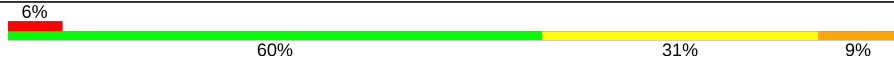

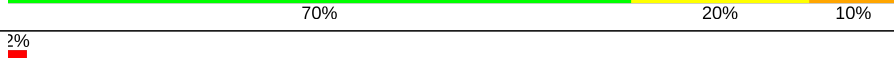






Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)
RNA backbone	3102	1006 (3.84-2.96)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A2	9	<div> <div>11%</div> <div>33%</div> <div>56%</div> </div>
2	AA	234	<div> <div>4%</div> <div>68%</div> <div>28%</div> <div>.</div> </div>
2	BA	234	<div> <div>7%</div> <div>70%</div> <div>27%</div> <div>.</div> </div>
3	AC	238	<div> <div>6%</div> <div>58%</div> <div>24%</div> <div>5%</div> <div>13%</div> </div>

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Mol	Chain	Length	Quality of chain
4	AD	208	
4	BD	208	
5	AE	150	
5	BE	150	
6	AF	101	
6	BF	101	
7	AG	155	
7	BG	155	
8	AH	138	
8	BH	138	
9	AI	127	
9	BI	127	
10	AJ	98	
10	BJ	98	
11	AK	119	
11	BK	119	
12	AL	124	
12	BL	124	
13	AM	124	
13	BM	124	
14	AN	60	
14	BN	60	
15	AO	88	
15	BO	88	
16	AP	83	

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Mol	Chain	Length	Quality of chain
16	BP	83	
17	AR	99	
17	BR	99	
18	AS	70	
18	BS	70	
19	AT	78	
19	BT	78	
20	AU	99	
20	BU	99	
21	AW	24	
21	BW	24	
22	Ab	1504	
22	Bb	1504	
23	B2	10	
24	BC	206	
25	C2	76	
25	C3	76	
25	D3	76	
26	C4	77	
27	CA	206	
28	CB	271	
28	DB	271	
29	CC	204	
29	DC	204	
30	CD	207	

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Mol	Chain	Length	Quality of chain
30	DD	207	
31	CE	181	
31	DE	181	
32	CF	159	
32	DF	159	
33	CI	145	
33	DI	145	
34	CJ	130	
34	DJ	130	
35	CM	138	
35	DM	138	
36	CN	122	
36	DN	122	
37	CO	146	
37	DO	146	
38	CP	141	
38	DP	141	
39	CQ	117	
39	DQ	117	
40	CR	98	
40	DR	98	
41	CS	137	
41	DS	137	
42	CT	117	
42	DT	117	

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Mol	Chain	Length	Quality of chain
43	CU	101	
43	DU	101	
44	CW	113	
45	CX	92	
45	DX	92	
46	CY	100	
46	DY	100	
47	CZ	176	
47	DZ	176	
48	Ca	84	
48	Da	84	
49	CH	93	
49	DH	93	
50	CK	71	
50	DK	71	
51	CL	59	
51	DL	59	
52	C5	30	
52	D5	30	
53	C6	59	
53	D6	59	
54	C7	44	
54	D7	44	
55	C8	48	
55	D8	48	

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Mol	Chain	Length	Quality of chain
56	C9	63	
56	D9	63	
57	C0	36	
57	D0	36	
58	C1	2899	
58	D1	2899	
59	Cs	119	
59	Ds	119	
60	D2	20	
61	D4	76	
62	DA	206	
63	DW	113	
64	DV	55	

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
66	3V6	D1	3001	-	-	X	-
67	MG	D1	3002	-	-	X	-

## 2 Entry composition

There are 67 unique types of molecules in this entry. The entry contains 295910 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 mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A2	9	Total	C	N	O	P	0	0	0
			173	76	29	59	9			

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AA	234	Total	C	N	O	S	0	0	0
			1901	1213	341	342	5			
2	BA	234	Total	C	N	O	S	0	0	0
			1901	1213	341	342	5			

- Molecule 3 is a protein called 30S ribosomal protein S3.

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

- Molecule 4 is a protein called 30S ribosomal protein S4.

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

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AE	150	Total	C	N	O	S	0	0	0
			1147	724	217	202	4			
5	BE	150	Total	C	N	O	S	0	0	0
			1147	724	217	202	4			



- Molecule 6 is a protein called 30S ribosomal protein S6.

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

- Molecule 7 is a protein called 30S ribosomal protein S7.

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

- Molecule 8 is a protein called 30S ribosomal protein S8.

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

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	AI	127	Total	C	N	O	0	0	0
			1011	639	198	174			
9	BI	127	Total	C	N	O	0	0	0
			1011	639	198	174			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AI	58	ARG	HIS	conflict	UNP P80374

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AJ	98	Total	C	N	O	S	0	0	0
			795	499	156	139	1			
10	BJ	98	Total	C	N	O	S	0	0	0
			795	499	156	139	1			

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AK	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			
11	BK	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AL	124	Total	C	N	O	S	0	0	0
			971	611	195	164	1			
12	BL	124	Total	C	N	O	S	0	0	0
			971	611	195	164	1			

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	124	Total	C	N	O	S	0	0	0
			988	611	205	170	2			
13	BM	124	Total	C	N	O	S	0	0	0
			988	611	205	170	2			

- Molecule 14 is a protein called 30S ribosomal protein S14 type Z.

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

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AO	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			
15	BO	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AP	83	Total	C	N	O	S	0	0	0
			701	443	139	118	1			
16	BP	83	Total	C	N	O	S	0	0	0
			701	443	139	118	1			

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AR	99	Total	C	N	O	S	0	0	0
			824	528	151	143	2			
17	BR	99	Total	C	N	O	S	0	0	0
			824	528	151	143	2			

- Molecule 18 is a protein called 30S ribosomal protein S18.

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

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AT	78	Total	C	N	O	S	0	0	0
			630	403	114	111	2			
19	BT	78	Total	C	N	O	S	0	0	0
			630	403	114	111	2			

- Molecule 20 is a protein called 30S ribosomal protein S20.

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

- Molecule 21 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	AW	24	Total	C	N	O	0	0	0
			209	128	50	31			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	BW	24	Total	C	N	O	0	0	0
			209	128	50	31			

- Molecule 22 is a RNA chain called RNA (1504-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	Ab	1504	Total	C	N	O	P	0	0	0
			32329	14390	5992	10444	1503			
22	Bb	1504	Total	C	N	O	P	0	0	0
			32329	14390	5992	10444	1503			

- Molecule 23 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	B2	10	Total	C	N	O	P	0	0	0
			194	86	34	64	10			

- Molecule 24 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	BC	206	Total	C	N	O	S	0	0	0
			1613	1016	314	282	1			

- Molecule 25 is a RNA chain called A site tNA, E site tNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	C2	75	Total	C	N	O	P	0	0	0
			1597	713	285	525	74			
25	C3	76	Total	C	N	O	P	0	0	0
			1619	723	290	531	75			
25	D3	76	Total	C	N	O	P	0	0	0
			1619	723	290	531	75			

- Molecule 26 is a RNA chain called P site trNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	C4	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			

- Molecule 27 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
27	CA	190	Total	C	N	O	0	0	0
			1156	706	220	230			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CA	106	ALA	GLY	conflict	UNP Q5SLP7

- Molecule 28 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	CB	271	Total	C	N	O	S	0	0	0
			2105	1329	416	357	3			
28	DB	271	Total	C	N	O	S	0	0	0
			2105	1329	416	357	3			

- Molecule 29 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	CC	204	Total	C	N	O	S	0	0	0
			1564	988	299	271	6			
29	DC	204	Total	C	N	O	S	0	0	0
			1564	988	299	271	6			

- Molecule 30 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	CD	207	Total	C	N	O	S	0	0	0
			1624	1035	303	283	3			
30	DD	207	Total	C	N	O	S	0	0	0
			1624	1035	303	283	3			

- Molecule 31 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	CE	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			
31	DE	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			

- Molecule 32 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	CF	159	Total	C	N	O	S	0	0	0
			1223	773	228	221	1			
32	DF	159	Total	C	N	O	S	0	0	0
			1223	773	228	221	1			

- Molecule 33 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	CI	145	Total	C	N	O	S	0	0	0
			1132	723	200	208	1			
33	DI	145	Total	C	N	O	S	0	0	0
			1132	723	200	208	1			

- Molecule 34 is a protein called ribosomal L10 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	CJ	130	Total	C	N	O		0	0	0
			651	390	130	131				
34	DJ	130	Total	C	N	O		0	0	0
			651	390	130	131				

- Molecule 35 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	CM	138	Total	C	N	O	S	0	0	0
			1105	712	206	183	4			
35	DM	138	Total	C	N	O	S	0	0	0
			1105	712	206	183	4			

- Molecule 36 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	CN	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			
36	DN	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

- Molecule 37 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	CO	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	DO	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			

- Molecule 38 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	CP	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			
38	DP	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

- Molecule 39 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	CQ	117	Total	C	N	O		0	0	0
			960	599	202	159				
39	DQ	117	Total	C	N	O		0	0	0
			960	599	202	159				

- Molecule 40 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	CR	98	Total	C	N	O		0	0	0
			771	486	154	131				
40	DR	98	Total	C	N	O		0	0	0
			771	486	154	131				

- Molecule 41 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	CS	137	Total	C	N	O	S	0	0	0
			1142	710	234	197	1			
41	DS	137	Total	C	N	O	S	0	0	0
			1142	710	234	197	1			

- Molecule 42 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	CT	117	Total	C	N	O	S	0	0	0
			958	604	202	151	1			
42	DT	117	Total	C	N	O	S	0	0	0
			958	604	202	151	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CT	32	ALA	PHE	conflict	UNP P60491
DT	32	ALA	PHE	conflict	UNP P60491

- Molecule 43 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	CU	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			
43	DU	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

- Molecule 44 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	CW	113	Total	C	N	O	S	0	0	0
			896	563	176	155	2			

- Molecule 45 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
45	CX	92	Total	C	N	O	0	0	0
			726	471	131	124			
45	DX	92	Total	C	N	O	0	0	0
			726	471	131	124			

- Molecule 46 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	CY	100	Total	C	N	O	S	0	0	0
			776	500	148	124	4			
46	DY	100	Total	C	N	O	S	0	0	0
			776	500	148	124	4			

- Molecule 47 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	CZ	176	Total	C	N	O	S	0	0	0
			1404	897	252	253	2			
47	DZ	176	Total	C	N	O	S	0	0	0
			1404	897	252	253	2			



- Molecule 48 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	Ca	84	Total	C	N	O	S	0	0	0
			662	410	140	111	1			
48	Da	84	Total	C	N	O	S	0	0	0
			662	410	140	111	1			

- Molecule 49 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	CH	93	Total	C	N	O	S	0	0	0
			734	460	147	126	1			
49	DH	93	Total	C	N	O	S	0	0	0
			734	460	147	126	1			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DH	81	ARG	LYS	conflict	UNP P60494

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	CK	71	Total	C	N	O	S	0	0	0
			598	370	121	106	1			
50	DK	71	Total	C	N	O	S	0	0	0
			598	370	121	106	1			

- Molecule 51 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	CL	59	Total	C	N	O	S	0	0	0
			468	298	90	79	1			
51	DL	59	Total	C	N	O	S	0	0	0
			468	298	90	79	1			

- Molecule 52 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	C5	30	Total	C	N	O	S	0	0	0
			226	142	36	44	4			
52	D5	30	Total	C	N	O	S	0	0	0
			226	142	36	44	4			

- Molecule 53 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	C6	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			
53	D6	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			

- Molecule 54 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	C7	44	Total	C	N	O	S	0	0	0
			381	235	77	65	4			
54	D7	44	Total	C	N	O	S	0	0	0
			381	235	77	65	4			

- Molecule 55 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	C8	48	Total	C	N	O	S	0	0	0
			419	257	104	56	2			
55	D8	48	Total	C	N	O	S	0	0	0
			419	257	104	56	2			

- Molecule 56 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	C9	63	Total	C	N	O	S	0	0	0
			508	326	101	79	2			
56	D9	63	Total	C	N	O	S	0	0	0
			508	326	101	79	2			

- Molecule 57 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	C0	36	Total	C	N	O	S	0	0	0
			299	183	67	46	3			
57	D0	36	Total	C	N	O	S	0	0	0
			299	183	67	46	3			

- Molecule 58 is a RNA chain called 23S rRNA (2899-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
58	C1	2807	Total	C	N	O	P	0	0	0
			60459	26907	11311	19435	2806			
58	D1	2807	Total	C	N	O	P	0	0	0
			60459	26907	11311	19435	2806			

- Molecule 59 is a RNA chain called 5S rRNA (119-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
59	Cs	119	Total	C	N	O	P	0	0	0
			2551	1136	471	826	118			
59	Ds	119	Total	C	N	O	P	0	0	0
			2551	1136	471	826	118			

- Molecule 60 is a RNA chain called tRNA (5'-D(\*AP\*UP\*CP\*CP\*CP\*CP\*GP\*UP\*GP\*UP\*CP\*CP\*UP\*UP\*GP\*GP\*UP\*UP\*CP\*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
60	D2	20	Total	C	N	O	P	0	0	0
			416	186	65	146	19			

- Molecule 61 is a RNA chain called tRNA (76-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
61	D4	76	Total	C	N	O	P	0	0	0
			1623	723	294	530	76			

- Molecule 62 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
62	DA	190	Total	C	N	O	0	0	0
			1155	705	220	230			

- Molecule 63 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
63	DW	113	Total	C	N	O	S	0	0	0
			896	563	176	155	2			

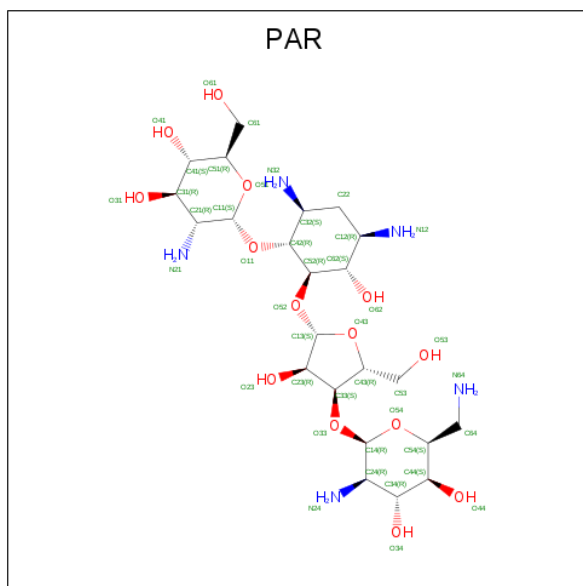
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DW	113	ALA	-	expression tag	UNP Q5SHP3

- Molecule 64 is a RNA chain called DNA (55-MER).

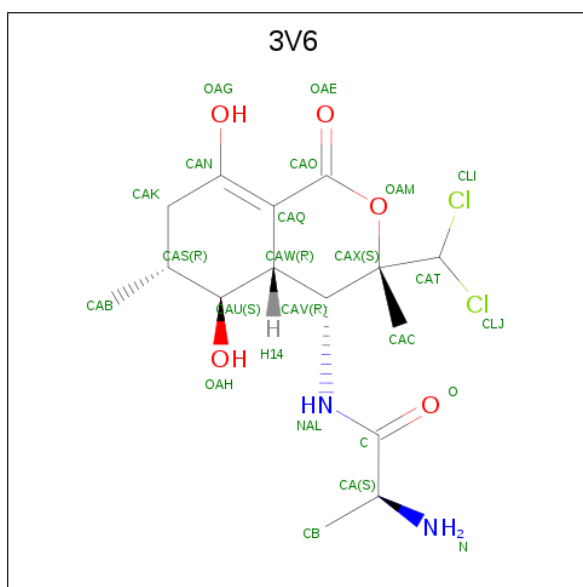
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
64	DV	55	Total	C	N	O	P	0	0	0
			1167	527	220	379	41			

- Molecule 65 is PAROMOMYCIN (three-letter code: PAR) (formula:  $C_{23}H_{45}N_5O_{14}$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
65	Ab	1	Total	C	N	O	0	0
			42	23	5	14		
65	Bb	1	Total	C	N	O	0	0
			42	23	5	14		

- Molecule 66 is Bactobolin A (three-letter code: 3V6) (formula:  $C_{15}H_{22}Cl_2N_2O_5$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
66	C1	1	Total 24	C 15	Cl 2	N 2	O 5	0	0
66	D1	1	Total 24	C 15	Cl 2	N 2	O 5	0	0

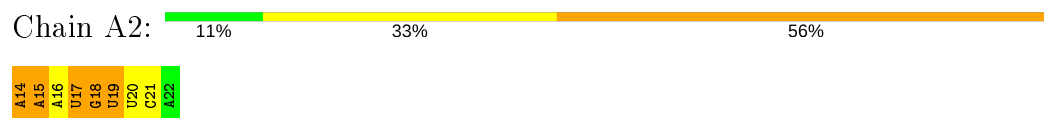
- Molecule 67 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
67	C1	1	Total Mg 1 1	0	0
67	D1	1	Total Mg 1 1	0	0

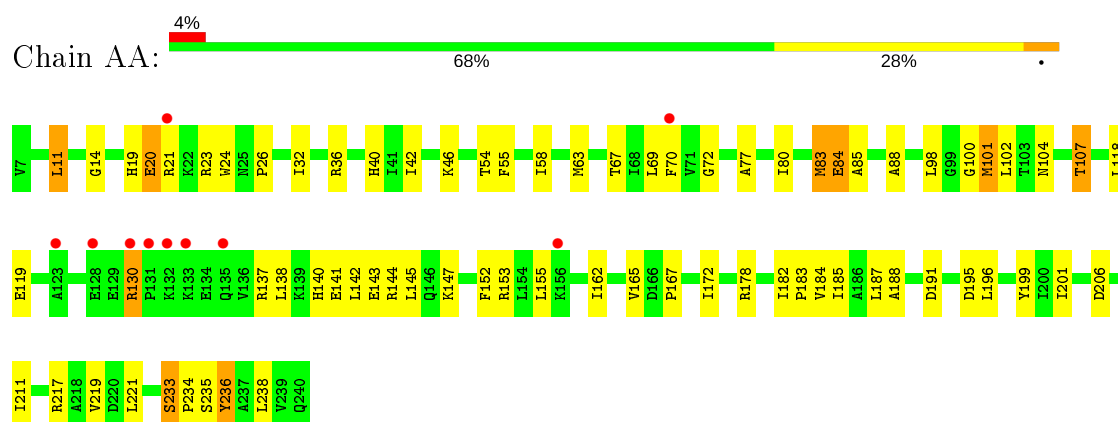
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

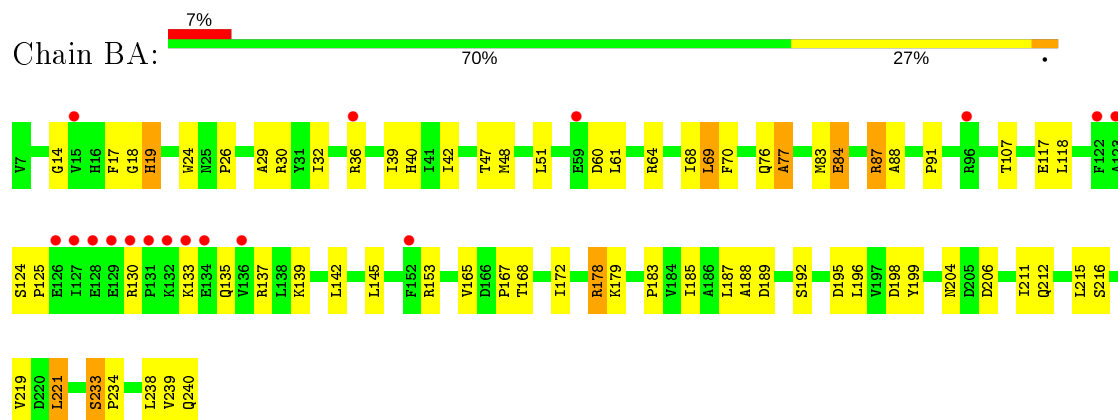
#### • Molecule 1: mRNA



#### • Molecule 2: 30S ribosomal protein S2

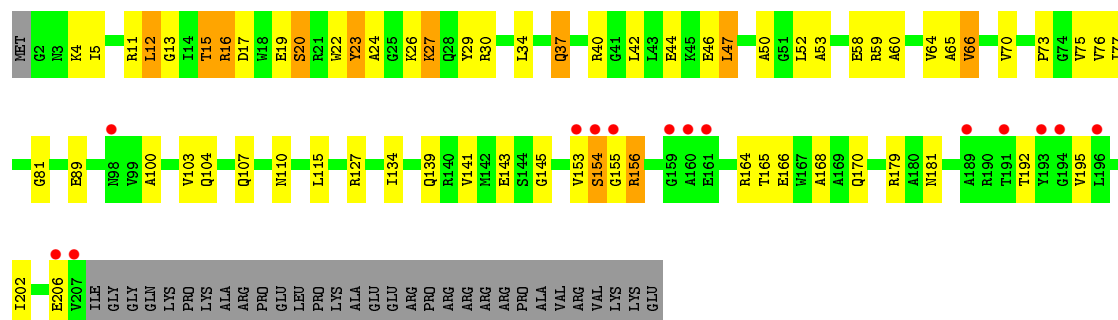


#### • Molecule 2: 30S ribosomal protein S2

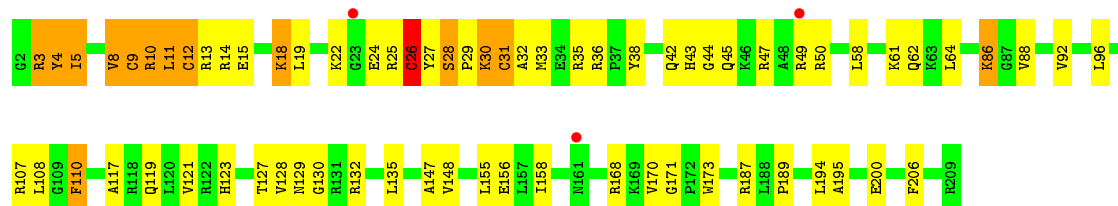


#### • Molecule 3: 30S ribosomal protein S3

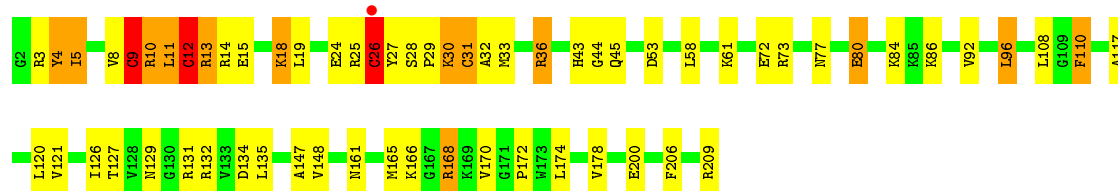




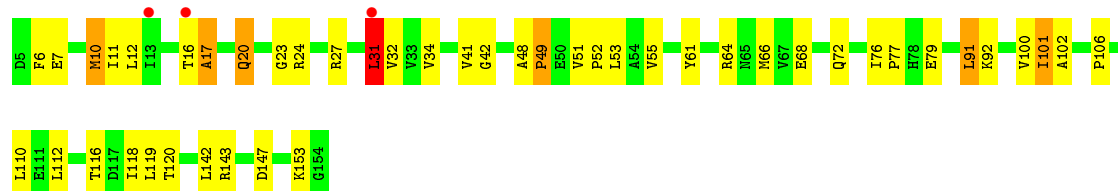
- Molecule 4: 30S ribosomal protein S4



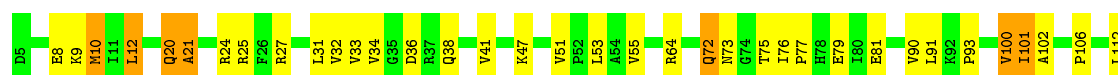
- Molecule 4: 30S ribosomal protein S4



- Molecule 5: 30S ribosomal protein S5

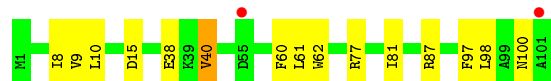
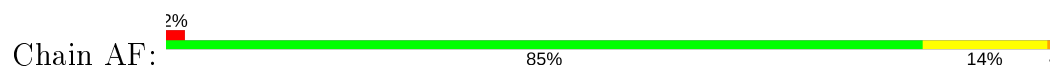


- Molecule 5: 30S ribosomal protein S5

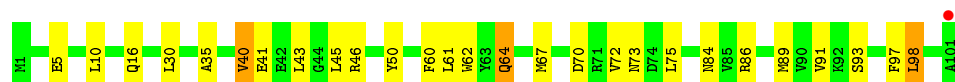
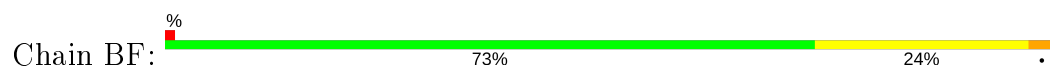




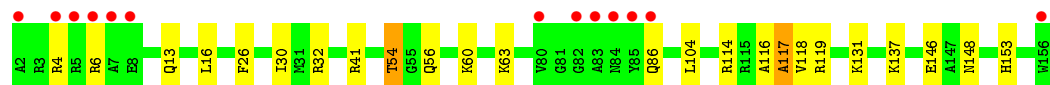
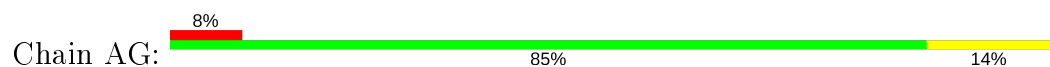
- Molecule 6: 30S ribosomal protein S6



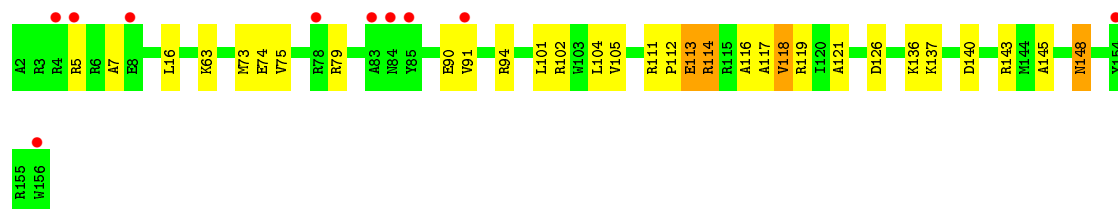
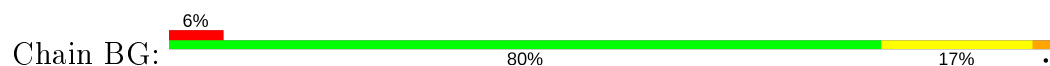
- Molecule 6: 30S ribosomal protein S6



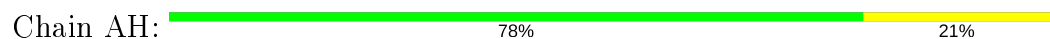
- Molecule 7: 30S ribosomal protein S7



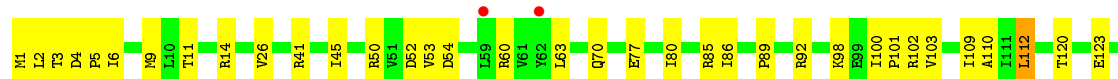
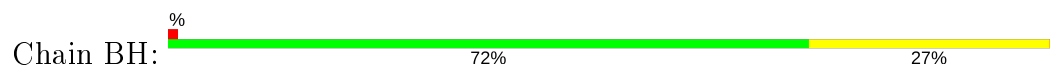
- Molecule 7: 30S ribosomal protein S7



- Molecule 8: 30S ribosomal protein S8



- Molecule 8: 30S ribosomal protein S8







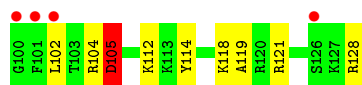
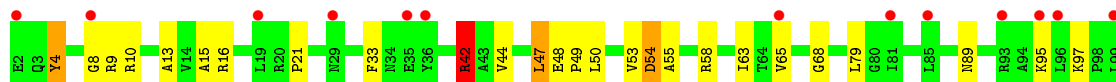
- Molecule 9: 30S ribosomal protein S9

Chain AI: 6% 61% 32% 6%



- Molecule 9: 30S ribosomal protein S9

Chain BI: 13% 72% 24%



- Molecule 10: 30S ribosomal protein S10

Chain AJ: 13% 66% 26% 8%



- Molecule 10: 30S ribosomal protein S10

Chain BJ: 22% 62% 28% 10%

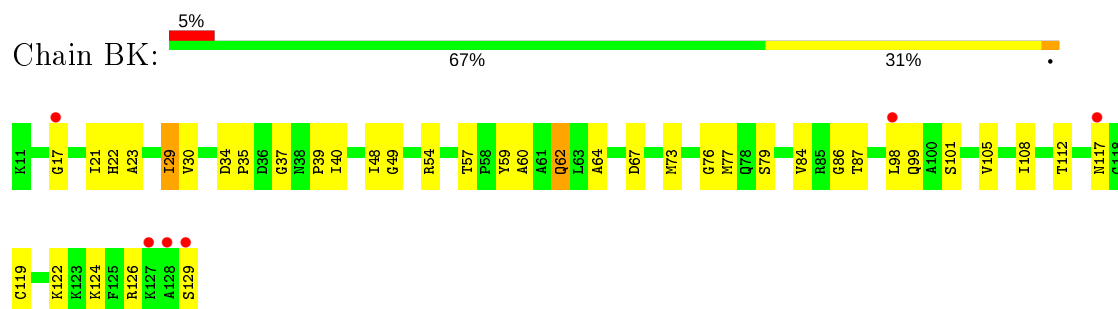


- Molecule 11: 30S ribosomal protein S11

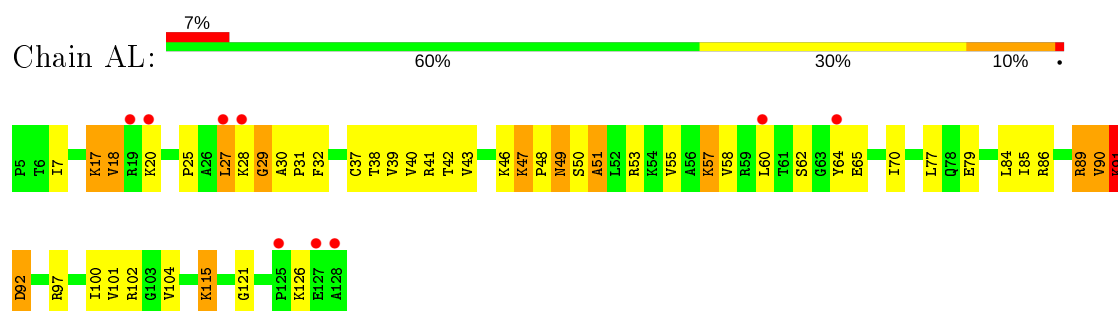
Chain AK: 4% 74% 26%



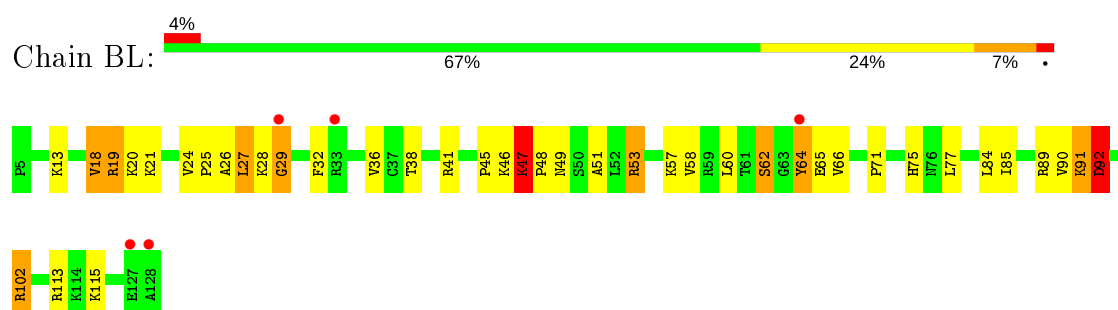
- Molecule 11: 30S ribosomal protein S11



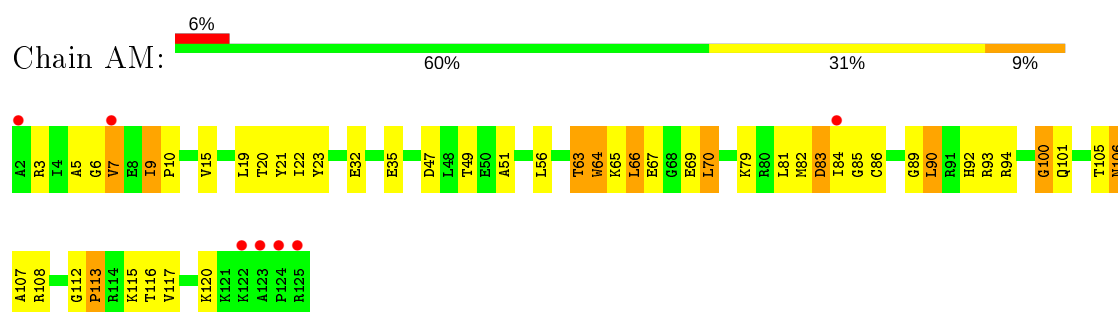
- Molecule 12: 30S ribosomal protein S12



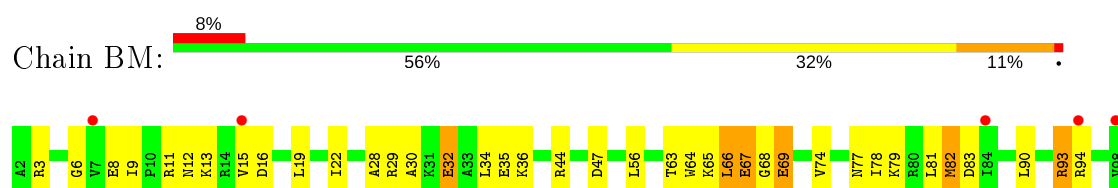
- Molecule 12: 30S ribosomal protein S12



- Molecule 13: 30S ribosomal protein S13

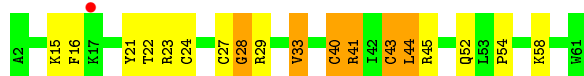
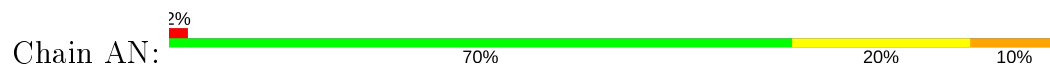


- Molecule 13: 30S ribosomal protein S13

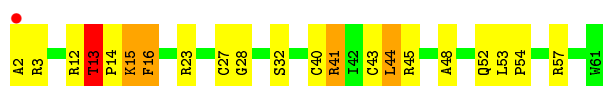




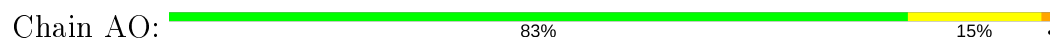
- Molecule 14: 30S ribosomal protein S14 type Z



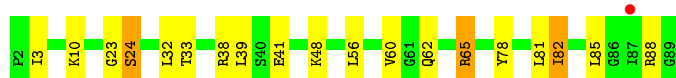
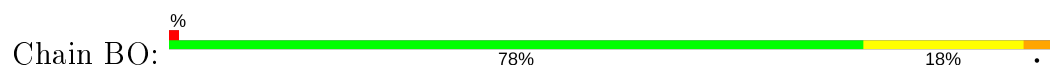
- Molecule 14: 30S ribosomal protein S14 type Z



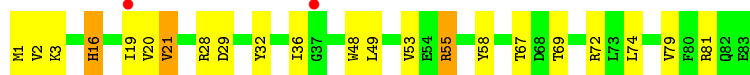
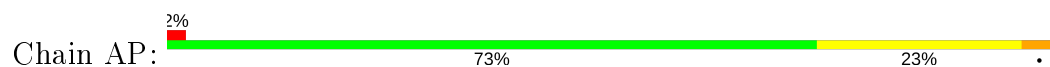
- Molecule 15: 30S ribosomal protein S15



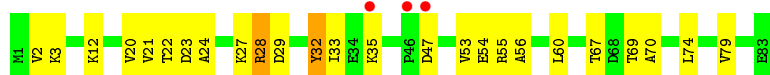
- Molecule 15: 30S ribosomal protein S15



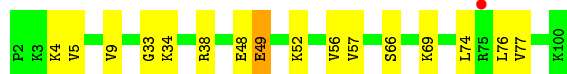
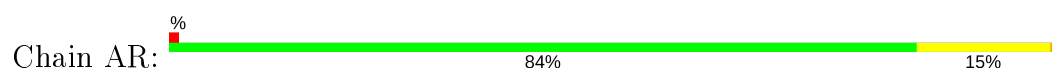
- Molecule 16: 30S ribosomal protein S16



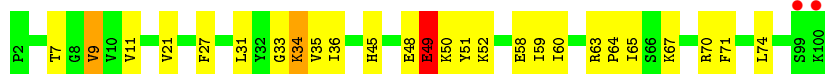
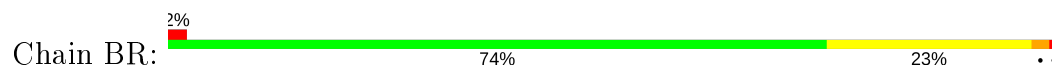
- Molecule 16: 30S ribosomal protein S16



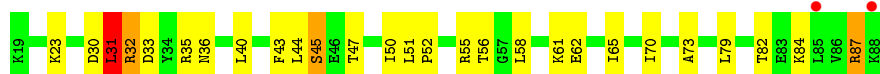
- Molecule 17: 30S ribosomal protein S17



- Molecule 17: 30S ribosomal protein S17



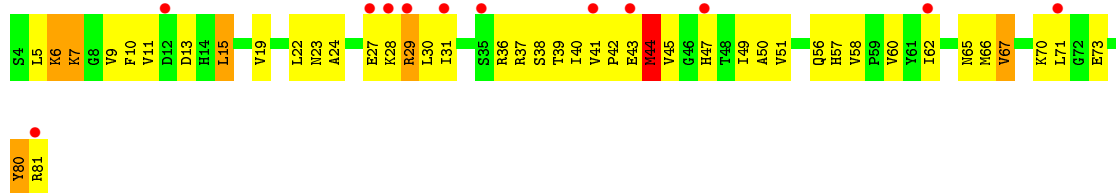
- Molecule 18: 30S ribosomal protein S18



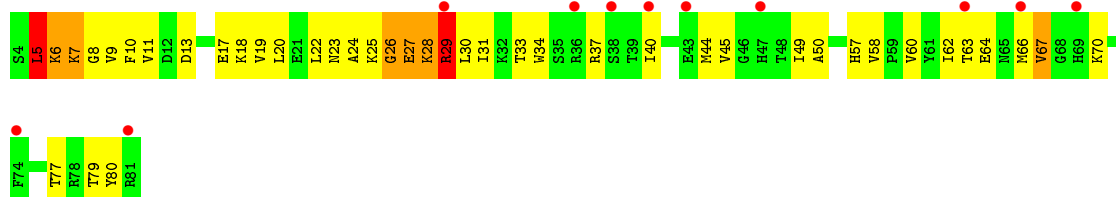
- Molecule 18: 30S ribosomal protein S18



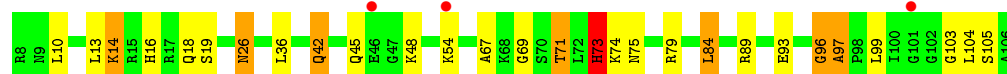
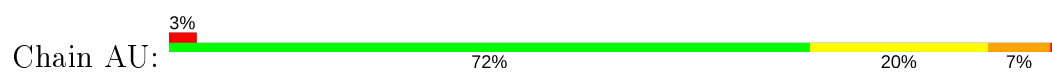
- Molecule 19: 30S ribosomal protein S19



- Molecule 19: 30S ribosomal protein S19



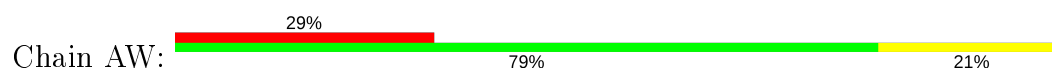
- Molecule 20: 30S ribosomal protein S20



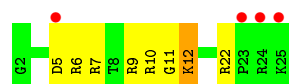
- Molecule 20: 30S ribosomal protein S20



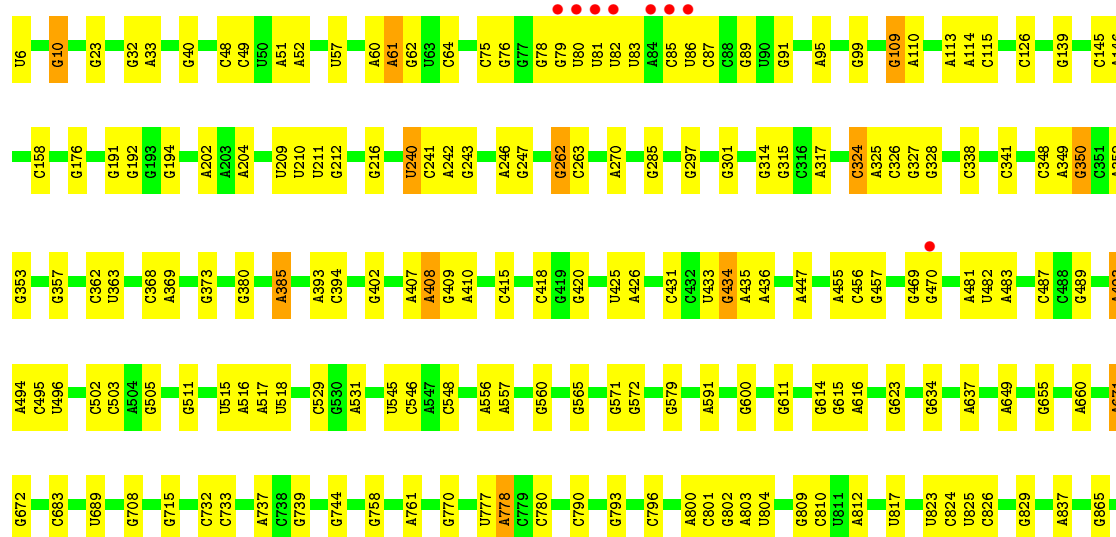
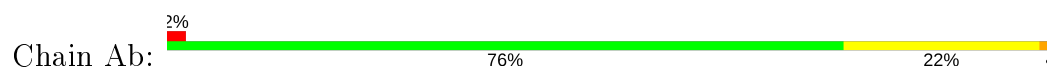
- Molecule 21: 30S ribosomal protein Thx

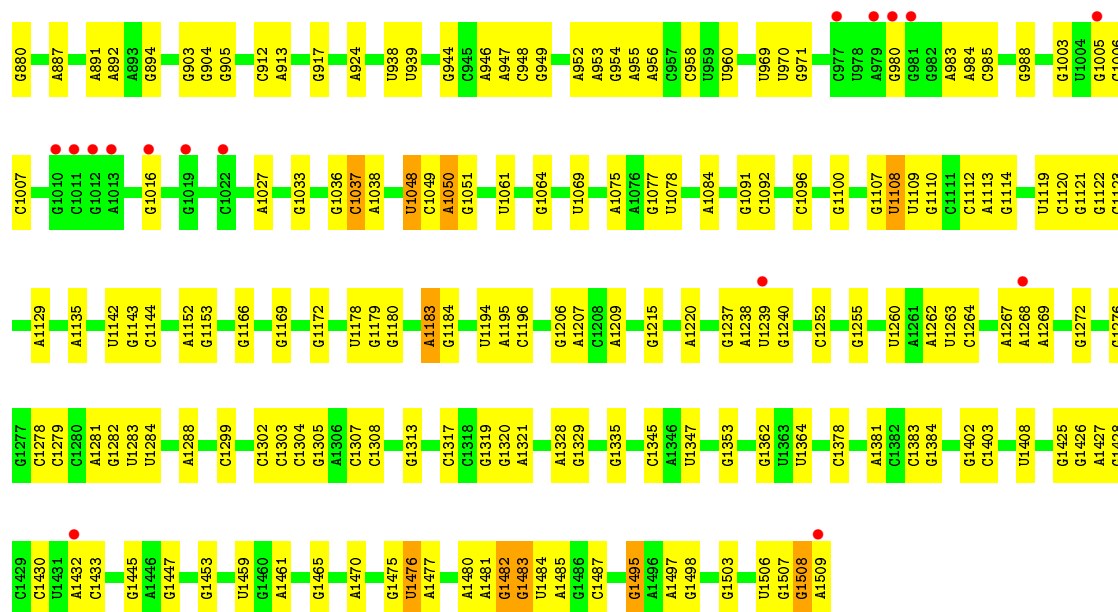


- Molecule 21: 30S ribosomal protein Thx

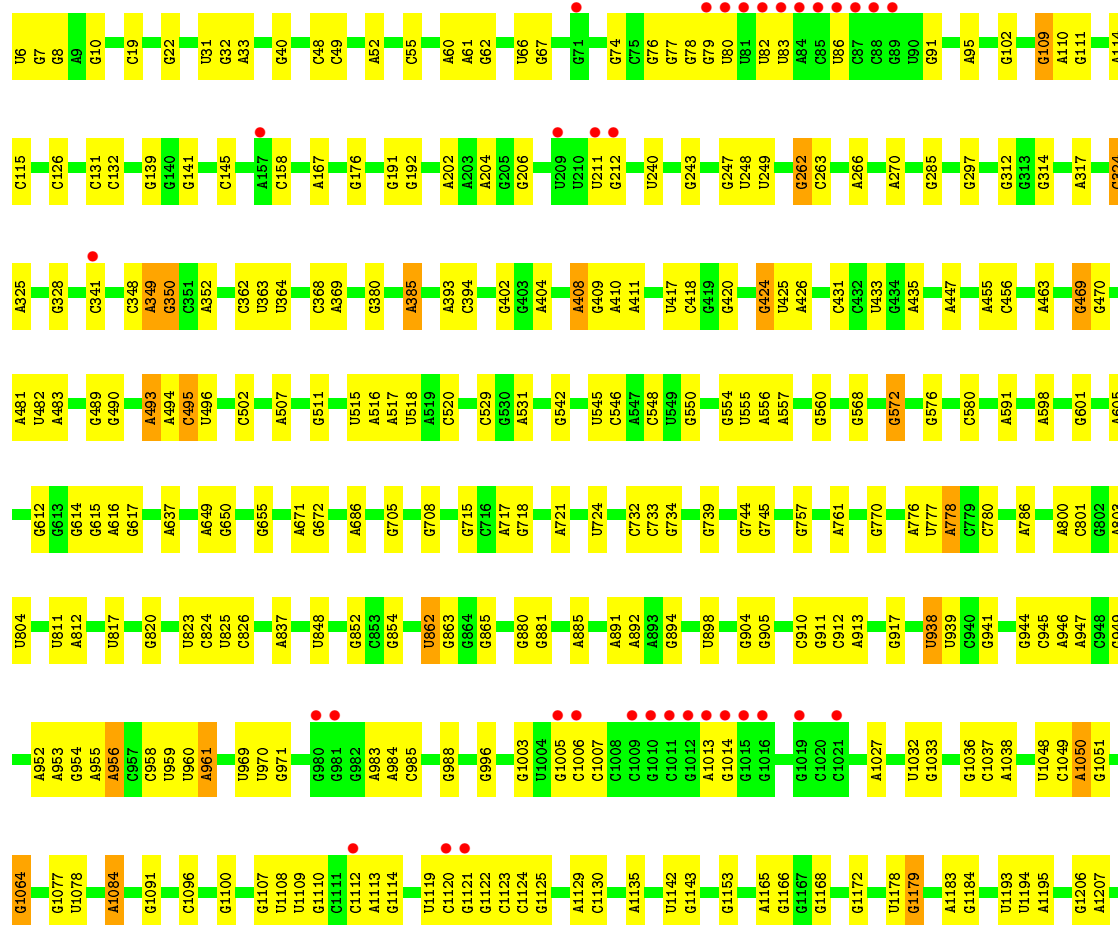
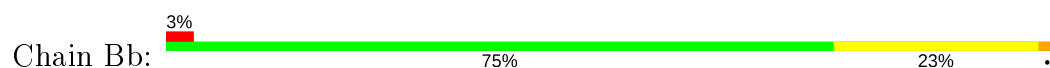


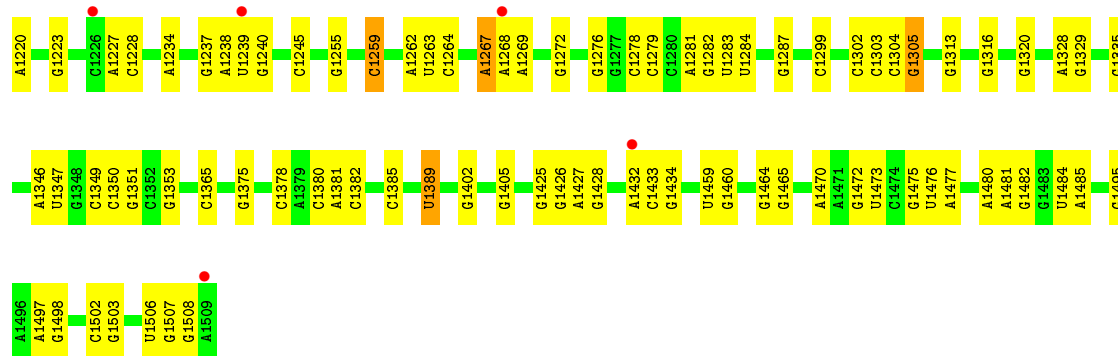
- Molecule 22: RNA (1504-MER)



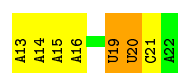


• Molecule 22: RNA (1504-MER)

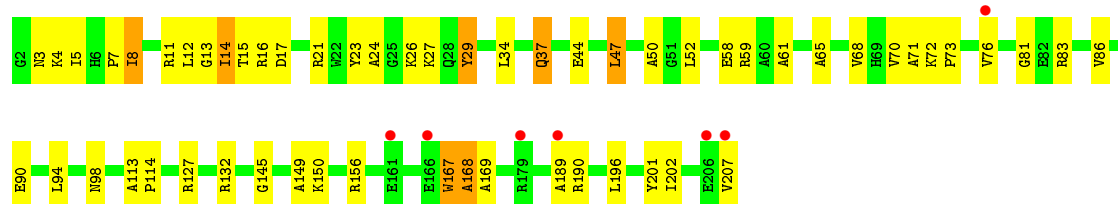
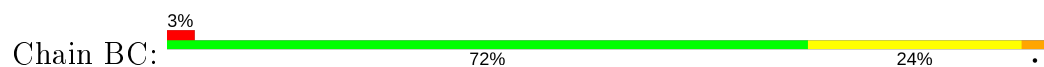




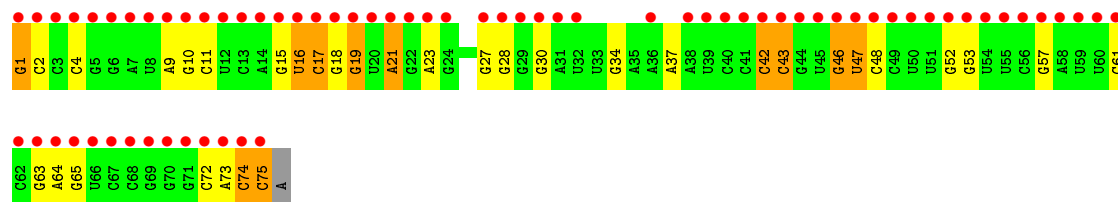
• Molecule 23: mRNA



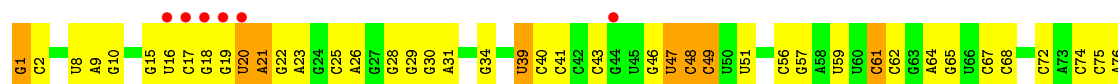
• Molecule 24: 30S ribosomal protein S3



• Molecule 25: A site tRNA, E site tRNA

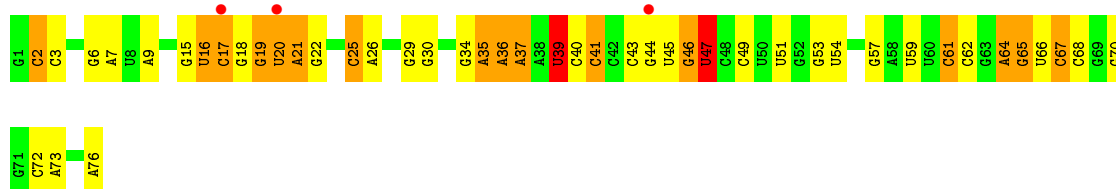


• Molecule 25: A site tRNA, E site tRNA



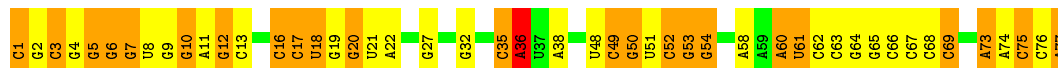
• Molecule 25: A site tRNA, E site tRNA





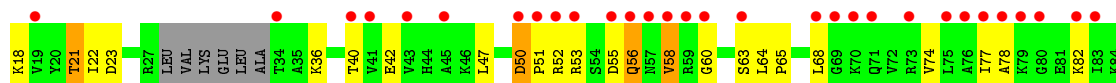
- Molecule 26: P site trNA

Chain C4: 38% 31% 30%



- Molecule 27: 50S ribosomal protein L1

Chain CA: 76% 14% 8%



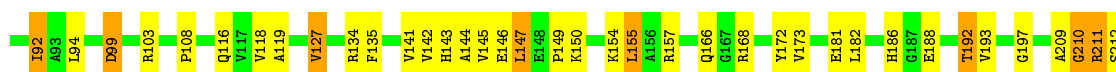
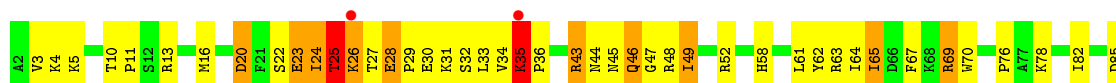
- Molecule 28: 50S ribosomal protein L2

Chain CB: 59% 29% 10%

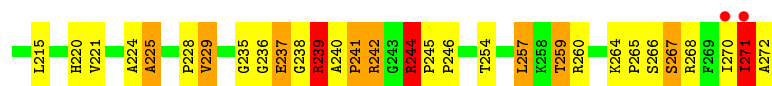


- Molecule 28: 50S ribosomal protein L2

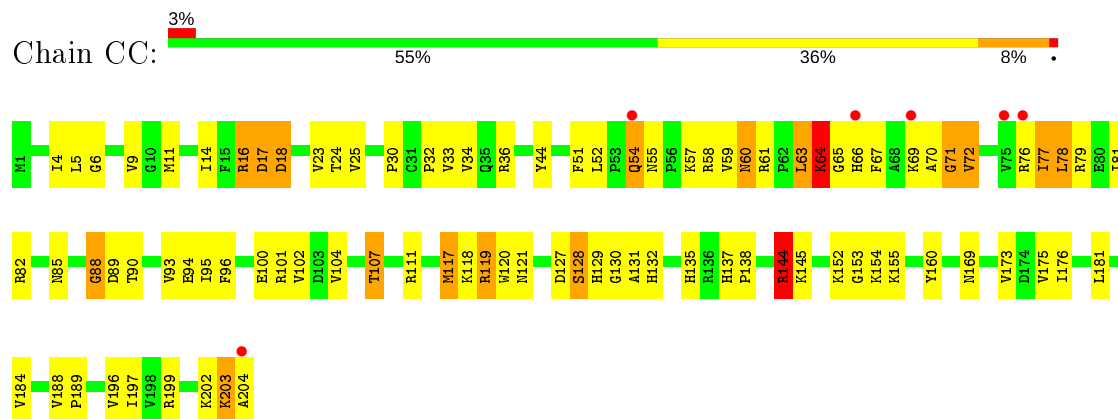
Chain DB: 59% 30% 10%



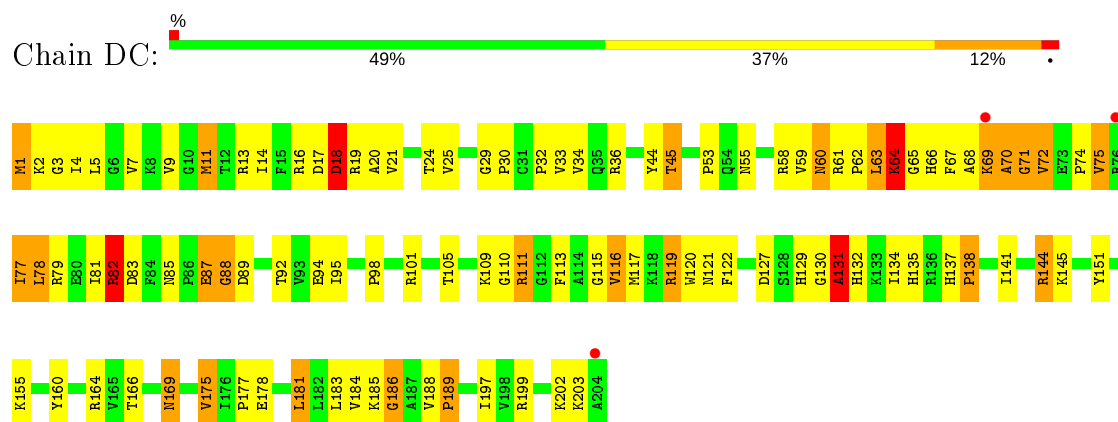




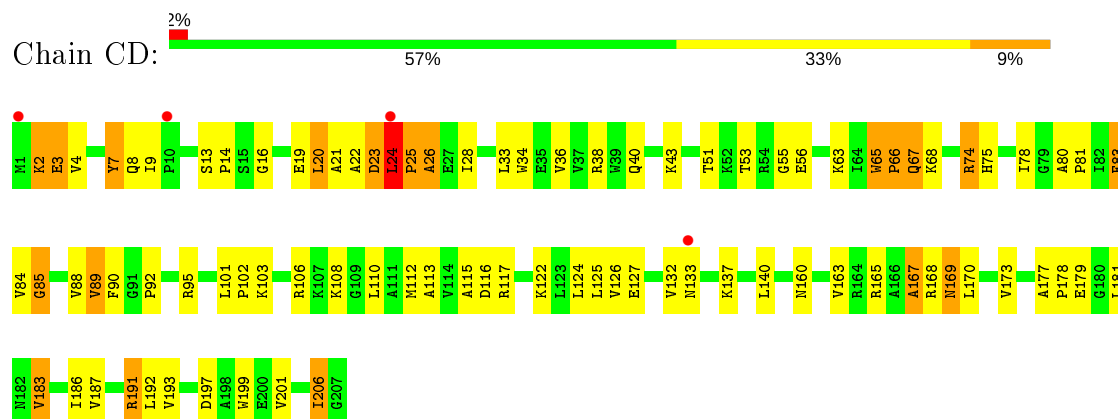
- Molecule 29: 50S ribosomal protein L3



- Molecule 29: 50S ribosomal protein L3

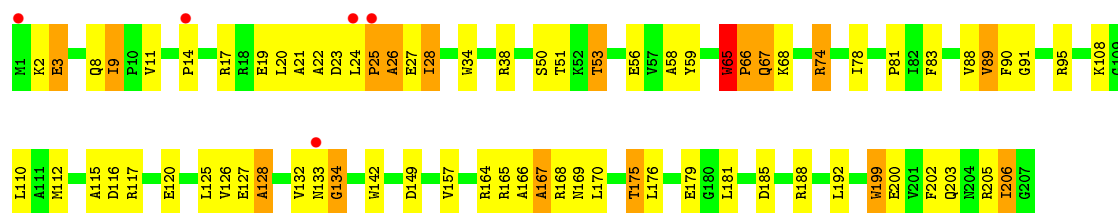


- Molecule 30: 50S ribosomal protein L4

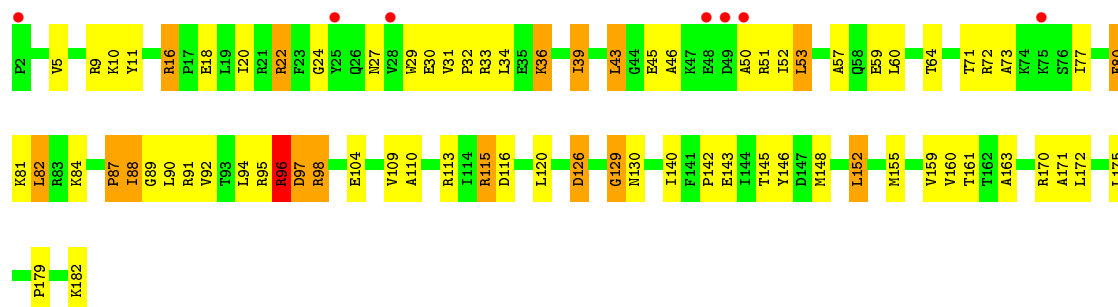


- Molecule 30: 50S ribosomal protein L4

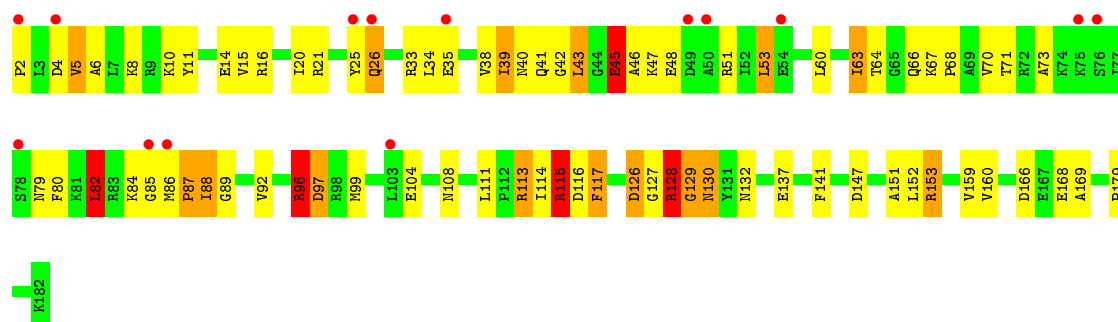




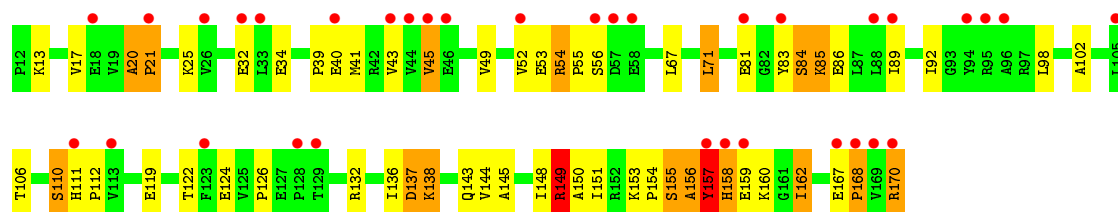
• Molecule 31: 50S ribosomal protein L5



• Molecule 31: 50S ribosomal protein L5

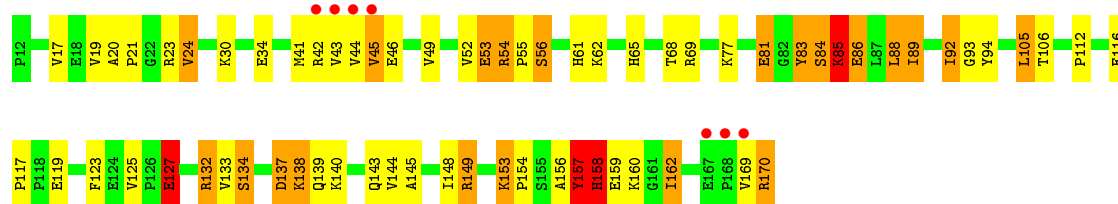


• Molecule 32: 50S ribosomal protein L6

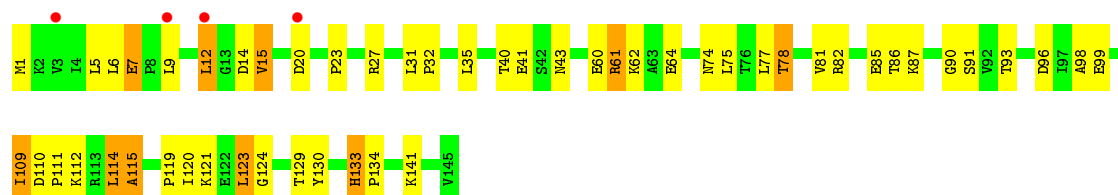


• Molecule 32: 50S ribosomal protein L6

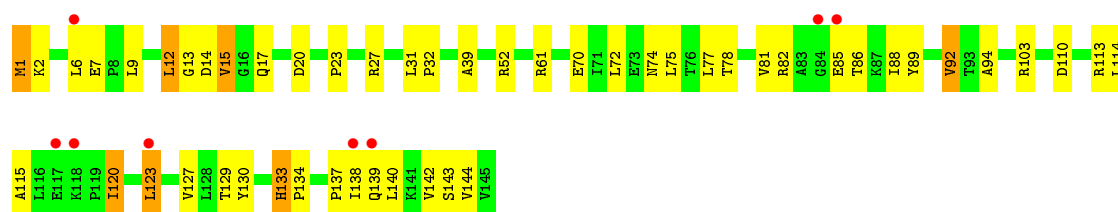




• Molecule 33: 50S ribosomal protein L9



• Molecule 33: 50S ribosomal protein L9



• Molecule 34: ribosomal L10 protein

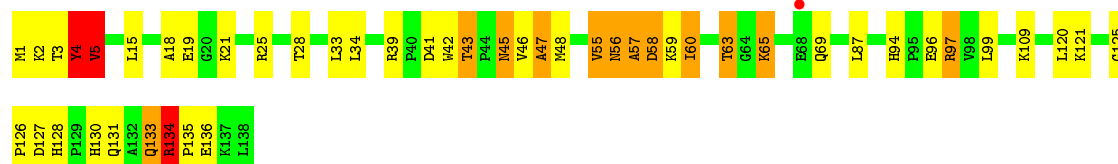


There are no outlier residues recorded for this chain.

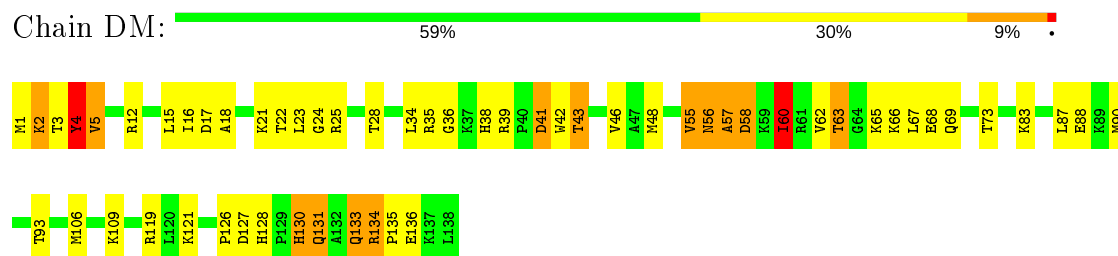
• Molecule 34: ribosomal L10 protein



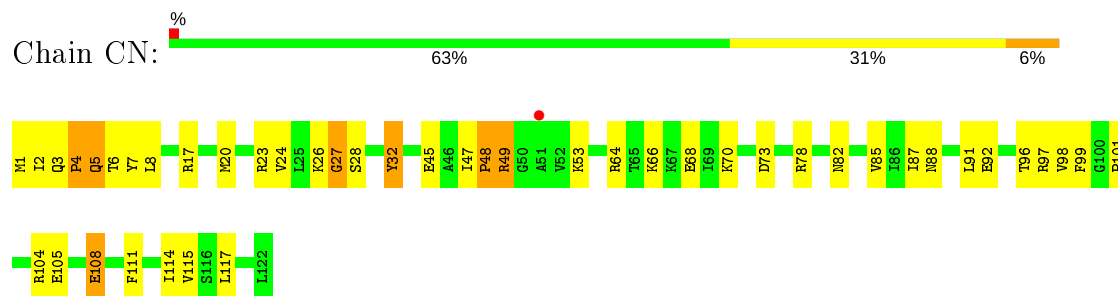
• Molecule 35: 50S ribosomal protein L13



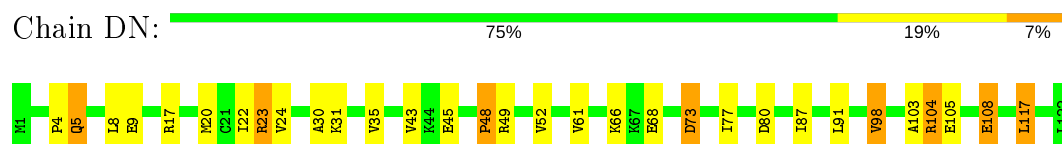
- Molecule 35: 50S ribosomal protein L13



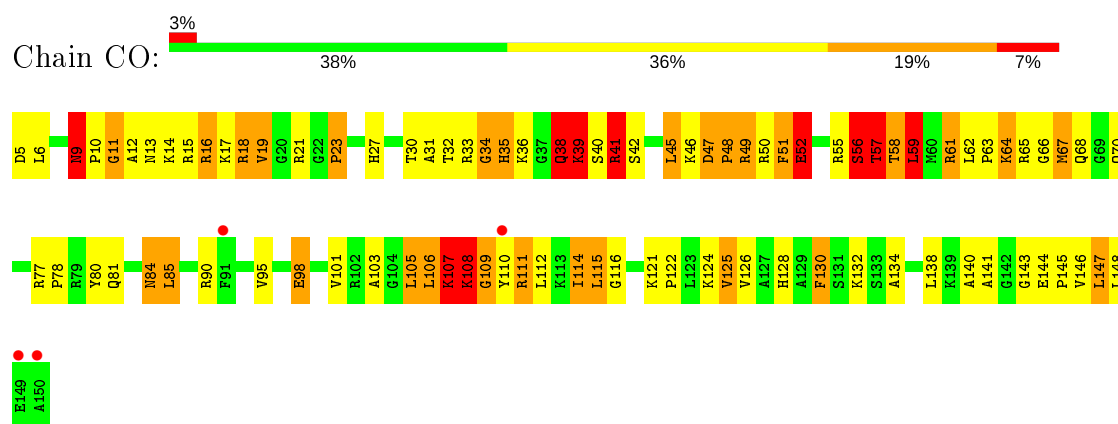
- Molecule 36: 50S ribosomal protein L14



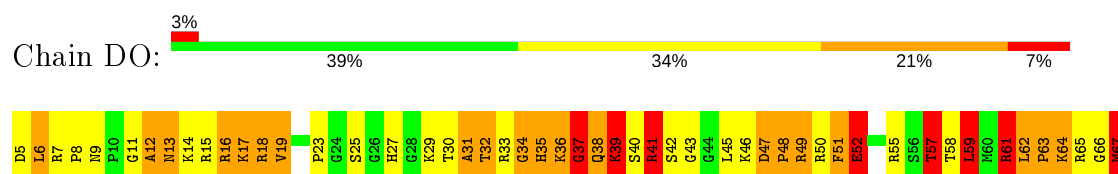
- Molecule 36: 50S ribosomal protein L14

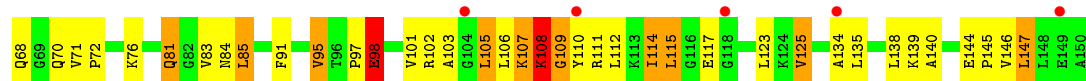


- Molecule 37: 50S ribosomal protein L15

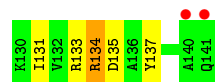
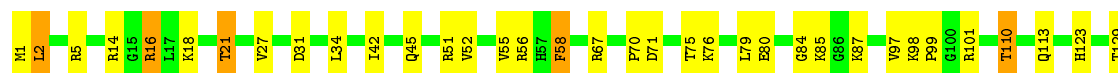
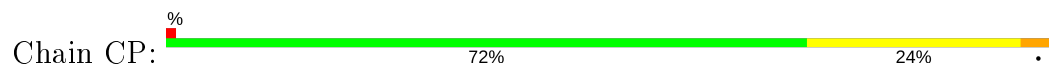


- Molecule 37: 50S ribosomal protein L15

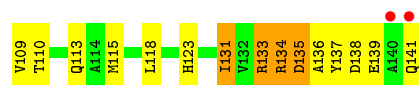
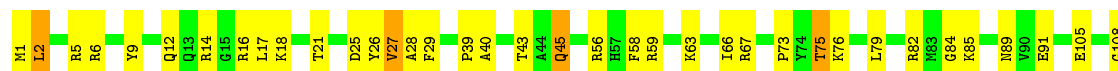




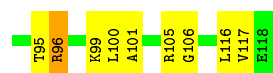
- Molecule 38: 50S ribosomal protein L16



- Molecule 38: 50S ribosomal protein L16



- Molecule 39: 50S ribosomal protein L17

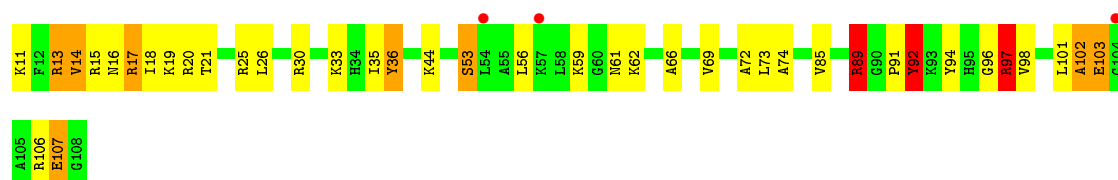


- Molecule 39: 50S ribosomal protein L17

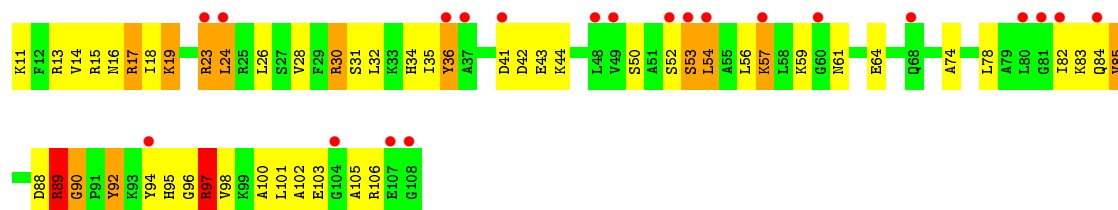


- Molecule 40: 50S ribosomal protein L18

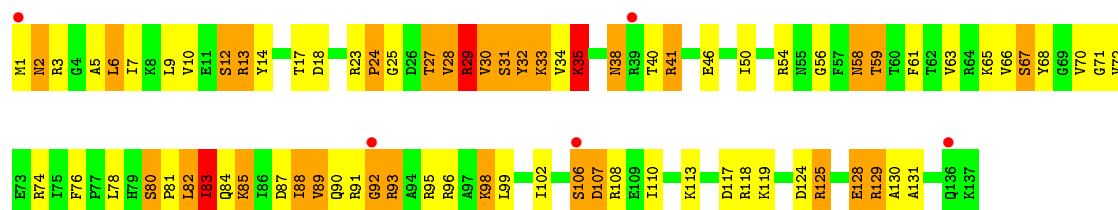
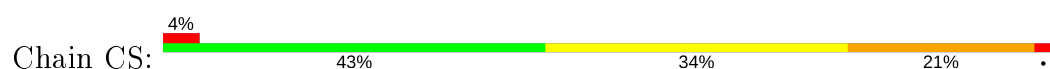




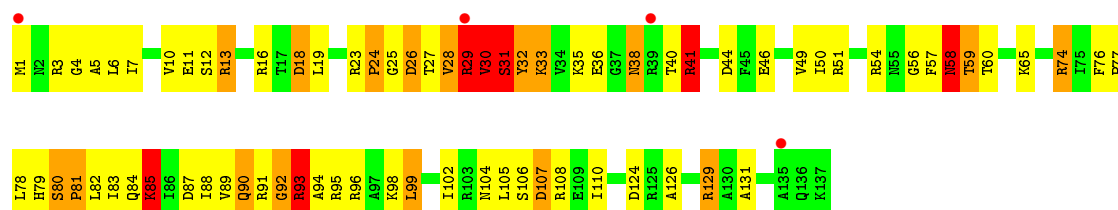
- Molecule 40: 50S ribosomal protein L18



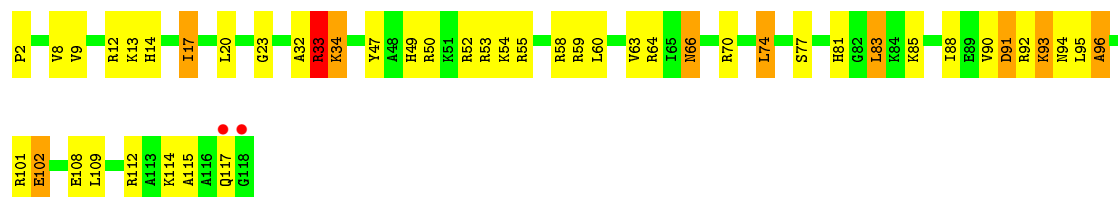
- Molecule 41: 50S ribosomal protein L19



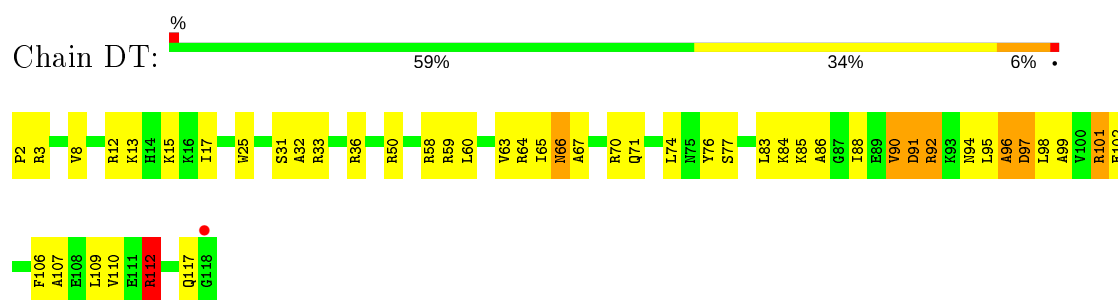
- Molecule 41: 50S ribosomal protein L19



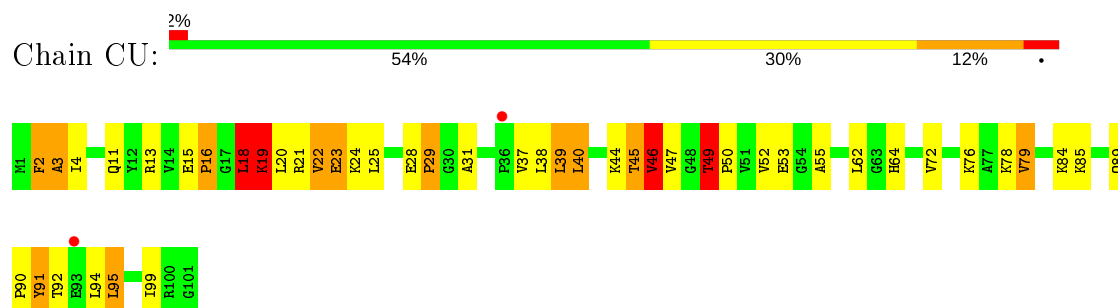
- Molecule 42: 50S ribosomal protein L20



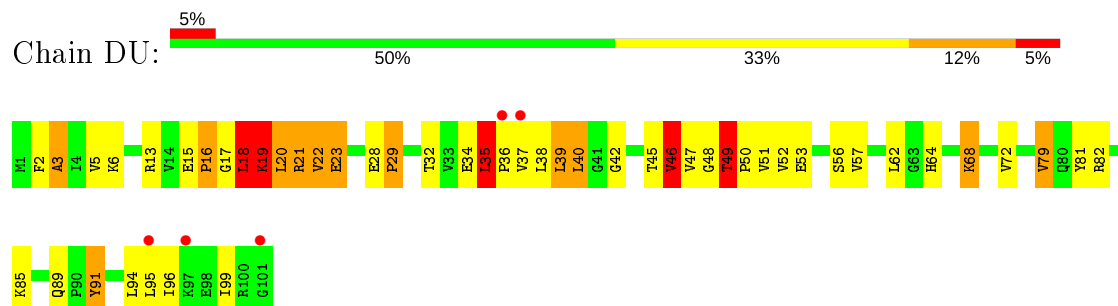
- Molecule 42: 50S ribosomal protein L20



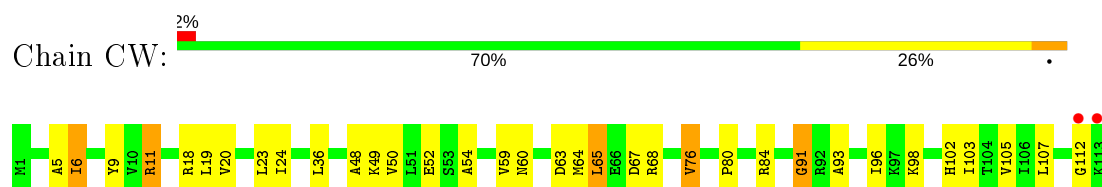
- Molecule 43: 50S ribosomal protein L21



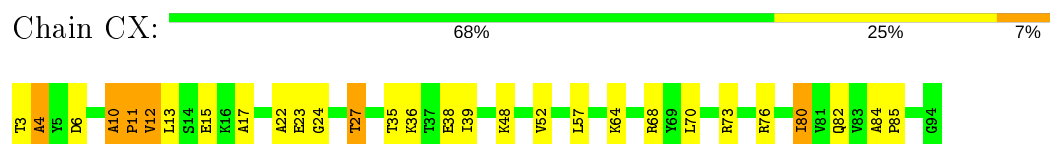
- Molecule 43: 50S ribosomal protein L21



- Molecule 44: 50S ribosomal protein L22

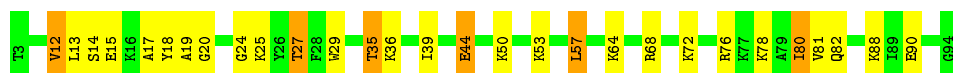


- Molecule 45: 50S ribosomal protein L23

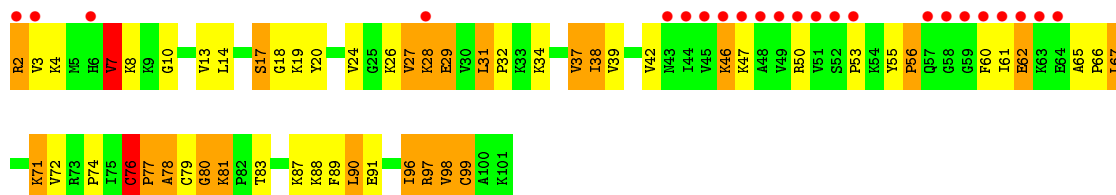


- Molecule 45: 50S ribosomal protein L23

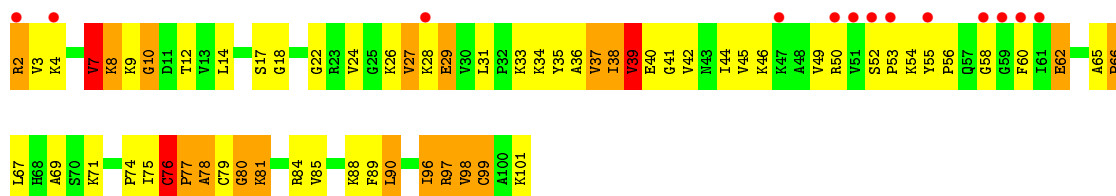




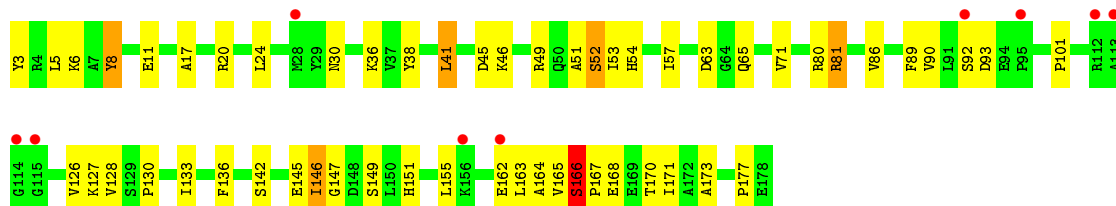
- Molecule 46: 50S ribosomal protein L24



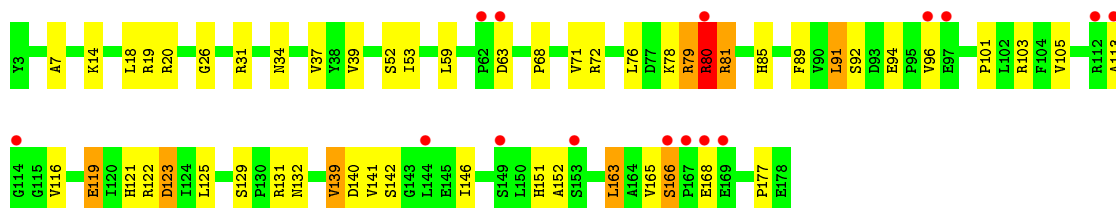
- Molecule 46: 50S ribosomal protein L24



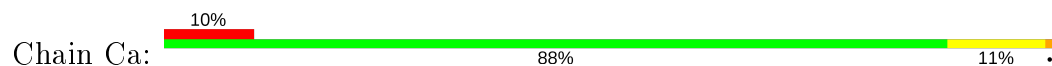
- Molecule 47: 50S ribosomal protein L25



- Molecule 47: 50S ribosomal protein L25



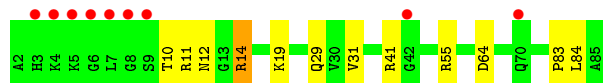
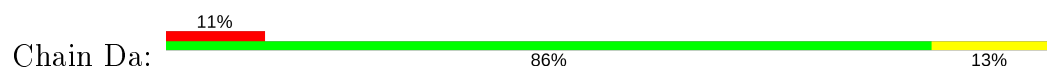
- Molecule 48: 50S ribosomal protein L27



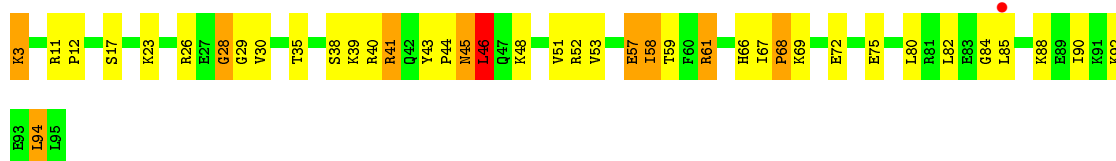




- Molecule 48: 50S ribosomal protein L27



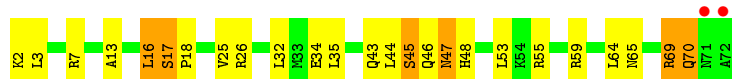
- Molecule 49: 50S ribosomal protein L28



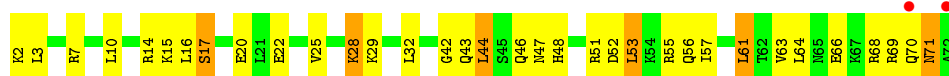
- Molecule 49: 50S ribosomal protein L28



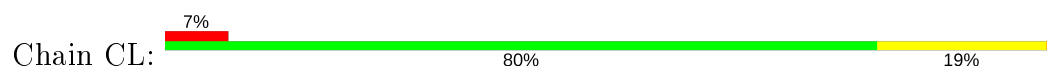
- Molecule 50: 50S ribosomal protein L29



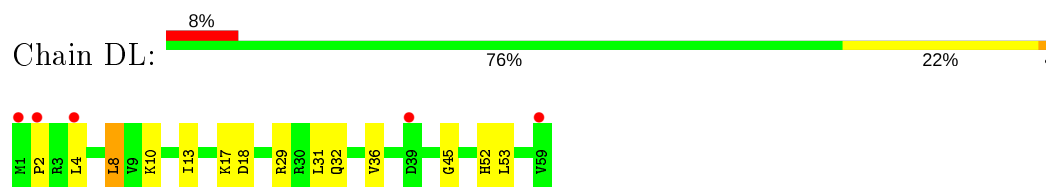
- Molecule 50: 50S ribosomal protein L29



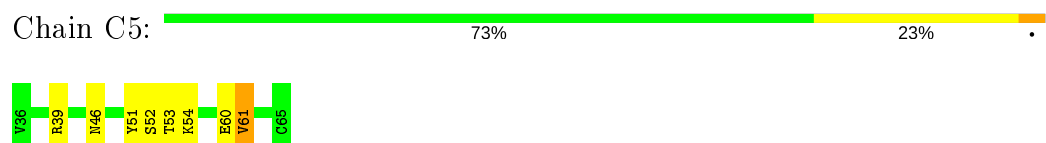
- Molecule 51: 50S ribosomal protein L30



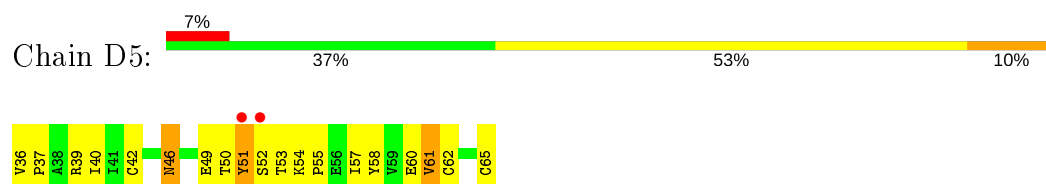
- Molecule 51: 50S ribosomal protein L30



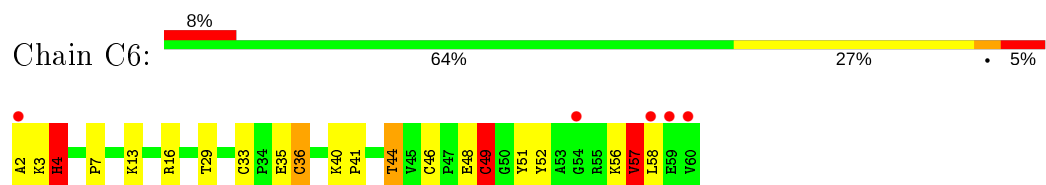
- Molecule 52: 50S ribosomal protein L31



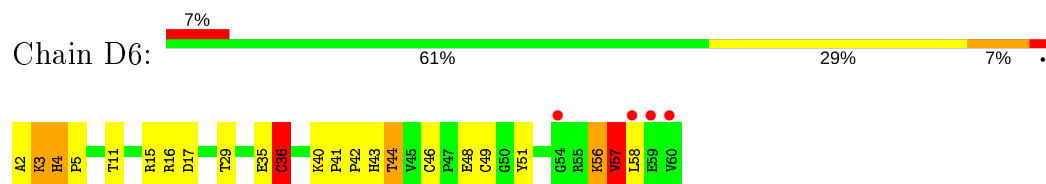
- Molecule 52: 50S ribosomal protein L31



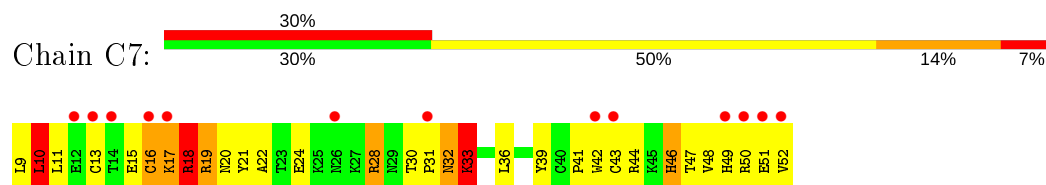
- Molecule 53: 50S ribosomal protein L32



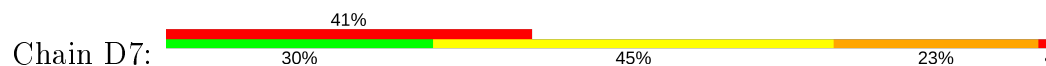
- Molecule 53: 50S ribosomal protein L32

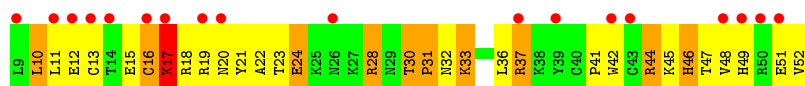


- Molecule 54: 50S ribosomal protein L33

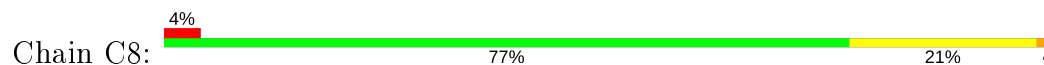


- Molecule 54: 50S ribosomal protein L33





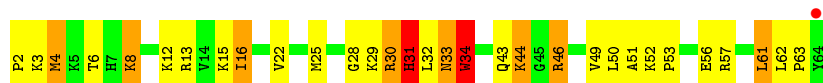
- Molecule 55: 50S ribosomal protein L34



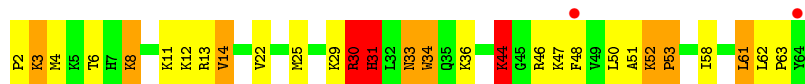
- Molecule 55: 50S ribosomal protein L34



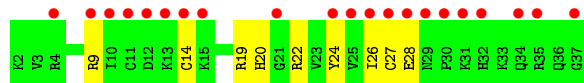
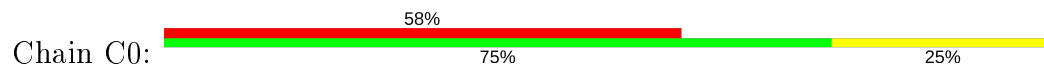
- Molecule 56: 50S ribosomal protein L35



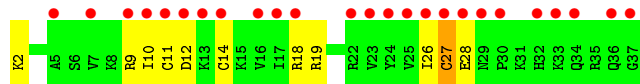
- Molecule 56: 50S ribosomal protein L35



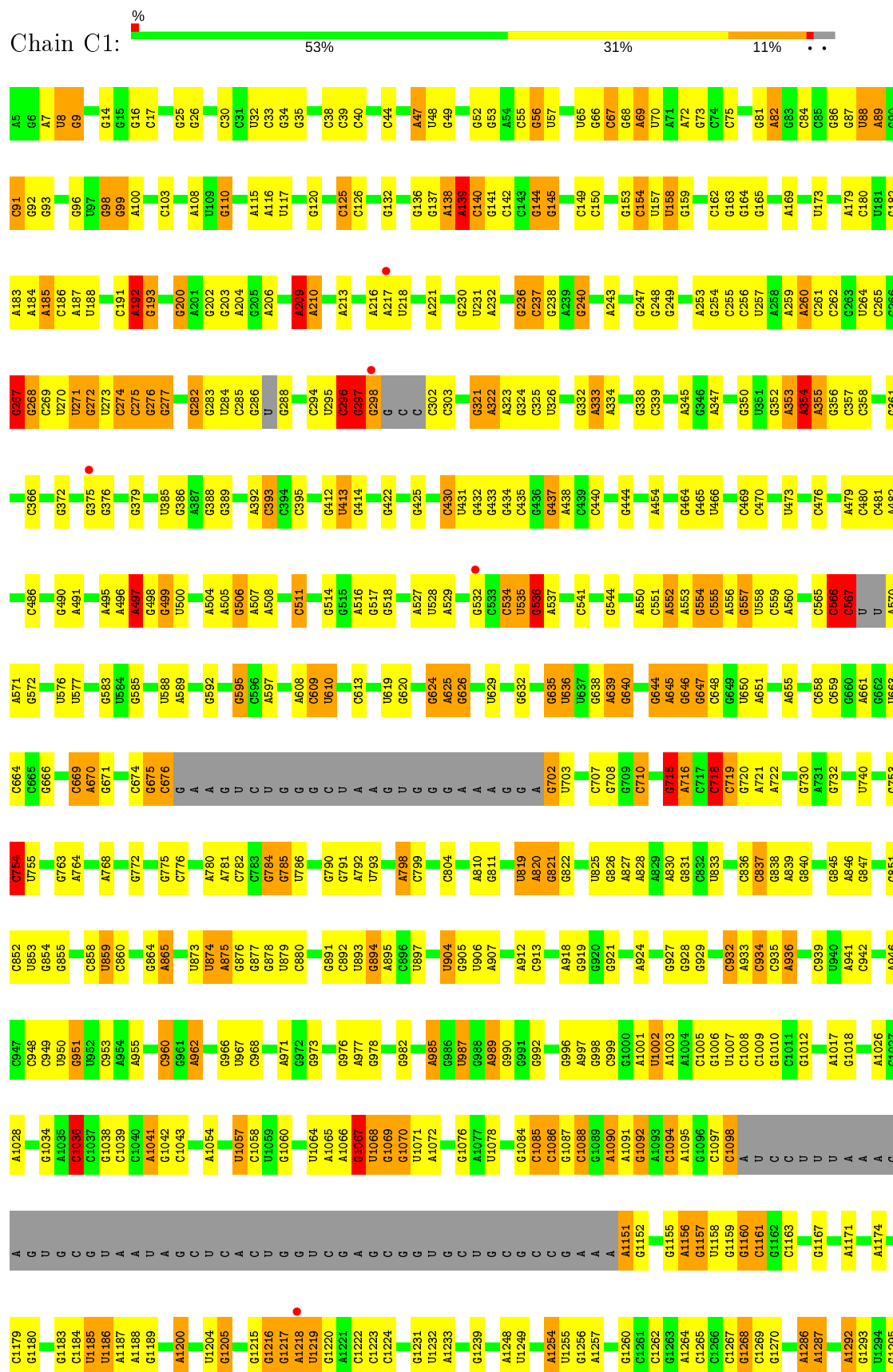
- Molecule 57: 50S ribosomal protein L36

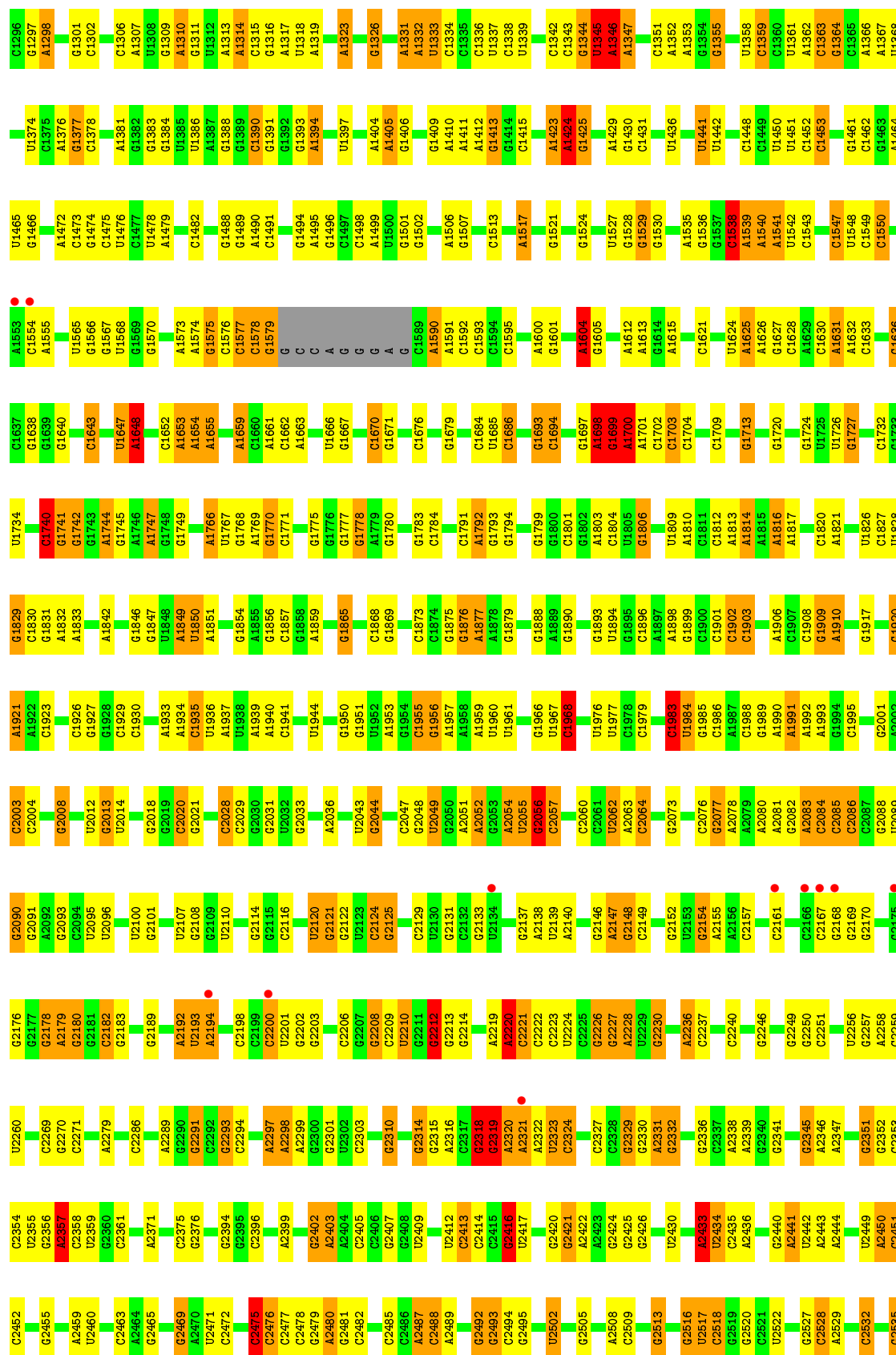


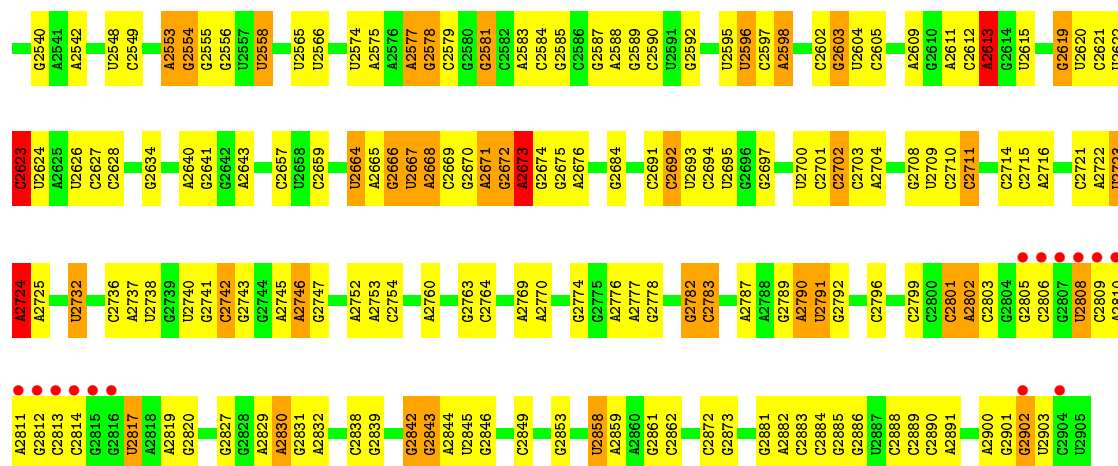
- Molecule 57: 50S ribosomal protein L36



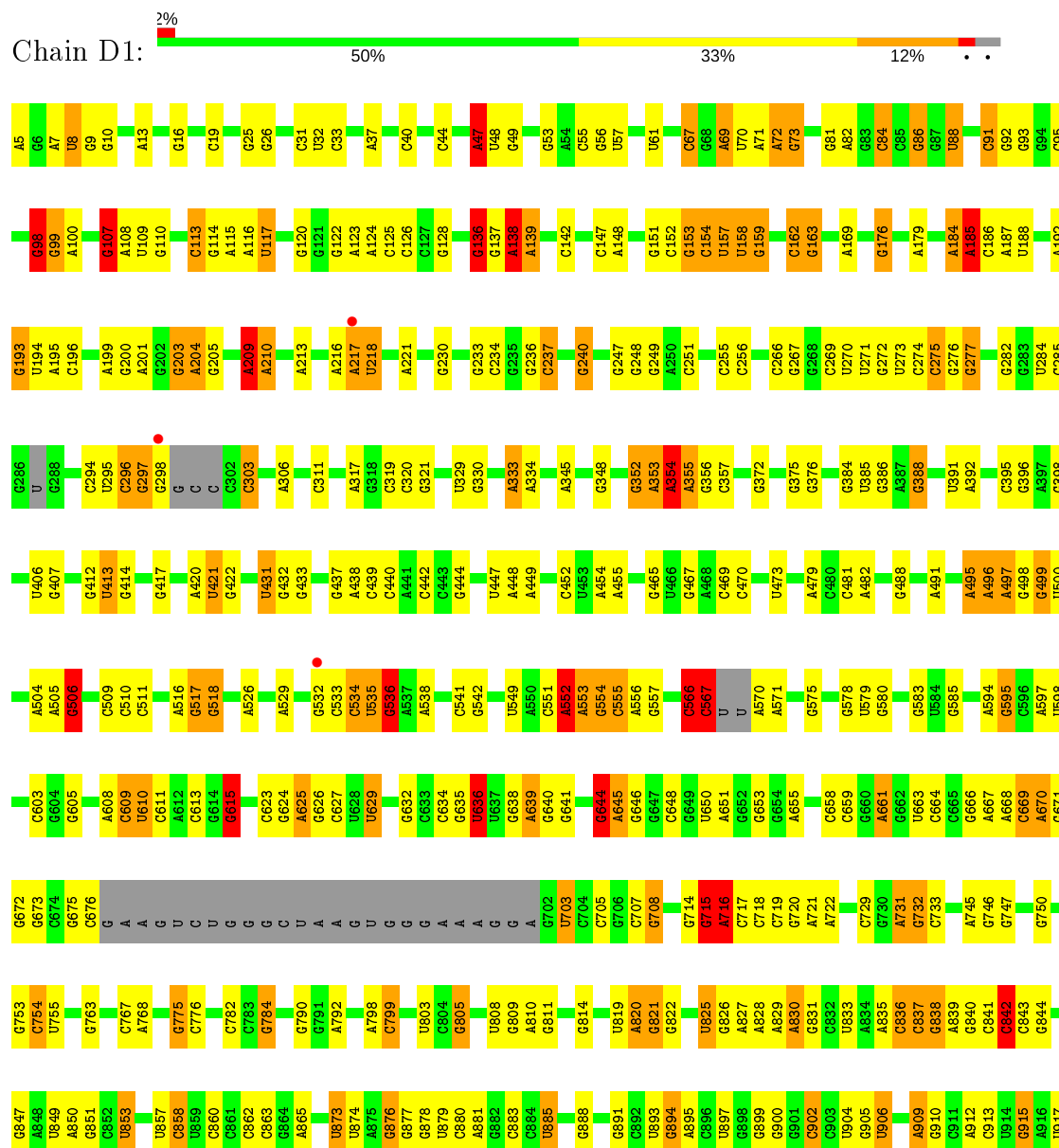
- Molecule 58: 23S rRNA (2899-MER)



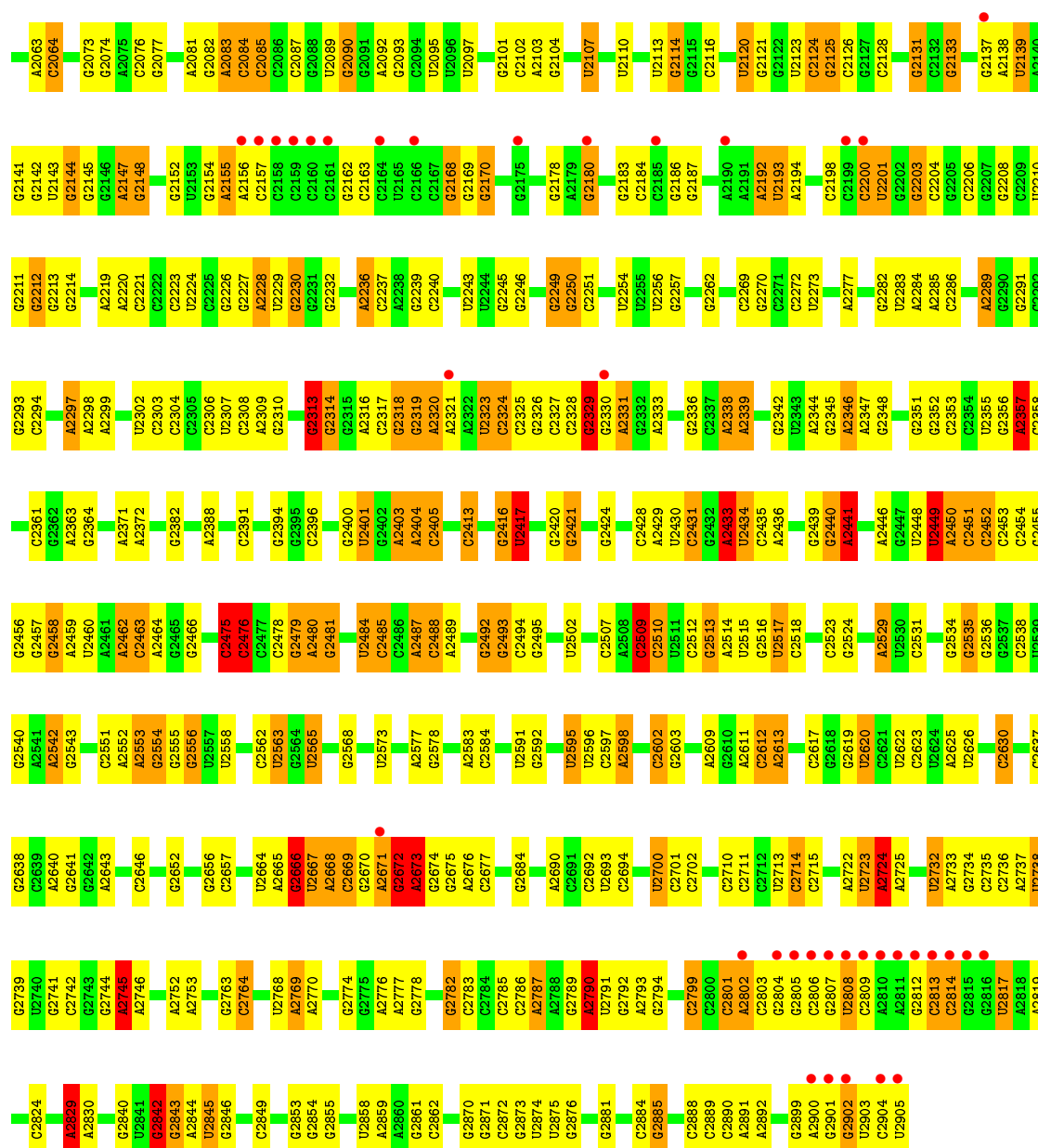




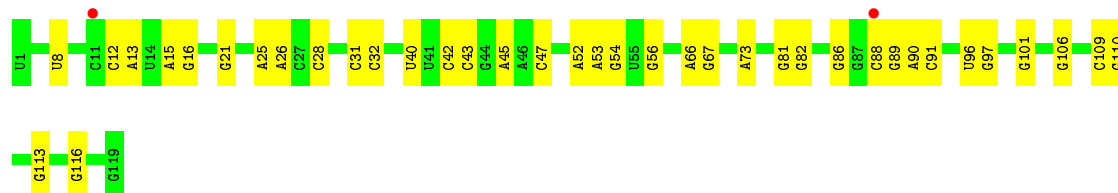
• Molecule 58: 23S rRNA (2899-MER)



G1985	C1900	U1828	G1732	G1640	C1554	C1477	G1392	G1304	C1222	G	G1084	U1002	U923
C1986	C1901	U1829	G1733	C1643	A1555	U1478	G1393	G1309	C1223	C	G1087	A1003	A924
C1988	C1903	C1830	U1734	G1646	A1556	C1482	A1394	G1310	C1224	C	G1088	C1005	G927
G1989	G1904	A1831	A1735	U1647	C1558	G1486	U1397	G1311	A1226	A	G1089	C1008	G928
A1990	A1905	A1832	C1740	G1648	U1559	G1487	G1400	U1312	G1229	A	A1090	C1009	G929
A1991	A1906	A1833	G1741	A1648	A1573	G1488	G1403	A1313	G1230	A1151	G1091	C1010	A933
A1992	C1907	A1842	G1742	C1652	A1574	G1489	G1404	A1314	U1230	U1152	G1092	C1011	C934
G1998	G1908	G1843	G1743	A1653	C1575	A1490	A1405	G1315	A1232	U1153	A1093	U1012	C935
A1999	G1909	A1844	A1744	A1654	G1576	G1495	G1406	G1316	A1233	C1154	C1094	U1013	A936
A1999	A1911	A1845	G1745	A1655	C1577	A1496	G1407	U1317	G1234	G1155	A1095	A1017	
C2000	G1912	G1846	A1746	A1656	C1578	G1497	U1409	U1318	G1235	A1156	G1096	G1018	A941
G2001	C1913		A1747	G1658	G1579	C1497	A1410	A1319	G1236	G1157	C1097	C1019	C942
A2002	G1917	A1849	G1763	C1660	G	C1498	A1411	A1320		U1158	A1098		C943
C2003	C2003	U1850	U1764	C1660	C	A1499	G1413	A1323	G1239	G1159	A	G1022	A944
C2004	A1851	G1852	G1765	A1661	A	U1500	G1414	G1324	C1244	G1160	C		A945
G2005	G1852	C1662	A1766	C1662	C	G1501	C1415	G1325	C1245		C	A1028	A946
G2006	G1853	G1767	U1767	A1663	G	G1505	C1420	G1326	C1246	G1167	U		
A2007	A1854	G1768	G1768	G1667	G	A1506	G1421	G1330	G1247	A1171	U	A1033	C949
C1923	A1855	A1769	A1769	G1671	A	G1507	G1422	A1331	A1248	A1172	U	A1034	U950
G1924	C1856	G1770	C1771	G1671	G	G1512	A1423	A1332	U1249	A1173	A	A1035	G951
G1925	G1857	G1771	G1771	G1672	A1590	C1513	A1424	U1332	G1250	U1174	A	C1036	U952
G1926	G1858	C1772	G1772	A1677	A1591	G1514	G1425	U1333	C1251	U1175	A	C1037	C953
G2012	C1927	C1773	C1773	A1678	A1592	A1515	G1426	C1334	C1252	G1176	G	G1038	A954
G2013	A1933	G1774	C1774	A1678	A1593	G1516	A1429	C1335	G1253	A1177	A	A1041	A956
U2014	A1934	G1775	G1775	A1678	C1594	A1517	G1430	C1336	A1254	U1178	A	G1042	
G2017	G1864	G1776	G1776	G1681	C1595	G1517	G1431	U1337	U1255	C1179	U	C1043	G961
G2018	G1865	G1778	G1778	G1681	C1596	C1520	G1432	C1338	G1260	G1181	C	U1044	C960
G2022	C1868	A1779	A1779	U1685	C1596	G1521	G1433	C1342	C1261	G1182	C	G1047	A962
G2023	G1869	G1780	G1780	C1686	A1600	C1522	U1436	C1343	C1262	G1183	U	G1048	A963
C2027	G1870	C1784	C1784	G1693	A1604	A1523	A1437	U1345	A1264	C1184	A	C1049	G972
C2028	A1785	C1694	A1785	C1694	G1605	G1524	A1438	U1346	C1265	U1186	U	C1050	G973
C2029	C1873	A1698	A1792	A1698	U1527	U1527	U1439	A1347	G1268	A1187	A		
A2036	G1874	G1699	G1793	G1699	G1528	G1528	A1440	G1348		A1188	G	C1053	G976
U2037	G1875	A1700	G1794	A1700	G1529	G1529	U1441	C1351	G1272	A1189	C	G1056	A977
U2038	G1876	C1795	C1795	C1795	G1530	G1530	U1448	A1352		C1190	U	U1057	G978
C2042	A1878	C1703	C1703	C1703	G1533	G1533	C1448	C1357	G1276	C1197	C	U1058	G982
U2043	G1879	C1704	C1704	C1704	U1534	U1534	U1450	U1357	G1277	C1198	A	U1059	
U2044	G1880	U1705	U1705	U1705	A1535	A1535	U1451	U1358		C1199	U	C1060	A985
G2045	C1881	C1706	C1706	C1706	G1536	G1536	C1452	C1359	G1281	A1200	G	U1064	G986
C2046	A1883	U1805	U1805	C1708	C1537	C1537	C1453	G1364	A1286	G1201	U	A1065	G988
C2047	A1884	G1806	G1806	C1708	A1625	A1538	G1459	C1365	A1287	C1202	C	A1066	A989
C2048	G1885	A1710	A1710	A1710	A1626	A1539	U1460	A1366	G1288	C1203	G	G1067	G990
U2049	G1886	A1711	A1711	A1711	G1627	G1627	G1461	G1373		U1210	A	U1068	G991
G2050	G1887	G1720	G1720	G1720	A1540	A1540	G1462	G1373	A1291	C1211	G	G1069	G992
A2051	C1888	C1811	C1811	C1811	U1542	U1542	G1463	G1373	A1292	U1212	C	G1070	C993
C2052	A1889	C1812	C1812	C1812	C1543	C1543	A1464	A1376	G1293	G1213	G	U1071	G994
G2053	G1890	A1813	A1813	A1813	C1544	C1544	U1465	G1377	U1294	G1216	G	A1072	C995
A1973	A1891	A1814	A1814	A1814	G1547	G1547	A1472	G1383	G1295	G1217	U	G1075	G996
A1974	U1894	U1726	U1726	U1726	C1549	C1549	C1473	G1384	A1298	A1218	C	G1076	G997
U2055	G1895	G1727	G1727	G1727	C1549	C1549	G1474	G1384	A1299	U1219	U	A1077	G998
U2056	G1896	C1729	C1729	C1729	C1550	C1550	G1475	C1390	U1300	U1220	G	U1078	C999
G2057	A1897	C1730	C1730	C1730	C1551	C1551	U1476	G1391	G1301	A1221	C	G1079	G1000
C2060	G1899	A1821	A1821	A1821	G1639	G1639							A1001



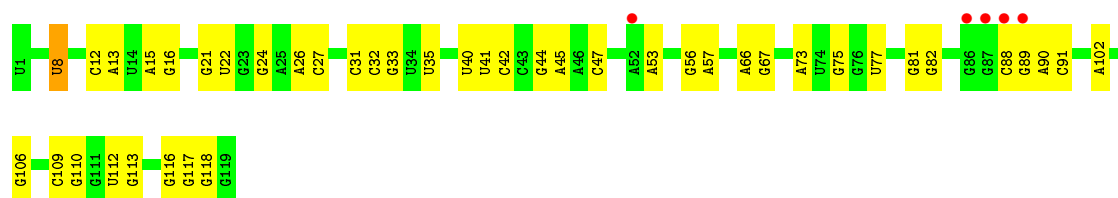
• Molecule 59: 5S rRNA (119-MER)



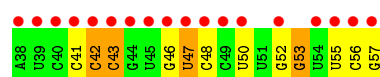
• Molecule 59: 5S rRNA (119-MER)







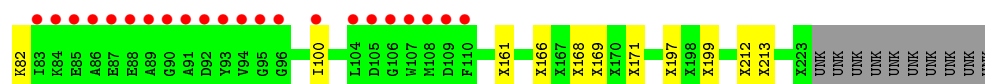
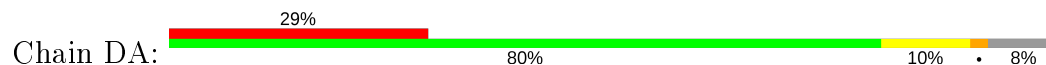
- Molecule 60: tRNA (5'-D(\*AP\*UP\*CP\*CP\*CP\*CP\*GP\*UP\*GP\*UP\*CP\*CP\*UP\*UP\*GP\*GP\*UP\*UP\*CP\*G)-3')



- Molecule 61: tRNA (76-MER)



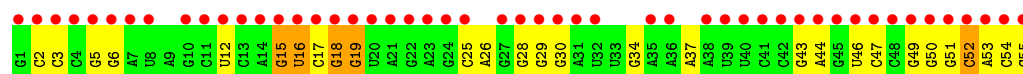
- Molecule 62: 50S ribosomal protein L1



- Molecule 63: 50S ribosomal protein L22



- Molecule 64: DNA (55-MER)



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	214.21Å 457.45Å 639.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.91 – 3.40 49.91 – 3.40	Depositor EDS
% Data completeness (in resolution range)	98.5 (49.91-3.40) 98.6 (49.91-3.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.28	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.46 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, $R_{free}$	0.204 , 0.241 0.207 , 0.241	Depositor DCC
$R_{free}$ test set	41975 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	74.2	Xtriage
Anisotropy	0.256	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 78.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	295910	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.91% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 3V6, PAR, 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	A2	0.48	0/192	0.82	0/297
2	AA	0.51	0/1936	0.74	0/2609
2	BA	0.50	0/1936	0.72	0/2609
3	AC	0.62	0/1636	0.82	2/2205 (0.1%)
4	AD	0.64	1/1733 (0.1%)	0.88	2/2318 (0.1%)
4	BD	0.68	2/1733 (0.1%)	0.98	9/2318 (0.4%)
5	AE	0.56	0/1163	0.82	1/1564 (0.1%)
5	BE	0.52	0/1163	0.78	0/1564
6	AF	0.52	0/856	0.78	0/1154
6	BF	0.56	0/856	0.81	0/1154
7	AG	0.51	0/1276	0.75	0/1709
7	BG	0.56	0/1276	0.78	2/1709 (0.1%)
8	AH	0.52	0/1136	0.75	0/1527
8	BH	0.52	0/1136	0.79	0/1527
9	AI	0.57	0/1029	0.82	0/1378
9	BI	0.54	0/1029	0.77	0/1378
10	AJ	0.58	0/808	0.84	0/1085
10	BJ	0.60	0/808	0.81	0/1085
11	AK	0.59	0/900	0.81	0/1213
11	BK	0.54	0/900	0.74	0/1213
12	AL	0.61	0/987	0.86	0/1320
12	BL	0.65	0/987	0.91	1/1320 (0.1%)
13	AM	0.57	0/999	0.86	1/1336 (0.1%)
13	BM	0.59	0/999	0.88	0/1336
14	AN	0.60	0/501	0.91	1/664 (0.2%)
14	BN	0.64	0/501	1.00	2/664 (0.3%)
15	AO	0.51	0/745	0.70	0/992
15	BO	0.53	0/745	0.80	0/992
16	AP	0.59	0/717	0.83	0/963
16	BP	0.56	0/717	0.81	0/963
17	AR	0.55	0/837	0.81	0/1117
17	BR	0.49	0/837	0.75	0/1117

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
18	AS	0.52	0/579	0.75	0/768
18	BS	0.54	0/579	0.73	0/768
19	AT	0.60	0/643	0.78	1/865 (0.1%)
19	BT	0.55	0/643	0.79	1/865 (0.1%)
20	AU	0.55	0/765	0.85	1/1007 (0.1%)
20	BU	0.50	0/765	0.80	0/1007
21	AW	0.61	0/213	0.90	0/277
21	BW	0.72	0/213	0.88	0/277
22	Ab	0.47	4/36190 (0.0%)	0.82	64/56486 (0.1%)
22	Bb	0.47	3/36190 (0.0%)	0.82	66/56486 (0.1%)
23	B2	0.42	0/216	0.86	0/334
24	BC	0.53	0/1637	0.76	1/2205 (0.0%)
25	C2	0.31	0/1784	0.72	1/2780 (0.0%)
25	C3	0.40	0/1809	0.77	3/2819 (0.1%)
25	D3	0.38	1/1809 (0.1%)	0.74	1/2819 (0.0%)
26	C4	0.49	0/1832	0.95	5/2855 (0.2%)
27	CA	0.55	0/646	0.72	0/869
28	CB	0.73	0/2155	0.99	3/2905 (0.1%)
28	DB	0.80	2/2155 (0.1%)	1.01	6/2905 (0.2%)
29	CC	0.70	1/1597 (0.1%)	0.93	2/2153 (0.1%)
29	DC	0.74	2/1597 (0.1%)	0.96	4/2153 (0.2%)
30	CD	0.65	0/1659	0.89	0/2244
30	DD	0.71	1/1659 (0.1%)	0.93	0/2244
31	CE	0.57	0/1499	0.84	0/2016
31	DE	0.58	0/1499	0.80	0/2016
32	CF	0.59	1/1246 (0.1%)	0.77	1/1682 (0.1%)
32	DF	0.69	1/1246 (0.1%)	0.92	2/1682 (0.1%)
33	CI	0.57	0/1147	0.84	1/1551 (0.1%)
33	DI	0.57	0/1147	0.81	0/1551
35	CM	0.60	0/1132	0.86	1/1525 (0.1%)
35	DM	0.63	0/1132	0.87	0/1525
36	CN	0.64	0/943	0.89	0/1269
36	DN	0.64	0/943	0.87	0/1269
37	CO	0.82	0/1131	1.17	4/1504 (0.3%)
37	DO	0.87	0/1131	1.16	2/1504 (0.1%)
38	CP	0.57	0/1143	0.80	0/1527
38	DP	0.63	0/1143	0.89	0/1527
39	CQ	0.67	0/974	0.99	2/1302 (0.2%)
39	DQ	0.74	0/974	1.08	6/1302 (0.5%)
40	CR	0.64	0/779	0.96	2/1036 (0.2%)
40	DR	0.71	0/779	1.04	2/1036 (0.2%)
41	CS	0.69	0/1156	1.04	0/1542
41	DS	0.73	0/1156	1.12	4/1542 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
42	CT	0.64	0/975	0.92	1/1297 (0.1%)
42	DT	0.75	0/975	1.07	4/1297 (0.3%)
43	CU	0.56	0/790	0.88	0/1057
43	DU	0.63	0/790	0.96	1/1057 (0.1%)
44	CW	0.64	0/907	0.89	0/1216
45	CX	0.63	0/740	0.85	0/993
45	DX	0.69	1/740 (0.1%)	1.01	2/993 (0.2%)
46	CY	0.75	0/789	0.98	0/1051
46	DY	0.80	0/789	1.00	1/1051 (0.1%)
47	CZ	0.51	0/1436	0.77	0/1949
47	DZ	0.53	0/1436	0.77	1/1949 (0.1%)
48	Ca	0.61	0/671	0.87	1/892 (0.1%)
48	Da	0.67	0/671	0.96	1/892 (0.1%)
49	CH	0.65	0/741	0.95	1/984 (0.1%)
49	DH	0.60	0/741	0.89	0/984
50	CK	0.54	0/600	0.83	0/793
50	DK	0.59	0/600	0.84	0/793
51	CL	0.54	0/473	0.80	0/634
51	DL	0.60	0/473	0.83	0/634
52	C5	0.63	0/229	0.86	0/309
52	D5	0.61	0/229	0.80	0/309
53	C6	0.67	0/473	0.91	1/639 (0.2%)
53	D6	0.64	0/473	0.94	1/639 (0.2%)
54	C7	0.89	0/387	1.06	1/515 (0.2%)
54	D7	0.71	0/387	1.01	1/515 (0.2%)
55	C8	0.72	0/427	1.01	1/561 (0.2%)
55	D8	0.78	0/427	0.99	1/561 (0.2%)
56	C9	0.74	0/516	1.08	0/679
56	D9	0.73	0/516	1.04	1/679 (0.1%)
57	C0	0.53	0/302	0.70	0/397
57	D0	0.59	0/302	0.87	0/397
58	C1	0.55	15/67709 (0.0%)	0.91	250/105690 (0.2%)
58	D1	0.58	32/67709 (0.0%)	0.96	353/105690 (0.3%)
59	Cs	0.45	0/2853	0.80	3/4451 (0.1%)
59	Ds	0.49	0/2853	0.85	4/4451 (0.1%)
60	D2	0.34	0/459	0.74	0/712
61	D4	0.48	0/1813	0.86	7/2825 (0.2%)
62	DA	0.55	0/645	0.73	0/867
63	DW	0.66	0/907	0.95	1/1216 (0.1%)
64	DV	0.28	0/1269	0.65	0/1956
All	All	0.56	67/318931 (0.0%)	0.89	845/476973 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	AA	0	1
3	AC	0	1
12	AL	0	1
13	AM	0	1
13	BM	0	1
14	BN	0	1
18	BS	0	1
19	AT	0	1
20	AU	0	1
22	Ab	1	0
22	Bb	1	0
25	C3	1	0
25	D3	1	0
28	CB	0	4
28	DB	0	3
29	DC	0	2
30	CD	0	1
31	CE	0	2
32	DF	0	1
33	CI	0	1
34	DJ	0	1
37	CO	0	6
37	DO	0	6
39	DQ	0	1
41	CS	0	1
41	DS	0	3
42	CT	0	1
42	DT	0	1
46	CY	0	1
46	DY	0	2
47	DZ	0	1
48	Da	0	1
53	C6	0	1
54	C7	0	1
54	D7	0	1
56	D9	0	1
58	C1	20	0
58	D1	21	0
All	All	45	52

All (67) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	C1	296	C	O3'-P	8.28	1.71	1.61
28	DB	237	GLU	CG-CD	8.11	1.64	1.51
29	DC	127	ASP	CB-CG	8.00	1.68	1.51
58	D1	1346	A	O3'-P	7.44	1.70	1.61
58	D1	1429	A	O3'-P	-7.22	1.52	1.61
58	C1	589	A	P-OP1	7.15	1.61	1.49
29	CC	127	ASP	CB-CG	6.73	1.65	1.51
58	D1	2027	C	P-OP1	6.46	1.59	1.49
22	Ab	1482	G	O3'-P	6.29	1.68	1.61
22	Bb	349	A	O3'-P	6.27	1.68	1.61
58	D1	2254	U	P-OP1	6.18	1.59	1.49
4	AD	12	CYS	CA-CB	6.17	1.67	1.53
58	C1	1648	A	O3'-P	6.09	1.68	1.61
4	BD	9	CYS	CB-SG	6.07	1.92	1.82
58	C1	2319	G	O3'-P	5.99	1.68	1.61
58	D1	1858	G	P-OP1	5.98	1.59	1.49
58	D1	1358	U	O3'-P	5.98	1.68	1.61
32	DF	157	TYR	CB-CG	5.97	1.60	1.51
58	D1	1151	A	O3'-P	5.93	1.68	1.61
58	D1	2056	G	O3'-P	5.91	1.68	1.61
58	D1	2603	G	P-OP1	5.91	1.58	1.49
29	DC	127	ASP	CG-OD2	5.88	1.38	1.25
58	D1	1097	C	O3'-P	5.81	1.68	1.61
58	D1	47	A	O3'-P	5.78	1.68	1.61
28	DB	220	HIS	C-O	5.70	1.34	1.23
22	Ab	246	A	O3'-P	5.70	1.68	1.61
32	CF	157	TYR	CB-CG	5.70	1.60	1.51
58	D1	833	U	P-OP1	5.69	1.58	1.49
58	D1	2745	A	O3'-P	-5.67	1.54	1.61
45	DX	44	GLU	CG-CD	5.63	1.60	1.51
58	D1	1816	A	O3'-P	5.63	1.68	1.61
58	C1	297	G	O3'-P	5.54	1.67	1.61
58	D1	625	A	O3'-P	5.52	1.67	1.61
58	C1	702	G	O3'-P	-5.52	1.54	1.61
58	D1	2095	U	P-OP1	5.49	1.58	1.49
58	D1	853	U	O3'-P	5.47	1.67	1.61
58	D1	2669	C	O3'-P	-5.39	1.54	1.61
30	DD	65	TRP	CB-CG	-5.33	1.40	1.50
4	BD	12	CYS	CA-CB	5.33	1.65	1.53
58	D1	1304	G	O3'-P	5.32	1.67	1.61
58	D1	1438	A	O3'-P	5.32	1.67	1.61
58	D1	209	A	O3'-P	5.32	1.67	1.61

*Continued on next page...*

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	C1	237	C	P-OP1	5.31	1.57	1.49
58	D1	830	A	O3'-P	5.30	1.67	1.61
58	D1	1711	A	P-OP2	5.29	1.57	1.49
58	D1	1313	A	P-OP1	5.28	1.57	1.49
58	C1	2695	U	O3'-P	-5.25	1.54	1.61
58	C1	846	A	O3'-P	5.24	1.67	1.61
58	C1	2251	C	O3'-P	5.24	1.67	1.61
58	D1	421	U	O3'-P	-5.18	1.54	1.61
58	D1	2609	A	P-OP1	5.16	1.57	1.49
58	D1	1804	C	P-OP1	5.15	1.57	1.49
58	C1	592	G	O3'-P	5.15	1.67	1.61
22	Ab	1108	U	O3'-P	5.14	1.67	1.61
58	C1	2634	G	O3'-P	5.14	1.67	1.61
58	D1	885	U	O3'-P	5.13	1.67	1.61
25	D3	39	U	O3'-P	5.13	1.67	1.61
58	C1	1804	C	O3'-P	5.12	1.67	1.61
58	D1	1806	G	P-OP2	5.09	1.57	1.49
58	D1	837	C	O3'-P	5.09	1.67	1.61
58	C1	855	G	O3'-P	5.09	1.67	1.61
58	C1	1806	G	P-OP2	5.09	1.57	1.49
22	Bb	786	A	O3'-P	-5.08	1.55	1.61
58	D1	2018	G	P-OP2	5.08	1.57	1.49
22	Ab	1495	G	O3'-P	5.07	1.67	1.61
22	Bb	572	G	O3'-P	5.05	1.67	1.61
58	D1	2250	G	O3'-P	-5.03	1.55	1.61

All (845) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	C4	36	A	O5'-P-OP2	-17.36	89.87	110.70
58	D1	2028	C	O5'-P-OP2	-16.34	90.99	105.70
58	D1	2603	G	O5'-P-OP2	-16.16	91.15	105.70
58	D1	598	U	O5'-P-OP2	-13.61	93.45	105.70
58	C1	2613	A	O5'-P-OP1	-12.83	94.15	105.70
58	D1	842	C	O5'-P-OP2	-12.77	94.21	105.70
58	D1	873	U	O5'-P-OP2	-12.68	94.29	105.70
58	D1	1424	A	N9-C1'-C2'	12.61	130.40	114.00
58	D1	1740	C	C2'-C3'-O3'	12.48	136.95	109.50
58	C1	1529	G	C2'-C3'-O3'	12.35	136.67	109.50
58	C1	534	C	O5'-P-OP2	-12.22	94.70	105.70
58	D1	2013	G	C2'-C3'-O3'	12.10	136.13	109.50
58	C1	185	A	O5'-P-OP1	-11.99	94.91	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	D1	1955	C	C2'-C3'-O3'	11.82	135.51	109.50
58	D1	2514	A	O5'-P-OP2	-11.81	95.07	105.70
58	D1	989	A	N9-C1'-C2'	11.79	129.32	114.00
58	C1	2623	C	O5'-P-OP2	-11.74	95.13	105.70
58	D1	1857	C	O5'-P-OP2	-11.73	95.14	105.70
58	D1	2808	U	N1-C1'-C2'	11.45	128.88	114.00
58	D1	534	C	O5'-P-OP2	-11.30	95.53	105.70
58	C1	1345	U	C2'-C3'-O3'	11.29	134.33	109.50
26	C4	36	A	O5'-P-OP1	11.23	124.18	110.70
58	D1	805	G	O5'-P-OP2	-11.19	95.63	105.70
58	D1	2431	C	O5'-P-OP1	-11.16	95.65	105.70
58	D1	1983	C	N1-C1'-C2'	11.15	128.49	114.00
22	Bb	1476	U	C2'-C3'-O3'	11.14	134.01	109.50
58	D1	535	U	O5'-P-OP1	-11.13	95.68	105.70
58	C1	1955	C	C2'-C3'-O3'	11.01	133.73	109.50
58	D1	909	A	O5'-P-OP2	-10.91	95.88	105.70
58	D1	1698	A	C2'-C3'-O3'	10.89	133.46	109.50
22	Bb	881	G	O5'-P-OP2	-10.80	95.98	105.70
58	D1	1850	U	O5'-P-OP1	-10.75	96.03	105.70
58	C1	2013	G	C2'-C3'-O3'	10.73	133.11	109.50
58	D1	1711	A	O5'-P-OP1	-10.71	96.06	105.70
58	C1	2513	G	O5'-P-OP1	-10.70	96.07	105.70
58	C1	989	A	N9-C1'-C2'	10.70	127.91	114.00
58	C1	1502	G	O5'-P-OP1	-10.64	96.12	105.70
58	C1	1983	C	N1-C1'-C2'	10.64	127.84	114.00
58	D1	1345	U	C5'-C4'-O4'	10.49	121.68	109.10
58	D1	1699	G	C2'-C3'-O3'	10.40	132.38	109.50
58	C1	1740	C	C2'-C3'-O3'	10.37	132.31	109.50
58	D1	2790	A	O5'-P-OP2	-10.34	96.39	105.70
58	D1	2603	G	O5'-P-OP1	10.32	123.09	110.70
58	C1	98	G	N9-C1'-C2'	10.26	127.34	114.00
58	C1	2587	G	O5'-P-OP2	-10.06	96.64	105.70
58	D1	1643	C	O5'-P-OP1	-10.02	96.69	105.70
4	BD	9	CYS	CA-CB-SG	10.01	132.02	114.00
58	C1	2623	C	O5'-P-OP1	9.97	122.66	110.70
58	C1	2236	A	C2'-C3'-O3'	9.96	131.40	109.50
58	C1	1829	G	C2'-C3'-O3'	9.95	131.39	109.50
22	Bb	408	A	N9-C1'-C2'	9.94	126.92	114.00
58	D1	1397	U	O5'-P-OP2	-9.78	96.90	105.70
58	C1	1345	U	N1-C1'-C2'	9.77	126.71	114.00
58	D1	2514	A	O5'-P-OP1	9.74	122.38	110.70
58	C1	833	U	O5'-P-OP2	-9.69	96.98	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	D1	805	G	O5'-P-OP1	9.68	122.32	110.70
58	D1	1985	G	O5'-P-OP1	-9.66	97.01	105.70
58	C1	2603	G	O5'-P-OP2	-9.65	97.01	105.70
58	D1	1659	A	O5'-P-OP2	-9.65	97.01	105.70
58	C1	785	G	O5'-P-OP1	9.64	122.27	110.70
14	BN	40	CYS	CA-CB-SG	9.63	131.34	114.00
58	C1	1659	A	O5'-P-OP2	-9.54	97.12	105.70
58	D1	1044	U	O5'-P-OP2	9.47	122.06	110.70
58	C1	2297	A	N9-C1'-C2'	9.45	126.29	114.00
58	D1	1590	A	N9-C1'-C2'	9.44	126.27	114.00
58	C1	536	G	O5'-P-OP1	-9.43	97.21	105.70
58	C1	2577	A	O5'-P-OP2	-9.40	97.24	105.70
22	Bb	1506	U	O5'-P-OP2	-9.39	97.25	105.70
58	D1	1044	U	O5'-P-OP1	-9.37	97.26	105.70
58	C1	1700	A	O5'-P-OP1	-9.37	97.26	105.70
58	D1	2236	A	C2'-C3'-O3'	9.36	130.09	109.50
58	D1	2339	A	O5'-P-OP1	-9.34	97.30	105.70
58	C1	715	G	C2'-C3'-O3'	9.32	130.01	109.50
58	C1	2673	A	N9-C1'-C2'	9.26	126.04	114.00
58	D1	782	C	O5'-P-OP1	-9.25	97.38	105.70
58	D1	2282	G	O5'-P-OP2	-9.20	97.42	105.70
4	BD	26	CYS	CA-CB-SG	9.19	130.53	114.00
58	C1	535	U	O5'-P-OP1	-9.18	97.44	105.70
58	C1	785	G	O5'-P-OP2	-9.16	97.45	105.70
58	D1	1053	C	O5'-P-OP1	-9.16	97.46	105.70
26	C4	77	A	O5'-P-OP2	-9.13	97.48	105.70
58	D1	2513	G	O5'-P-OP1	-9.13	97.48	105.70
4	BD	12	CYS	CA-CB-SG	9.13	130.43	114.00
58	D1	847	G	O5'-P-OP1	-9.09	97.52	105.70
58	C1	589	A	O5'-P-OP2	-9.07	97.53	105.70
58	D1	1424	A	O4'-C1'-N9	9.06	115.45	108.20
22	Ab	408	A	N9-C1'-C2'	9.05	125.76	114.00
58	D1	883	C	O5'-P-OP1	-9.04	97.56	105.70
58	D1	186	C	O5'-P-OP1	-9.02	97.58	105.70
58	D1	847	G	O5'-P-OP2	9.00	121.50	110.70
22	Bb	885	A	O5'-P-OP2	-8.94	97.65	105.70
58	D1	2431	C	O5'-P-OP2	8.91	121.40	110.70
58	C1	1413	G	O5'-P-OP2	-8.90	97.69	105.70
58	C1	1857	C	O5'-P-OP2	-8.89	97.70	105.70
58	C1	2212	G	C2'-C3'-O3'	8.89	129.05	109.50
58	D1	2457	G	O5'-P-OP2	-8.88	97.71	105.70
22	Ab	1050	A	C2'-C3'-O3'	8.86	129.00	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	C1	497	A	C2'-C3'-O3'	8.86	129.00	109.50
58	D1	1345	U	C5'-C4'-C3'	8.86	130.17	116.00
58	C1	1017	A	O5'-P-OP1	-8.77	97.81	105.70
58	D1	2212	G	C2'-C3'-O3'	8.73	128.70	109.50
58	D1	992	G	O5'-P-OP1	8.71	121.15	110.70
58	D1	98	G	N9-C1'-C2'	8.69	125.30	114.00
58	C1	1424	A	N9-C1'-C2'	8.69	125.29	114.00
58	D1	2297	A	N9-C1'-C2'	8.65	125.25	114.00
25	C3	47	U	N1-C1'-C2'	8.64	125.23	114.00
22	Ab	1476	U	C2'-C3'-O3'	8.63	128.50	109.50
22	Bb	111	G	O5'-P-OP1	-8.63	97.94	105.70
58	C1	1699	G	C2'-C3'-O3'	8.62	128.47	109.50
58	D1	1529	G	C2'-C3'-O3'	8.62	128.47	109.50
58	D1	833	U	O5'-P-OP2	-8.62	97.94	105.70
58	C1	1323	A	O5'-P-OP2	-8.62	97.95	105.70
58	D1	497	A	C2'-C3'-O3'	8.61	128.44	109.50
58	D1	1060	G	O5'-P-OP2	-8.60	97.96	105.70
58	D1	518	G	O5'-P-OP2	8.60	121.02	110.70
58	C1	2518	C	O5'-P-OP2	-8.59	97.97	105.70
22	Bb	891	A	C2'-C3'-O3'	8.56	128.34	109.50
22	Bb	956	A	O5'-P-OP1	-8.54	98.02	105.70
58	D1	2243	U	O5'-P-OP2	-8.48	98.07	105.70
58	D1	2027	C	O5'-P-OP2	-8.48	98.07	105.70
58	C1	1968	C	O5'-P-OP2	-8.44	98.11	105.70
58	D1	2357	A	O5'-P-OP1	-8.39	98.15	105.70
58	C1	715	G	N9-C1'-C2'	8.38	124.90	114.00
58	C1	1983	C	C2'-C3'-O3'	8.37	127.92	109.50
58	C1	715	G	C4'-C3'-O3'	8.36	129.72	113.00
58	D1	992	G	O5'-P-OP2	-8.34	98.20	105.70
58	C1	2791	U	O4'-C1'-N1	8.31	114.85	108.20
22	Ab	778	A	O5'-P-OP2	8.31	120.67	110.70
22	Ab	683	C	O5'-P-OP1	-8.31	98.22	105.70
58	D1	827	A	O5'-P-OP1	-8.28	98.24	105.70
58	D1	497	A	C4'-C3'-O3'	8.28	129.56	113.00
22	Ab	240	U	O5'-P-OP1	-8.20	98.32	105.70
58	D1	906	U	O5'-P-OP2	-8.17	98.35	105.70
58	D1	2724	A	O5'-P-OP1	8.16	120.49	110.70
58	C1	491	A	O5'-P-OP2	-8.11	98.40	105.70
22	Bb	109	G	C2'-C3'-O3'	8.07	127.26	109.50
58	D1	715	G	N9-C1'-C2'	8.05	124.47	114.00
58	C1	1590	A	N9-C1'-C2'	8.04	124.44	114.00
58	C1	1703	C	O5'-P-OP2	-8.03	98.47	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	D1	2452	C	O5'-P-OP1	-8.01	98.49	105.70
58	C1	1693	G	O5'-P-OP1	-8.00	98.50	105.70
58	D1	784	G	O5'-P-OP2	-7.95	98.54	105.70
22	Ab	1180	G	O5'-P-OP2	7.94	120.23	110.70
58	D1	1828	U	O5'-P-OP2	-7.94	98.55	105.70
22	Ab	1459	U	O5'-P-OP1	-7.94	98.56	105.70
58	C1	819	U	O5'-P-OP2	-7.93	98.56	105.70
58	D1	1643	C	O5'-P-OP2	7.87	120.14	110.70
58	C1	877	G	O5'-P-OP1	-7.85	98.64	105.70
58	C1	1983	C	C5'-C4'-O4'	7.83	118.49	109.10
58	D1	2613	A	N9-C1'-C2'	7.81	124.16	114.00
58	D1	1067	G	C2'-C3'-O3'	7.80	126.66	109.50
58	C1	2057	C	O5'-P-OP2	-7.74	98.73	105.70
58	D1	1984	U	O5'-P-OP2	-7.72	98.75	105.70
19	AT	5	LEU	CA-CB-CG	7.72	133.06	115.30
58	D1	1488	G	C2'-C3'-O3'	7.72	126.49	109.50
58	D1	1424	A	C2'-C3'-O3'	7.72	126.48	109.50
58	C1	2743	G	O5'-P-OP1	-7.71	98.76	105.70
58	D1	1711	A	O5'-P-OP2	7.70	119.94	110.70
58	D1	715	G	C4'-C3'-O3'	7.70	128.40	113.00
22	Bb	1206	G	O5'-P-OP1	7.70	119.93	110.70
58	D1	708	G	O5'-P-OP2	-7.69	98.78	105.70
58	D1	1323	A	O5'-P-OP2	-7.69	98.78	105.70
58	C1	2609	A	O5'-P-OP2	-7.68	98.78	105.70
58	C1	1036	C	O5'-P-OP1	-7.68	98.79	105.70
58	D1	1659	A	O5'-P-OP1	7.68	119.91	110.70
58	C1	1323	A	O5'-P-OP1	7.67	119.90	110.70
58	D1	1820	C	O5'-P-OP2	7.66	119.89	110.70
58	D1	2790	A	O5'-P-OP1	7.65	119.88	110.70
58	D1	465	G	O5'-P-OP1	-7.62	98.84	105.70
58	D1	117	U	O5'-P-OP1	-7.61	98.85	105.70
58	D1	2212	G	C4'-C3'-O3'	7.61	128.23	113.00
4	BD	31	CYS	CA-CB-SG	-7.61	100.30	114.00
58	D1	2424	G	O5'-P-OP2	-7.61	98.85	105.70
58	C1	144	G	O5'-P-OP2	-7.58	98.88	105.70
58	D1	2028	C	O5'-P-OP1	7.57	119.78	110.70
58	D1	1010	G	O5'-P-OP2	-7.57	98.89	105.70
58	D1	2102	C	O5'-P-OP2	-7.57	98.89	105.70
58	C1	2791	U	C1'-O4'-C4'	-7.55	103.86	109.90
22	Ab	1206	G	O5'-P-OP1	7.54	119.75	110.70
58	C1	2416	G	C2'-C3'-O3'	7.54	126.10	109.50
58	D1	644	G	O5'-P-OP1	-7.54	98.91	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	D1	2282	G	O5'-P-OP1	7.54	119.75	110.70
58	C1	1344	G	O5'-P-OP1	-7.54	98.92	105.70
22	Bb	424	G	C2'-C3'-O3'	7.54	126.08	109.50
58	C1	1346	A	O5'-P-OP1	-7.54	98.92	105.70
58	D1	2023	G	O5'-P-OP1	-7.51	98.94	105.70
58	D1	1313	A	O5'-P-OP2	-7.49	98.96	105.70
58	D1	906	U	O5'-P-OP1	7.47	119.67	110.70
58	D1	784	G	O5'-P-OP1	7.47	119.66	110.70
37	CO	41	ARG	NE-CZ-NH2	7.46	124.03	120.30
22	Ab	891	A	C2'-C3'-O3'	7.45	125.90	109.50
58	D1	186	C	O5'-P-OP2	7.44	119.63	110.70
58	D1	1345	U	N1-C1'-C2'	7.43	123.67	114.00
58	C1	718	C	O5'-P-OP2	-7.43	99.01	105.70
22	Ab	793	G	O5'-P-OP2	-7.43	99.01	105.70
58	D1	625	A	C2'-C3'-O3'	7.41	125.81	109.50
22	Ab	790	C	O5'-P-OP1	-7.41	99.03	105.70
58	D1	1345	U	C2'-C3'-O3'	7.41	125.79	109.50
58	C1	555	C	O5'-P-OP1	-7.40	99.04	105.70
58	D1	2027	C	O5'-P-OP1	7.38	119.56	110.70
58	D1	2092	A	O5'-P-OP2	-7.38	99.06	105.70
58	C1	2359	U	O5'-P-OP2	-7.37	99.07	105.70
58	D1	2670	G	C2'-C3'-O3'	7.36	125.69	109.50
22	Ab	1183	A	C2'-C3'-O3'	7.34	125.66	109.50
58	D1	2457	G	O5'-P-OP1	7.34	119.51	110.70
58	D1	989	A	O5'-P-OP1	7.34	119.50	110.70
58	D1	518	G	O5'-P-OP1	-7.33	99.10	105.70
22	Ab	350	G	O5'-P-OP2	-7.29	99.14	105.70
58	D1	2417	U	O5'-P-OP2	-7.29	99.14	105.70
22	Ab	434	G	O5'-P-OP2	-7.27	99.16	105.70
58	D1	1678	A	O5'-P-OP1	-7.27	99.16	105.70
58	D1	2515	U	O5'-P-OP2	-7.26	99.17	105.70
58	C1	2587	G	O5'-P-OP1	7.25	119.40	110.70
58	D1	1983	C	C5'-C4'-O4'	7.24	117.79	109.10
48	Da	14	ARG	NE-CZ-NH2	-7.24	116.68	120.30
22	Bb	1378	C	O5'-P-OP1	-7.24	99.19	105.70
58	C1	1397	U	O5'-P-OP2	-7.24	99.19	105.70
58	D1	1286	A	O5'-P-OP1	-7.23	99.19	105.70
58	C1	566	C	C2'-C3'-O3'	7.23	125.40	109.50
58	D1	1344	G	O5'-P-OP2	7.23	119.37	110.70
58	D1	536	G	O4'-C1'-N9	7.20	113.96	108.20
58	D1	2308	C	O5'-P-OP1	-7.17	99.25	105.70
58	D1	1857	C	O5'-P-OP1	7.15	119.28	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	CR	89	ARG	NE-CZ-NH2	-7.15	116.73	120.30
22	Bb	262	G	C2'-C3'-O3'	7.14	125.20	109.50
58	D1	2403	A	O5'-P-OP1	-7.13	99.28	105.70
58	D1	2673	A	N9-C1'-C2'	7.13	123.26	114.00
22	Ab	1180	G	O5'-P-OP1	-7.12	99.29	105.70
58	C1	1804	C	O5'-P-OP2	-7.10	99.31	105.70
58	C1	1816	A	N9-C1'-C2'	7.10	123.23	114.00
58	C1	625	A	C2'-C3'-O3'	7.10	125.11	109.50
58	C1	784	G	O5'-P-OP2	-7.07	99.33	105.70
58	D1	1816	A	N9-C1'-C2'	7.07	123.19	114.00
22	Bb	605	A	O5'-P-OP1	-7.03	99.38	105.70
58	C1	847	G	O5'-P-OP1	-7.02	99.38	105.70
58	D1	1984	U	O4'-C1'-C2'	-7.02	98.78	105.80
58	C1	209	A	O5'-P-OP1	-7.00	99.40	105.70
58	D1	72	A	C2'-C3'-O3'	6.99	124.89	113.70
58	D1	1473	C	O5'-P-OP1	-6.99	99.41	105.70
58	D1	836	C	C2'-C3'-O3'	6.99	124.88	113.70
61	D4	33	C	O5'-P-OP1	-6.98	99.42	105.70
58	C1	1968	C	O5'-P-OP1	6.98	119.08	110.70
58	D1	1344	G	O5'-P-OP1	-6.97	99.42	105.70
58	D1	598	U	O5'-P-OP1	6.96	119.06	110.70
37	CO	41	ARG	NE-CZ-NH1	-6.96	116.82	120.30
58	D1	2038	U	O5'-P-OP2	-6.96	99.44	105.70
22	Ab	109	G	C2'-C3'-O3'	6.96	124.83	113.70
58	C1	511	C	O5'-P-OP1	-6.95	99.44	105.70
58	C1	534	C	O5'-P-OP1	6.95	119.05	110.70
58	D1	1829	G	C2'-C3'-O3'	6.95	124.82	113.70
58	C1	435	C	O5'-P-OP1	6.92	119.00	110.70
58	D1	1233	A	O5'-P-OP1	-6.92	99.47	105.70
22	Ab	1267	A	C2'-C3'-O3'	6.91	124.76	113.70
58	D1	2029	C	O5'-P-OP1	6.91	118.99	110.70
58	C1	2212	G	C4'-C3'-O3'	6.90	126.79	113.00
22	Ab	357	G	O5'-P-OP2	6.88	118.96	110.70
4	BD	31	CYS	N-CA-CB	6.88	122.99	110.60
58	C1	1817	A	O5'-P-OP1	-6.88	99.51	105.70
58	D1	1313	A	O5'-P-OP1	6.87	118.94	110.70
58	D1	2666	G	N9-C1'-C2'	6.87	122.93	114.00
22	Bb	542	G	O5'-P-OP2	-6.86	99.53	105.70
58	C1	1424	A	O4'-C1'-N9	6.86	113.69	108.20
58	C1	259	A	C2'-C3'-O3'	6.85	124.66	113.70
53	C6	49	CYS	CA-CB-SG	6.85	126.33	114.00
22	Bb	22	G	O5'-P-OP1	6.85	118.92	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	C1	354	A	C2'-C3'-O3'	6.84	124.64	113.70
42	DT	112	ARG	NE-CZ-NH1	6.83	123.72	120.30
58	D1	1604	A	C2'-C3'-O3'	6.83	124.63	113.70
58	C1	1036	C	O5'-P-OP2	6.83	118.89	110.70
58	C1	1424	A	O5'-P-OP2	-6.83	99.56	105.70
58	D1	1348	G	O5'-P-OP2	-6.83	99.56	105.70
58	C1	2329	G	C2'-C3'-O3'	6.82	124.61	113.70
58	D1	1323	A	O5'-P-OP1	6.81	118.88	110.70
59	Ds	66	A	C2'-C3'-O3'	6.81	124.60	113.70
58	D1	138	A	C2'-C3'-O3'	6.80	124.58	113.70
58	D1	2329	G	C2'-C3'-O3'	6.80	124.58	113.70
58	C1	992	G	O5'-P-OP2	-6.79	99.58	105.70
58	D1	2022	A	O5'-P-OP1	-6.76	99.61	105.70
58	C1	2581	G	O5'-P-OP1	-6.76	99.62	105.70
58	D1	1662	C	O5'-P-OP1	-6.75	99.62	105.70
58	D1	715	G	C5'-C4'-O4'	6.75	117.20	109.10
58	C1	200	G	O5'-P-OP2	-6.75	99.63	105.70
22	Ab	385	A	C5'-C4'-O4'	6.74	117.19	109.10
58	D1	2441	A	O5'-P-OP1	-6.73	99.65	105.70
58	D1	1648	A	O5'-P-OP1	-6.72	99.65	105.70
58	C1	2791	U	C5'-C4'-O4'	6.71	117.16	109.10
58	D1	1286	A	O5'-P-OP2	6.71	118.76	110.70
58	D1	2602	C	O5'-P-OP2	6.71	118.76	110.70
58	C1	2465	G	O5'-P-OP2	-6.71	99.66	105.70
58	D1	113	C	O5'-P-OP2	-6.71	99.66	105.70
4	AD	9	CYS	CA-CB-SG	6.70	126.06	114.00
40	CR	89	ARG	NE-CZ-NH1	6.69	123.65	120.30
58	C1	1740	C	C5'-C4'-O4'	6.69	117.13	109.10
58	C1	754	C	O5'-P-OP1	-6.68	99.69	105.70
26	C4	36	A	C5'-C4'-O4'	6.67	117.11	109.10
58	D1	124	A	O5'-P-OP2	-6.67	99.69	105.70
58	C1	1666	U	O5'-P-OP1	-6.66	99.70	105.70
58	D1	2808	U	O4'-C1'-N1	6.65	113.52	108.20
58	C1	1857	C	O5'-P-OP1	6.64	118.67	110.70
58	D1	2449	U	O5'-P-OP1	-6.64	99.73	105.70
58	C1	98	G	O4'-C1'-N9	6.63	113.51	108.20
58	D1	2515	U	O5'-P-OP1	6.63	118.65	110.70
58	D1	2289	A	C5'-C4'-O4'	6.62	117.05	109.10
58	C1	192	A	O5'-P-OP2	-6.62	99.75	105.70
4	BD	36	ARG	NE-CZ-NH1	6.61	123.60	120.30
58	D1	1011	C	O5'-P-OP2	-6.61	99.75	105.70
22	Bb	1506	U	O5'-P-OP1	6.61	118.63	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	D3	47	U	N1-C1'-C2'	6.61	122.59	114.00
22	Ab	327	G	O5'-P-OP1	-6.60	99.76	105.70
29	DC	127	ASP	CB-CG-OD2	6.60	124.24	118.30
58	C1	2609	A	O5'-P-OP1	6.59	118.61	110.70
58	C1	1344	G	O5'-P-OP2	6.58	118.60	110.70
58	D1	185	A	O5'-P-OP1	-6.57	99.78	105.70
58	D1	1373	G	C2'-C3'-O3'	6.57	124.21	113.70
58	C1	2220	A	C2'-C3'-O3'	6.56	124.20	113.70
58	D1	1345	U	O4'-C1'-N1	6.56	113.45	108.20
22	Bb	1267	A	C2'-C3'-O3'	6.55	124.18	113.70
22	Bb	778	A	O5'-P-OP2	6.55	118.56	110.70
58	D1	2672	G	N9-C1'-C2'	6.54	122.50	114.00
58	D1	1358	U	O5'-P-OP2	-6.54	99.81	105.70
58	C1	30	C	O5'-P-OP2	-6.54	99.81	105.70
58	C1	2518	C	O5'-P-OP1	6.54	118.54	110.70
58	C1	435	C	O5'-P-OP2	-6.53	99.82	105.70
58	C1	2619	G	O5'-P-OP2	-6.53	99.82	105.70
58	C1	1489	G	O5'-P-OP2	-6.52	99.83	105.70
58	C1	182	G	O5'-P-OP2	-6.51	99.84	105.70
58	D1	1075	G	O5'-P-OP2	-6.51	99.84	105.70
58	C1	430	C	O5'-P-OP1	-6.51	99.84	105.70
22	Ab	655	G	O5'-P-OP2	-6.50	99.85	105.70
22	Bb	1464	G	O5'-P-OP2	-6.50	99.85	105.70
58	D1	200	G	O5'-P-OP1	6.50	118.50	110.70
58	D1	2458	G	O5'-P-OP1	-6.50	99.85	105.70
58	D1	839	A	O5'-P-OP2	-6.49	99.86	105.70
58	C1	1067	G	C2'-C3'-O3'	6.48	124.07	113.70
58	C1	1698	A	C2'-C3'-O3'	6.47	124.06	113.70
58	C1	2028	C	O5'-P-OP2	-6.47	99.88	105.70
58	C1	1941	C	O5'-P-OP2	-6.46	99.88	105.70
58	D1	2022	A	O5'-P-OP2	6.46	118.45	110.70
58	D1	107	G	O5'-P-OP2	-6.45	99.89	105.70
58	C1	511	C	O5'-P-OP2	6.45	118.44	110.70
22	Bb	19	C	O5'-P-OP1	-6.43	99.91	105.70
58	D1	833	U	O5'-P-OP1	6.43	118.42	110.70
58	D1	1229	C	O5'-P-OP2	-6.42	99.92	105.70
58	D1	1852	G	O5'-P-OP1	6.42	118.41	110.70
58	C1	32	U	O5'-P-OP1	-6.42	99.92	105.70
58	C1	288	G	O5'-P-OP1	-6.42	99.92	105.70
58	D1	465	G	O5'-P-OP2	6.42	118.40	110.70
58	C1	1345	U	C5'-C4'-O4'	6.41	116.78	109.10
58	C1	740	U	O5'-P-OP2	-6.40	99.94	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	C1	798	A	C2'-C3'-O3'	6.40	123.94	113.70
58	D1	1984	U	N1-C1'-C2'	6.39	122.31	114.00
58	D1	963	A	O5'-P-OP1	-6.39	99.95	105.70
58	C1	1850	U	C4'-C3'-O3'	6.38	125.75	113.00
58	D1	998	G	O5'-P-OP1	-6.38	99.96	105.70
58	D1	1473	C	O5'-P-OP2	6.37	118.34	110.70
29	DC	127	ASP	CB-CG-OD1	-6.36	112.57	118.30
58	D1	955	A	O5'-P-OP2	-6.36	99.98	105.70
22	Bb	493	A	C2'-C3'-O3'	6.35	123.86	113.70
28	DB	69	ARG	NE-CZ-NH2	-6.35	117.13	120.30
58	C1	1345	U	C5'-C4'-C3'	6.34	126.15	116.00
58	C1	1069	G	O5'-P-OP1	-6.34	99.99	105.70
61	D4	76	C	P-O5'-C5'	-6.34	110.75	120.90
22	Ab	61	A	C2'-C3'-O3'	6.33	123.83	113.70
58	D1	2672	G	O4'-C1'-N9	6.33	113.27	108.20
22	Ab	262	G	C2'-C3'-O3'	6.33	123.82	113.70
58	C1	2004	C	O5'-P-OP1	-6.31	100.02	105.70
58	C1	640	G	O5'-P-OP1	-6.31	100.02	105.70
22	Bb	22	G	O5'-P-OP2	-6.30	100.03	105.70
58	D1	19	C	O5'-P-OP2	-6.30	100.03	105.70
58	C1	413	U	C2'-C3'-O3'	6.30	123.78	113.70
58	D1	1924	G	O5'-P-OP1	-6.30	100.03	105.70
22	Bb	111	G	O5'-P-OP2	6.30	118.26	110.70
22	Ab	408	A	O4'-C1'-N9	6.29	113.23	108.20
58	D1	1983	C	C2'-C3'-O3'	6.29	123.76	113.70
58	C1	1817	A	O5'-P-OP2	6.29	118.24	110.70
58	C1	186	C	O5'-P-OP1	-6.29	100.04	105.70
58	C1	1893	G	O5'-P-OP2	-6.28	100.04	105.70
58	D1	199	A	O5'-P-OP2	-6.28	100.05	105.70
58	D1	873	U	O5'-P-OP1	6.27	118.23	110.70
58	C1	2691	C	O5'-P-OP1	6.25	118.20	110.70
58	D1	835	A	O5'-P-OP1	-6.25	100.08	105.70
58	D1	1654	A	O5'-P-OP1	-6.24	100.08	105.70
28	DB	229	VAL	CB-CA-C	-6.24	99.54	111.40
22	Bb	1305	G	O5'-P-OP1	-6.22	100.10	105.70
58	D1	2005	G	C5'-C4'-O4'	6.22	116.56	109.10
58	D1	2045	G	O5'-P-OP2	-6.22	100.10	105.70
59	Cs	66	A	C2'-C3'-O3'	6.21	123.63	113.70
22	Ab	1378	C	O5'-P-OP1	-6.19	100.12	105.70
58	D1	2223	C	O5'-P-OP1	-6.19	100.13	105.70
58	C1	845	G	O5'-P-OP2	-6.19	100.13	105.70
58	D1	2451	C	O5'-P-OP1	-6.19	100.13	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	D1	2666	G	C1'-O4'-C4'	-6.19	104.95	109.90
22	Bb	507	A	O5'-P-OP2	6.19	118.13	110.70
58	C1	120	G	O5'-P-OP2	-6.19	100.13	105.70
58	D1	506	G	O5'-P-OP2	-6.19	100.13	105.70
58	C1	1995	C	O5'-P-OP2	-6.17	100.15	105.70
58	D1	625	A	P-O3'-C3'	6.17	127.10	119.70
58	C1	992	G	O5'-P-OP1	6.16	118.09	110.70
58	D1	716	A	O5'-P-OP2	-6.16	100.16	105.70
22	Ab	408	A	O4'-C1'-C2'	6.15	113.13	107.60
58	D1	2054	A	C4'-C3'-O3'	6.15	125.30	113.00
58	C1	1604	A	C2'-C3'-O3'	6.15	123.53	113.70
4	AD	26	CYS	CA-CB-SG	6.14	125.05	114.00
58	C1	589	A	O5'-P-OP1	6.14	118.06	110.70
58	C1	490	G	O5'-P-OP2	6.13	118.06	110.70
58	D1	1795	C	O5'-P-OP2	-6.13	100.18	105.70
58	C1	1727	G	O5'-P-OP1	-6.13	100.18	105.70
58	D1	1384	G	O5'-P-OP2	6.13	118.05	110.70
58	C1	1726	U	C2'-C3'-O3'	6.12	123.49	113.70
22	Bb	956	A	O5'-P-OP2	6.12	118.04	110.70
40	DR	54	LEU	CA-CB-CG	6.12	129.37	115.30
58	C1	2289	A	C5'-C4'-O4'	6.12	116.44	109.10
58	D1	2584	C	O5'-P-OP2	-6.11	100.20	105.70
58	C1	2657	C	O5'-P-OP2	-6.11	100.20	105.70
22	Bb	885	A	O5'-P-OP1	6.11	118.03	110.70
58	C1	1538	C	N1-C1'-C2'	6.10	121.93	114.00
58	C1	1820	C	O5'-P-OP1	-6.09	100.21	105.70
54	D7	10	LEU	CA-CB-CG	6.09	129.31	115.30
41	DS	30	VAL	N-CA-C	6.09	127.43	111.00
22	Ab	809	G	O5'-P-OP2	-6.08	100.22	105.70
58	C1	506	G	C2'-C3'-O3'	6.08	123.43	113.70
58	D1	1017	A	O5'-P-OP1	-6.08	100.23	105.70
58	D1	2440	G	O5'-P-OP2	-6.08	100.23	105.70
58	C1	2031	G	O5'-P-OP2	6.07	117.99	110.70
25	C3	1	G	C5'-C4'-O4'	6.07	116.39	109.10
58	C1	2221	C	C2'-C3'-O3'	6.07	123.41	113.70
25	C2	1	G	C5'-C4'-O4'	6.07	116.39	109.10
37	CO	41	ARG	N-CA-C	-6.07	94.61	111.00
58	C1	2522	U	O5'-P-OP2	-6.07	100.24	105.70
26	C4	1	C	C5'-C4'-O4'	6.06	116.38	109.10
22	Bb	324	C	C2'-C3'-O3'	6.05	123.38	113.70
58	C1	1953	A	O5'-P-OP1	-6.05	100.25	105.70
58	D1	1017	A	O5'-P-OP2	6.05	117.96	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	Bb	555	U	O5'-P-OP1	-6.04	100.26	105.70
58	D1	1984	U	C3'-C2'-C1'	-6.04	96.67	101.50
58	D1	1991	A	C5'-C4'-O4'	6.03	116.34	109.10
58	C1	1850	U	P-O3'-C3'	6.03	126.94	119.70
58	D1	1681	G	O5'-P-OP2	-6.02	100.28	105.70
22	Ab	357	G	O5'-P-OP1	-6.01	100.29	105.70
58	D1	1403	G	O5'-P-OP2	-6.01	100.29	105.70
22	Bb	1502	C	O5'-P-OP1	-6.01	100.29	105.70
22	Bb	385	A	C5'-C4'-O4'	6.00	116.30	109.10
58	D1	2700	U	P-O3'-C3'	5.99	126.89	119.70
58	D1	1424	A	O4'-C1'-C2'	5.98	112.98	107.60
32	CF	149	ARG	NE-CZ-NH1	5.97	123.29	120.30
58	C1	2020	C	O5'-P-OP1	5.96	117.86	110.70
58	D1	1740	C	N1-C1'-C2'	5.96	121.75	114.00
58	D1	2329	G	C5'-C4'-O4'	5.96	116.25	109.10
58	C1	2357	A	C1'-O4'-C4'	-5.96	105.13	109.90
58	C1	2482	C	C2'-C3'-O3'	5.95	123.22	113.70
22	Ab	1487	C	O5'-P-OP2	-5.95	100.35	105.70
22	Ab	903	G	O5'-P-OP2	-5.94	100.35	105.70
58	D1	1816	A	O4'-C1'-C2'	-5.94	99.86	105.80
58	D1	2102	C	O5'-P-OP1	5.94	117.83	110.70
55	D8	21	ARG	NE-CZ-NH2	-5.93	117.33	120.30
58	D1	535	U	O5'-P-OP2	5.93	117.81	110.70
22	Bb	1206	G	O5'-P-OP2	-5.93	100.37	105.70
58	C1	1343	C	O5'-P-OP1	-5.92	100.37	105.70
58	C1	837	C	O5'-P-OP2	-5.92	100.37	105.70
58	C1	253	A	N9-C1'-C2'	5.92	121.70	114.00
22	Ab	1508	G	O5'-P-OP2	-5.90	100.39	105.70
19	BT	5	LEU	CA-CB-CG	5.89	128.86	115.30
58	C1	2293	G	C4'-C3'-O3'	5.89	124.79	113.00
58	D1	201	A	O5'-P-OP2	-5.89	100.40	105.70
58	D1	1646	G	O5'-P-OP1	5.89	117.77	110.70
22	Ab	1206	G	O5'-P-OP2	-5.89	100.40	105.70
58	C1	1345	U	O4'-C1'-N1	5.87	112.90	108.20
22	Bb	1389	U	O5'-P-OP1	5.87	117.74	110.70
55	C8	12	ARG	NE-CZ-NH1	5.86	123.23	120.30
58	C1	2577	A	O5'-P-OP1	5.86	117.73	110.70
58	D1	952	U	O5'-P-OP2	-5.86	100.43	105.70
58	D1	2000	C	O5'-P-OP2	-5.86	100.43	105.70
58	C1	2627	C	O5'-P-OP1	-5.86	100.43	105.70
58	D1	575	G	O5'-P-OP2	5.85	117.72	110.70
3	AC	156	ARG	NE-CZ-NH1	5.84	123.22	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	D1	2052	A	O5'-P-OP1	-5.84	100.44	105.70
14	BN	43	CYS	CA-CB-SG	-5.84	103.49	114.00
58	D1	731	A	O5'-P-OP1	-5.84	100.45	105.70
58	D1	1991	A	C1'-O4'-C4'	-5.84	105.23	109.90
58	D1	204	A	O5'-P-OP1	-5.83	100.46	105.70
59	Ds	116	G	C2'-C3'-O3'	5.83	123.02	113.70
58	D1	552	A	C1'-C2'-O2'	5.83	128.08	110.60
58	C1	1820	C	O5'-P-OP2	5.82	117.69	110.70
58	D1	1925	G	O5'-P-OP2	-5.82	100.46	105.70
32	DF	149	ARG	NE-CZ-NH1	5.82	123.21	120.30
58	D1	718	C	O5'-P-OP2	-5.82	100.46	105.70
22	Bb	469	G	C2'-C3'-O3'	5.82	123.00	113.70
58	D1	1248	A	N9-C1'-C2'	5.81	121.56	114.00
58	C1	490	G	O5'-P-OP1	-5.81	100.47	105.70
58	D1	1643	C	C2'-C3'-O3'	5.80	122.99	113.70
58	D1	2107	U	O5'-P-OP2	-5.80	100.48	105.70
58	D1	2509	C	O5'-P-OP1	-5.79	100.48	105.70
58	D1	352	G	O5'-P-OP2	-5.79	100.49	105.70
58	D1	1953	A	O5'-P-OP1	-5.79	100.49	105.70
22	Ab	1288	A	O5'-P-OP2	-5.78	100.50	105.70
22	Bb	548	C	O5'-P-OP1	-5.78	100.50	105.70
39	DQ	10	LEU	CB-CG-CD2	5.78	120.83	111.00
58	C1	1698	A	C4'-C3'-O3'	5.77	124.55	113.00
58	C1	1740	C	C4'-C3'-O3'	5.76	124.53	113.00
22	Ab	671	A	C2'-C3'-O3'	5.75	122.90	113.70
58	D1	2339	A	O5'-P-OP2	5.75	117.60	110.70
22	Bb	1349	C	O5'-P-OP1	-5.75	100.53	105.70
58	D1	136	G	C5'-C4'-O4'	5.75	116.00	109.10
22	Ab	1445	G	O5'-P-OP2	-5.74	100.53	105.70
58	D1	838	G	O5'-P-OP2	-5.74	100.54	105.70
58	D1	2107	U	O5'-P-OP1	5.74	117.58	110.70
61	D4	73	A	O4'-C4'-C3'	-5.74	98.27	104.00
32	DF	132	ARG	NE-CZ-NH1	5.74	123.17	120.30
58	C1	639	A	C4'-C3'-O3'	5.73	124.46	113.00
33	CI	27	ARG	NE-CZ-NH1	5.73	123.16	120.30
58	D1	2008	G	C2'-C3'-O3'	5.73	122.86	113.70
39	CQ	4	LEU	CB-CG-CD1	5.73	120.73	111.00
58	D1	1849	A	C4'-C3'-O3'	5.72	124.45	113.00
58	C1	2472	C	O5'-P-OP1	-5.72	100.55	105.70
58	D1	1436	U	O5'-P-OP2	5.72	117.56	110.70
22	Bb	1064	G	O5'-P-OP2	-5.71	100.56	105.70
58	D1	567	C	O5'-P-OP1	-5.71	100.56	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	D1	2232	G	O5'-P-OP1	-5.71	100.56	105.70
58	C1	647	G	C2'-C3'-O3'	5.71	122.83	113.70
58	D1	2842	G	O5'-P-OP2	-5.71	100.56	105.70
22	Ab	6	U	C5'-C4'-O4'	5.70	115.94	109.10
24	BC	59	ARG	NE-CZ-NH2	-5.70	117.45	120.30
58	C1	2049	U	N1-C1'-C2'	5.70	121.41	114.00
7	BG	114	ARG	NE-CZ-NH1	5.70	123.15	120.30
58	D1	2018	G	C5'-C4'-O4'	5.69	115.93	109.10
58	C1	715	G	C5'-C4'-O4'	5.69	115.92	109.10
58	D1	203	G	O5'-P-OP2	5.69	117.53	110.70
58	D1	636	U	O5'-P-OP1	-5.69	100.58	105.70
22	Ab	78	G	C2'-C3'-O3'	5.68	122.79	113.70
45	DX	44	GLU	OE1-CD-OE2	-5.68	116.48	123.30
7	BG	102	ARG	NE-CZ-NH1	5.68	123.14	120.30
58	D1	136	G	O4'-C1'-N9	5.67	112.73	108.20
58	D1	1300	U	O5'-P-OP1	-5.67	100.60	105.70
4	BD	12	CYS	CB-CA-C	5.67	121.73	110.40
58	C1	262	C	O5'-P-OP2	-5.66	100.60	105.70
39	DQ	58	GLY	N-CA-C	5.66	127.26	113.10
22	Bb	350	G	O5'-P-OP2	-5.66	100.61	105.70
58	D1	639	A	C4'-C3'-O3'	5.66	124.31	113.00
63	DW	51	LEU	CA-CB-CG	5.65	128.30	115.30
58	D1	55	C	O5'-P-OP1	-5.65	100.62	105.70
22	Ab	1403	C	O5'-P-OP1	-5.65	100.62	105.70
22	Ab	493	A	C2'-C3'-O3'	5.64	122.72	113.70
42	CT	33	ARG	NE-CZ-NH2	-5.63	117.48	120.30
58	C1	193	G	O5'-P-OP2	5.63	117.46	110.70
58	D1	899	G	C2'-C3'-O3'	5.63	122.71	113.70
25	C3	47	U	O4'-C1'-N1	5.62	112.70	108.20
22	Ab	1038	A	O5'-P-OP1	-5.62	100.64	105.70
58	D1	2342	G	O5'-P-OP1	5.62	117.45	110.70
58	C1	1955	C	C4'-C3'-O3'	5.62	124.24	113.00
58	D1	200	G	O5'-P-OP2	-5.62	100.64	105.70
58	D1	1814	A	C2'-C3'-O3'	-5.62	97.14	109.50
58	C1	302	C	O5'-P-OP1	5.61	117.44	110.70
58	C1	2783	C	O5'-P-OP2	5.61	117.44	110.70
58	D1	1331	A	O5'-P-OP2	-5.61	100.65	105.70
58	C1	125	C	C4'-C3'-O3'	5.61	124.21	113.00
58	D1	179	A	O5'-P-OP2	-5.61	100.65	105.70
58	D1	615	G	O5'-P-OP2	-5.60	100.66	105.70
58	C1	2319	G	C4'-C3'-O3'	5.60	124.19	113.00
3	AC	16	ARG	NE-CZ-NH1	5.59	123.10	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	Bb	1084	A	O5'-P-OP2	-5.59	100.67	105.70
49	CH	46	LEU	CA-CB-CG	5.59	128.16	115.30
28	DB	43	ARG	NE-CZ-NH2	-5.59	117.51	120.30
37	DO	59	LEU	CB-CG-CD2	5.59	120.50	111.00
58	D1	998	G	O5'-P-OP2	5.59	117.40	110.70
58	D1	1033	A	O5'-P-OP1	-5.59	100.67	105.70
58	C1	1956	G	C2'-C3'-O3'	5.58	122.64	113.70
58	C1	2341	G	O5'-P-OP1	-5.58	100.68	105.70
58	C1	499	G	C4'-C3'-O3'	5.58	124.15	113.00
58	D1	1436	U	O5'-P-OP1	-5.58	100.68	105.70
58	C1	754	C	O5'-P-OP2	5.57	117.38	110.70
58	C1	202	G	O4'-C4'-C3'	-5.57	98.43	104.00
58	D1	499	G	P-O3'-C3'	5.57	126.38	119.70
58	D1	1709	C	C2'-C3'-O3'	5.56	122.60	113.70
58	C1	2627	C	O5'-P-OP2	5.56	117.37	110.70
58	D1	888	G	O5'-P-OP2	5.56	117.37	110.70
58	D1	1069	G	O5'-P-OP1	-5.54	100.71	105.70
58	D1	1985	G	O5'-P-OP2	5.54	117.34	110.70
61	D4	33	C	O5'-P-OP2	5.53	117.34	110.70
22	Bb	1375	G	O5'-P-OP2	-5.53	100.72	105.70
58	D1	536	G	C1'-O4'-C4'	-5.53	105.48	109.90
58	D1	1998	A	O5'-P-OP2	-5.52	100.73	105.70
58	C1	2303	C	O5'-P-OP1	5.52	117.32	110.70
58	D1	1420	C	O5'-P-OP2	5.52	117.32	110.70
54	C7	10	LEU	CA-CB-CG	5.52	127.99	115.30
59	Cs	96	U	O5'-P-OP1	-5.52	100.73	105.70
28	DB	69	ARG	NE-CZ-NH1	5.52	123.06	120.30
58	C1	144	G	O5'-P-OP1	5.52	117.32	110.70
58	C1	2477	C	O5'-P-OP2	5.51	117.32	110.70
22	Bb	1305	G	O5'-P-OP2	5.51	117.31	110.70
22	Bb	961	A	O5'-P-OP1	-5.51	100.74	105.70
58	D1	176	G	O5'-P-OP1	-5.51	100.74	105.70
58	D1	2630	C	O5'-P-OP2	-5.51	100.74	105.70
22	Ab	1061	U	O5'-P-OP2	5.51	117.31	110.70
58	C1	185	A	O5'-P-OP2	5.50	117.31	110.70
58	C1	557	G	O5'-P-OP1	5.50	117.30	110.70
28	DB	210	GLY	N-CA-C	-5.50	99.36	113.10
22	Bb	6	U	C5'-C4'-O4'	5.50	115.70	109.10
58	C1	535	U	O5'-P-OP2	5.48	117.28	110.70
58	D1	1397	U	O5'-P-OP1	5.48	117.28	110.70
58	C1	1346	A	C1'-O4'-C4'	-5.47	105.52	109.90
22	Ab	113	A	O5'-P-OP1	-5.47	100.78	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	D1	2313	G	C2'-C3'-O3'	5.47	122.46	113.70
35	CM	120	LEU	CA-CB-CG	5.47	127.88	115.30
58	D1	1968	C	C2'-C3'-O3'	5.47	122.45	113.70
22	Bb	131	C	O5'-P-OP2	-5.47	100.78	105.70
58	C1	780	A	O5'-P-OP1	5.46	117.26	110.70
58	D1	1744	A	O4'-C1'-N9	5.46	112.57	108.20
58	C1	877	G	O5'-P-OP2	5.46	117.25	110.70
58	C1	1816	A	O4'-C1'-C2'	-5.46	100.34	105.80
58	C1	2613	A	N9-C1'-C2'	5.46	121.09	114.00
59	Ds	77	U	C2'-C3'-O3'	5.46	122.43	113.70
22	Ab	324	C	C1'-O4'-C4'	-5.45	105.54	109.90
58	C1	2029	C	O5'-P-OP2	-5.45	100.80	105.70
58	C1	715	G	O5'-P-OP1	5.45	117.24	110.70
43	DU	35	LEU	CA-CB-CG	5.45	127.83	115.30
58	D1	488	G	O5'-P-OP2	-5.44	100.80	105.70
58	D1	1772	C	C2'-C3'-O3'	5.44	122.40	113.70
58	C1	1659	A	O5'-P-OP1	5.44	117.22	110.70
58	C1	2724	A	O5'-P-OP2	-5.44	100.81	105.70
58	D1	784	G	C5'-C4'-O4'	5.44	115.62	109.10
39	CQ	96	ARG	NE-CZ-NH2	-5.43	117.58	120.30
29	DC	144	ARG	NE-CZ-NH1	5.43	123.02	120.30
58	D1	2329	G	O4'-C4'-C3'	-5.43	98.57	104.00
58	C1	1700	A	O5'-P-OP2	5.43	117.21	110.70
58	C1	1842	A	O5'-P-OP2	-5.43	100.81	105.70
58	C1	1286	A	O5'-P-OP2	5.42	117.21	110.70
22	Bb	881	G	O5'-P-OP1	5.42	117.20	110.70
58	C1	2796	C	O5'-P-OP2	-5.42	100.82	105.70
22	Ab	660	A	O5'-P-OP1	-5.42	100.82	105.70
58	D1	2056	G	O5'-P-OP2	-5.42	100.83	105.70
13	AM	9	ILE	CB-CA-C	-5.42	100.77	111.60
58	C1	1991	A	O5'-P-OP2	-5.41	100.83	105.70
58	D1	1991	A	C5'-C4'-C3'	5.41	124.66	116.00
58	D1	2005	G	O5'-P-OP2	-5.41	100.83	105.70
58	D1	2013	G	O5'-P-OP1	-5.41	100.83	105.70
58	D1	2403	A	O5'-P-OP2	5.41	117.19	110.70
53	D6	15	ARG	NE-CZ-NH2	-5.40	117.60	120.30
58	D1	205	G	O5'-P-OP1	-5.40	100.84	105.70
22	Bb	1459	U	O5'-P-OP1	-5.40	100.84	105.70
58	C1	267	G	C4'-C3'-O3'	5.40	123.80	113.00
22	Ab	924	A	O5'-P-OP1	-5.40	100.84	105.70
58	D1	715	G	O5'-P-OP1	5.39	117.17	110.70
58	D1	1792	A	C2'-C3'-O3'	-5.39	97.63	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	D1	354	A	C2'-C3'-O3'	5.39	122.33	113.70
58	C1	715	G	O5'-P-OP2	-5.39	100.85	105.70
58	C1	2403	A	O5'-P-OP1	-5.39	100.85	105.70
58	C1	827	A	C2'-C3'-O3'	5.39	122.32	113.70
58	C1	437	G	O5'-P-OP2	-5.38	100.86	105.70
22	Bb	911	G	O5'-P-OP1	-5.38	100.86	105.70
22	Bb	1050	A	C2'-C3'-O3'	5.38	122.31	113.70
58	C1	486	C	O5'-P-OP1	-5.38	100.86	105.70
58	D1	157	U	O5'-P-OP1	5.38	117.16	110.70
58	D1	913	C	O5'-P-OP1	-5.38	100.86	105.70
14	AN	43	CYS	CA-CB-SG	-5.37	104.33	114.00
58	C1	544	G	O5'-P-OP2	-5.37	100.87	105.70
41	DS	29	ARG	C-N-CA	5.37	135.12	121.70
58	D1	1384	G	O5'-P-OP1	-5.37	100.87	105.70
58	D1	2885	G	O5'-P-OP1	5.37	117.14	110.70
22	Bb	862	U	O5'-P-OP2	-5.36	100.87	105.70
58	C1	2475	C	N1-C1'-C2'	-5.36	106.10	112.00
58	C1	2522	U	O5'-P-OP1	5.36	117.13	110.70
12	BL	53	ARG	NE-CZ-NH1	5.36	122.98	120.30
58	D1	1744	A	N9-C1'-C2'	5.36	120.97	114.00
22	Ab	113	A	C2'-C3'-O3'	5.36	122.27	113.70
58	C1	30	C	O5'-P-OP1	5.36	117.13	110.70
28	DB	237	GLU	OE1-CD-OE2	-5.36	116.87	123.30
56	D9	30	ARG	NE-CZ-NH1	5.36	122.98	120.30
58	D1	1049	C	O5'-P-OP1	-5.35	100.88	105.70
29	DC	117	MET	CA-CB-CG	5.35	122.40	113.30
58	C1	1849	A	C2'-C3'-O3'	5.35	122.25	113.70
58	D1	1740	C	C5'-C4'-O4'	5.35	115.52	109.10
58	D1	1236	G	O5'-P-OP2	-5.34	100.89	105.70
22	Bb	1259	C	C4'-C3'-O3'	5.34	123.68	113.00
58	C1	960	C	C5'-C4'-O4'	5.34	115.51	109.10
58	D1	1862	C	O5'-P-OP2	-5.34	100.90	105.70
42	DT	3	ARG	NE-CZ-NH1	5.33	122.97	120.30
58	D1	2466	G	O5'-P-OP2	-5.33	100.90	105.70
58	C1	1740	C	C5'-C4'-C3'	5.33	124.52	116.00
22	Ab	1075	A	O5'-P-OP2	5.33	117.09	110.70
58	D1	960	C	C5'-C4'-O4'	5.32	115.49	109.10
58	D1	994	G	O5'-P-OP2	-5.32	100.91	105.70
58	D1	1698	A	C4'-C3'-O3'	5.32	123.64	113.00
58	D1	708	G	O5'-P-OP1	5.32	117.08	110.70
22	Bb	408	A	O4'-C1'-C2'	5.32	112.38	107.60
28	CB	237	GLU	OE1-CD-OE2	-5.32	116.92	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	C1	276	G	N9-C1'-C2'	-5.32	106.15	112.00
22	Ab	1506	U	O5'-P-OP1	5.31	117.08	110.70
61	D4	73	A	C1'-O4'-C4'	-5.31	105.65	109.90
58	D1	1849	A	P-O3'-C3'	5.31	126.07	119.70
22	Ab	1061	U	O5'-P-OP1	-5.31	100.92	105.70
58	C1	139	A	C1'-O4'-C4'	-5.31	105.66	109.90
58	C1	236	G	O5'-P-OP2	-5.31	100.92	105.70
22	Bb	424	G	P-O3'-C3'	5.30	126.06	119.70
22	Bb	776	A	O4'-C1'-C2'	-5.30	100.50	105.80
58	C1	236	G	O5'-P-OP1	5.30	117.06	110.70
58	D1	534	C	O5'-P-OP1	5.29	117.05	110.70
58	C1	1744	A	O4'-C1'-N9	5.29	112.43	108.20
58	D1	953	C	O5'-P-OP1	5.29	117.04	110.70
58	D1	1678	A	O5'-P-OP2	5.29	117.04	110.70
59	Ds	8	U	O5'-P-OP1	5.28	117.03	110.70
58	C1	675	G	C2'-C3'-O3'	5.28	122.14	113.70
48	Ca	12	ASN	N-CA-C	5.27	125.23	111.00
58	C1	499	G	P-O3'-C3'	5.27	126.02	119.70
58	D1	526	A	O5'-P-OP1	-5.26	100.97	105.70
58	D1	98	G	O4'-C1'-C2'	5.26	112.33	107.60
29	CC	117	MET	CA-CB-CG	5.25	122.22	113.30
58	D1	2317	C	C2'-C3'-O3'	5.25	122.09	113.70
42	DT	36	ARG	NE-CZ-NH1	5.25	122.92	120.30
58	D1	1448	C	C5'-C4'-O4'	5.24	115.39	109.10
58	C1	1791	C	O5'-P-OP2	-5.24	100.99	105.70
58	D1	1538	C	N1-C1'-C2'	5.24	120.81	114.00
58	D1	1962	C	O5'-P-OP1	-5.23	100.99	105.70
58	D1	715	G	C5'-C4'-C3'	5.23	124.37	116.00
58	D1	1740	C	C1'-O4'-C4'	-5.23	105.72	109.90
22	Bb	490	G	O5'-P-OP2	5.23	116.97	110.70
42	DT	101	ARG	NE-CZ-NH1	5.23	122.91	120.30
58	C1	2310	G	C2'-C3'-O3'	5.22	122.05	113.70
22	Ab	1453	G	O5'-P-OP2	5.22	116.96	110.70
4	BD	12	CYS	N-CA-C	-5.22	96.91	111.00
58	D1	47	A	C2'-C3'-O3'	5.21	122.04	113.70
22	Ab	1461	A	O5'-P-OP1	-5.21	101.01	105.70
58	D1	1288	G	O5'-P-OP1	-5.21	101.01	105.70
22	Bb	1179	G	O5'-P-OP2	-5.21	101.01	105.70
58	D1	2428	C	O5'-P-OP2	-5.20	101.02	105.70
22	Ab	1483	G	O5'-P-OP1	-5.20	101.02	105.70
22	Bb	1476	U	P-O3'-C3'	5.20	125.94	119.70
58	D1	2745	A	C5'-C4'-O4'	5.20	115.34	109.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	Bb	1234	A	O5'-P-OP2	-5.19	101.03	105.70
22	Ab	1037	C	O5'-P-OP1	-5.19	101.03	105.70
22	Bb	938	U	N1-C1'-C2'	5.19	120.75	114.00
61	D4	76	C	O5'-P-OP1	-5.19	101.03	105.70
58	D1	499	G	C4'-C3'-O3'	5.18	123.36	113.00
58	D1	566	C	C2'-C3'-O3'	5.18	121.99	113.70
58	D1	605	G	O5'-P-OP2	-5.18	101.04	105.70
58	D1	1625	A	C2'-C3'-O3'	5.18	121.99	113.70
22	Ab	10	G	O5'-P-OP1	5.18	116.91	110.70
58	D1	2625	A	O5'-P-OP2	5.18	116.91	110.70
58	C1	186	C	O5'-P-OP2	5.17	116.91	110.70
58	C1	1424	A	O4'-C1'-C2'	5.17	112.25	107.60
58	C1	913	C	O5'-P-OP1	-5.17	101.05	105.70
58	D1	541	C	O5'-P-OP1	-5.17	101.05	105.70
58	D1	775	G	O5'-P-OP2	-5.17	101.05	105.70
58	D1	2475	C	C4'-C3'-O3'	5.17	123.34	113.00
58	C1	1829	G	P-O3'-C3'	5.17	125.90	119.70
58	D1	782	C	O5'-P-OP2	5.17	116.90	110.70
58	D1	1060	G	O5'-P-OP1	5.16	116.90	110.70
58	D1	1187	A	O5'-P-OP1	-5.16	101.05	105.70
58	C1	2056	G	N9-C1'-C2'	5.16	120.70	114.00
39	DQ	17	ARG	NE-CZ-NH1	5.16	122.88	120.30
58	D1	1549	C	C4'-C3'-O3'	5.16	123.31	113.00
58	D1	2433	A	C4'-C3'-O3'	5.15	123.31	113.00
22	Ab	1048	U	C2'-C3'-O3'	5.15	121.94	113.70
22	Ab	1408	U	O5'-P-OP1	-5.15	101.06	105.70
58	D1	1706	C	O5'-P-OP2	-5.15	101.06	105.70
58	D1	1859	A	O5'-P-OP2	-5.15	101.06	105.70
22	Bb	408	A	O4'-C1'-N9	5.15	112.32	108.20
22	Bb	1350	C	O5'-P-OP1	-5.15	101.06	105.70
39	DQ	18	LEU	CA-CB-CG	5.15	127.14	115.30
58	D1	2221	C	C2'-C3'-O3'	5.14	121.93	113.70
58	D1	1960	U	O5'-P-OP1	-5.14	101.07	105.70
28	CB	210	GLY	N-CA-C	-5.14	100.25	113.10
58	D1	2591	U	C4'-C3'-O3'	-5.14	98.61	109.40
58	C1	1744	A	C1'-O4'-C4'	-5.14	105.79	109.90
20	AU	14	LYS	CD-CE-NZ	5.13	123.50	111.70
22	Ab	683	C	O5'-P-OP2	5.13	116.85	110.70
5	AE	31	LEU	CA-CB-CG	5.12	127.08	115.30
22	Bb	404	A	O5'-P-OP2	-5.12	101.09	105.70
58	C1	1267	C	O5'-P-OP1	-5.12	101.09	105.70
22	Bb	1473	U	O5'-P-OP2	-5.11	101.10	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	D1	203	G	O5'-P-OP1	-5.11	101.10	105.70
58	D1	2476	C	O5'-P-OP2	-5.11	101.10	105.70
58	C1	1298	A	O5'-P-OP1	-5.11	101.10	105.70
58	D1	84	C	C2'-C3'-O3'	5.11	121.88	113.70
58	C1	2110	U	C2'-C3'-O3'	5.11	121.87	113.70
58	D1	1974	A	O5'-P-OP1	-5.10	101.11	105.70
58	C1	820	A	C2'-C3'-O3'	-5.10	98.28	109.50
58	D1	1342	C	O5'-P-OP1	5.10	116.82	110.70
39	DQ	4	LEU	CA-CB-CG	5.10	127.03	115.30
22	Ab	796	C	O5'-P-OP2	-5.10	101.11	105.70
58	D1	1263	G	O5'-P-OP1	5.10	116.82	110.70
58	D1	1330	G	O5'-P-OP1	-5.10	101.11	105.70
58	D1	2538	C	C2'-C3'-O3'	5.10	121.86	113.70
28	CB	69	ARG	NE-CZ-NH2	-5.09	117.75	120.30
47	DZ	19	ARG	NE-CZ-NH1	5.09	122.85	120.30
58	D1	114	G	O5'-P-OP1	5.09	116.81	110.70
58	D1	909	A	O5'-P-OP1	5.09	116.81	110.70
58	D1	1022	G	O5'-P-OP2	-5.09	101.12	105.70
58	D1	1190	C	O5'-P-OP2	5.09	116.81	110.70
22	Bb	495	C	C2'-C3'-O3'	5.09	121.84	113.70
22	Ab	948	C	O5'-P-OP2	5.09	116.80	110.70
58	D1	1707	G	O5'-P-OP2	-5.09	101.12	105.70
58	D1	2829	A	P-O3'-C3'	5.09	125.80	119.70
22	Ab	548	C	O5'-P-OP1	-5.08	101.13	105.70
58	C1	434	G	O5'-P-OP2	-5.08	101.13	105.70
58	D1	413	U	P-O3'-C3'	5.08	125.80	119.70
61	D4	73	A	O5'-P-OP2	-5.08	101.13	105.70
58	C1	2619	G	O5'-P-OP1	5.08	116.79	110.70
58	D1	842	C	O5'-P-OP1	5.08	116.79	110.70
58	D1	954	A	O5'-P-OP1	5.08	116.79	110.70
58	D1	114	G	O5'-P-OP2	-5.07	101.13	105.70
58	C1	833	U	O5'-P-OP1	5.07	116.79	110.70
58	C1	626	G	O5'-P-OP1	-5.07	101.14	105.70
58	C1	987	U	O5'-P-OP1	5.07	116.78	110.70
58	C1	1364	G	O5'-P-OP1	-5.07	101.14	105.70
58	D1	2799	C	O5'-P-OP1	-5.07	101.14	105.70
58	C1	567	C	O5'-P-OP1	-5.07	101.14	105.70
58	D1	1424	A	C4'-C3'-O3'	-5.07	98.76	109.40
40	DR	88	ASP	CB-CG-OD2	5.06	122.86	118.30
22	Ab	1215	G	O5'-P-OP1	5.06	116.78	110.70
22	Ab	57	U	O5'-P-OP1	-5.06	101.15	105.70
58	C1	209	A	O5'-P-OP2	5.06	116.77	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	D1	803	U	O5'-P-OP2	-5.06	101.15	105.70
4	BD	36	ARG	NE-CZ-NH2	-5.06	117.77	120.30
39	DQ	33	ARG	NE-CZ-NH1	5.06	122.83	120.30
41	DS	30	VAL	CB-CA-C	-5.06	101.79	111.40
58	D1	2741	G	C2'-C3'-O3'	5.06	121.79	113.70
58	C1	1699	G	O5'-P-OP1	-5.06	101.15	105.70
37	CO	59	LEU	CA-CB-CG	5.05	126.92	115.30
58	C1	2520	G	O5'-P-OP1	-5.05	101.15	105.70
58	C1	2008	G	C2'-C3'-O3'	5.05	121.78	113.70
37	DO	41	ARG	NE-CZ-NH2	5.05	122.83	120.30
58	D1	2095	U	O5'-P-OP2	-5.05	101.15	105.70
29	CC	44	TYR	N-CA-C	5.05	124.63	111.00
58	C1	989	A	O5'-P-OP1	5.05	116.76	110.70
58	C1	864	G	C2'-C3'-O3'	-5.04	98.41	109.50
58	C1	2433	A	C4'-C3'-O3'	5.04	123.08	113.00
58	D1	1681	G	O5'-P-OP1	5.04	116.75	110.70
22	Bb	721	A	O5'-P-OP1	-5.03	101.17	105.70
58	C1	2588	A	O5'-P-OP2	-5.03	101.17	105.70
59	Cs	116	G	C2'-C3'-O3'	5.03	121.74	113.70
45	DX	57	LEU	CA-CB-CG	5.03	126.86	115.30
58	D1	1951	G	O5'-P-OP2	-5.03	101.18	105.70
58	C1	1744	A	N9-C1'-C2'	5.02	120.53	114.00
58	D1	1640	G	O5'-P-OP1	-5.02	101.18	105.70
58	C1	2318	G	C2'-C3'-O3'	5.02	121.73	113.70
58	D1	2625	A	O5'-P-OP1	-5.02	101.18	105.70
22	Bb	550	G	O5'-P-OP2	-5.02	101.19	105.70
41	DS	95	ARG	NE-CZ-NH2	-5.01	117.79	120.30
58	D1	1983	C	C5'-C4'-C3'	5.01	124.02	116.00
22	Ab	373	G	O5'-P-OP2	-5.01	101.19	105.70
46	DY	84	ARG	NE-CZ-NH1	5.01	122.81	120.30
58	D1	2382	G	O5'-P-OP1	-5.01	101.19	105.70
58	C1	372	G	C2'-C3'-O3'	5.01	121.71	113.70
58	C1	2691	C	O5'-P-OP2	-5.01	101.19	105.70
58	D1	2700	U	C2'-C3'-O3'	5.00	121.70	113.70

All (45) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	Ab	408	A	C1'
22	Bb	408	A	C1'
25	C3	47	U	C1'
58	C1	98	G	C1'

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Mol	Chain	Res	Type	Atom
58	C1	715	G	C4',C1',C3'
58	C1	989	A	C1'
58	C1	1345	U	C4',C3',C1'
58	C1	1424	A	C1'
58	C1	1529	G	C3'
58	C1	1590	A	C1'
58	C1	1740	C	C4',C3'
58	C1	1955	C	C3'
58	C1	1983	C	C4',C1'
58	C1	2212	G	C3'
58	C1	2297	A	C1'
58	C1	2673	A	C1'
58	C1	2808	U	C1'
25	D3	47	U	C1'
58	D1	98	G	C1'
58	D1	497	A	C3'
58	D1	715	G	C4',C3',C1'
58	D1	989	A	C1'
58	D1	1345	U	C4',C3',C1'
58	D1	1424	A	C1'
58	D1	1590	A	C1'
58	D1	1698	A	C3'
58	D1	1740	C	C4',C3'
58	D1	1955	C	C3'
58	D1	1983	C	C4',C1'
58	D1	2212	G	C3'
58	D1	2297	A	C1'
58	D1	2673	A	C1'
58	D1	2808	U	C1'

All (52) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	AA	23	ARG	Peptide
3	AC	26	LYS	Peptide
12	AL	91	LYS	Peptide
13	AM	69	GLU	Peptide
19	AT	28	LYS	Peptide
20	AU	73	HIS	Peptide
13	BM	69	GLU	Peptide
14	BN	2	ALA	Peptide
18	BS	84	LYS	Peptide

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Group</b>
53	C6	4	HIS	Peptide
54	C7	32	ASN	Peptide
28	CB	237	GLU	Peptide
28	CB	24	ILE	Peptide
28	CB	244	ARG	Peptide
28	CB	47	GLY	Peptide
30	CD	85	GLY	Peptide
31	CE	53	LEU	Peptide
31	CE	88	ILE	Peptide
33	CI	12	LEU	Peptide
37	CO	115	LEU	Peptide
37	CO	41	ARG	Peptide
37	CO	51	PHE	Peptide
37	CO	52	GLU	Peptide
37	CO	57	THR	Peptide
37	CO	9	ASN	Peptide
41	CS	29	ARG	Peptide
42	CT	96	ALA	Peptide
46	CY	76	CYS	Peptide
54	D7	24	GLU	Peptide
56	D9	44	LYS	Peptide
28	DB	197	GLY	Peptide
28	DB	237	GLU	Peptide
28	DB	244	ARG	Peptide
29	DC	115	GLY	Peptide
29	DC	131	ALA	Peptide
32	DF	158	HIS	Peptide
34	DJ	109	UNK	Peptide
37	DO	115	LEU	Peptide
37	DO	37	GLY	Peptide
37	DO	51	PHE	Peptide
37	DO	52	GLU	Peptide
37	DO	57	THR	Peptide
37	DO	9	ASN	Peptide
39	DQ	5	LYS	Peptide
41	DS	29	ARG	Peptide
41	DS	31	SER	Peptide
41	DS	79	HIS	Peptide
42	DT	96	ALA	Peptide
46	DY	39	VAL	Peptide
46	DY	76	CYS	Peptide
47	DZ	151	HIS	Peptide

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Mol	Chain	Res	Type	Group
48	Da	83	PRO	Peptide

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A2	173	0	85	16	0
2	AA	1901	0	1951	33	0
2	BA	1901	0	1951	32	0
3	AC	1612	0	1677	30	0
4	AD	1703	0	1763	41	0
4	BD	1703	0	1763	43	0
5	AE	1147	0	1207	27	0
5	BE	1147	0	1207	23	0
6	AF	843	0	857	6	0
6	BF	843	0	857	19	0
7	AG	1257	0	1296	8	0
7	BG	1257	0	1296	15	0
8	AH	1116	0	1177	11	0
8	BH	1116	0	1177	17	0
9	AI	1011	0	1043	29	0
9	BI	1011	0	1043	18	0
10	AJ	795	0	840	22	0
10	BJ	795	0	840	21	0
11	AK	885	0	904	13	0
11	BK	885	0	904	21	0
12	AL	971	0	1057	24	0
12	BL	971	0	1057	17	0
13	AM	988	0	1059	35	0
13	BM	988	0	1059	27	0
14	AN	492	0	529	20	0
14	BN	492	0	529	13	0
15	AO	734	0	771	7	0
15	BO	734	0	771	8	0
16	AP	701	0	720	10	0
16	BP	701	0	720	14	0
17	AR	824	0	891	5	0
17	BR	824	0	891	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	AS	574	0	644	17	0
18	BS	574	0	644	15	0
19	AT	630	0	652	24	0
19	BT	630	0	652	26	0
20	AU	763	0	861	16	0
20	BU	763	0	861	13	0
21	AW	209	0	221	1	0
21	BW	209	0	221	3	0
22	Ab	32329	0	16318	0	0
22	Bb	32329	0	16318	0	1
23	B2	194	0	95	12	0
24	BC	1613	0	1677	26	0
25	C2	1597	0	811	18	0
25	C3	1619	0	822	28	0
25	D3	1619	0	822	46	0
26	C4	1640	0	837	56	0
27	CA	1156	0	755	15	0
28	CB	2105	0	2182	95	0
28	DB	2105	0	2182	88	0
29	CC	1564	0	1629	60	0
29	DC	1564	0	1629	79	0
30	CD	1624	0	1677	61	0
30	DD	1624	0	1677	47	0
31	CE	1474	0	1535	44	0
31	DE	1474	0	1535	57	0
32	CF	1223	0	1282	26	0
32	DF	1223	0	1282	49	0
33	CI	1132	0	1218	25	1
33	DI	1132	0	1218	29	0
34	CJ	651	0	155	0	0
34	DJ	651	0	155	4	0
35	CM	1105	0	1180	34	0
35	DM	1105	0	1180	37	0
36	CN	933	0	996	23	0
36	DN	933	0	996	21	0
37	CO	1114	0	1187	84	0
37	DO	1114	0	1187	103	0
38	CP	1122	0	1179	26	0
38	DP	1122	0	1179	37	0
39	CQ	960	0	1021	30	0
39	DQ	960	0	1021	34	0
40	CR	771	0	832	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	DR	771	0	832	29	0
41	CS	1142	0	1202	79	0
41	DS	1142	0	1202	80	0
42	CT	958	0	1018	45	0
42	DT	958	0	1018	44	0
43	CU	779	0	852	44	0
43	DU	779	0	852	45	0
44	CW	896	0	953	22	0
45	CX	726	0	778	17	0
45	DX	726	0	778	19	0
46	CY	776	0	870	50	0
46	DY	776	0	868	60	0
47	CZ	1404	0	1432	34	0
47	DZ	1404	0	1432	23	0
48	Ca	662	0	688	0	0
48	Da	662	0	688	0	0
49	CH	734	0	808	16	0
49	DH	734	0	808	17	0
50	CK	598	0	653	11	0
50	DK	598	0	653	17	0
51	CL	468	0	523	9	0
51	DL	468	0	523	8	0
52	C5	226	0	229	2	0
52	D5	226	0	229	11	0
53	C6	459	0	478	13	0
53	D6	459	0	477	15	0
54	C7	381	0	390	17	0
54	D7	381	0	390	21	0
55	C8	419	0	467	8	0
55	D8	419	0	467	5	0
56	C9	508	0	576	36	0
56	D9	508	0	576	33	0
57	C0	299	0	326	4	0
57	D0	299	0	324	5	0
58	C1	60459	0	30486	641	0
58	D1	60459	0	30488	729	0
59	Cs	2551	0	1295	0	0
59	Ds	2551	0	1295	0	0
60	D2	416	0	215	8	0
61	D4	1623	0	825	46	0
62	DA	1155	0	757	14	0
63	DW	896	0	956	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
64	DV	1167	0	624	15	0
65	Ab	42	0	45	0	0
65	Bb	42	0	45	0	0
66	C1	24	0	20	5	0
66	D1	24	0	21	11	0
67	C1	1	0	0	0	0
67	D1	1	0	0	2	0
All	All	295910	0	199849	3935	1

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 9.

All (3935) 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)
61:D4:2:G:C2	61:D4:73:A:N3	1.85	1.31
58:C1:1331:A:O2'	58:C1:1333:U:OP2	1.54	1.25
58:D1:927:G:O2'	64:DV:19:G:C6	1.93	1.22
58:C1:2492:G:O2'	58:C1:2493:G:OP2	1.60	1.17
29:DC:132:HIS:ND1	58:D1:1704:C:OP1	1.79	1.16
25:C2:19:G:N1	58:C1:927:G:O2'	1.80	1.15
37:DO:58:THR:O	37:DO:61:ARG:NE	1.83	1.12
58:C1:26:G:N2	58:C1:536:G:HO2'	1.46	1.11
58:C1:26:G:N2	58:C1:536:G:O2'	1.82	1.09
1:A2:17:U:H2'	1:A2:18:G:H5''	1.33	1.05
58:D1:927:G:O2'	64:DV:19:G:N1	1.81	1.05
46:CY:79:CYS:SG	46:CY:80:GLY:N	2.30	1.05
28:DB:24:ILE:O	28:DB:25:THR:O	1.73	1.04
58:D1:2672:G:H2'	58:D1:2673:A:C2	1.94	1.02
41:CS:13:ARG:HA	41:CS:13:ARG:CZ	1.89	1.02
37:DO:58:THR:O	37:DO:61:ARG:CZ	2.08	1.00
41:CS:27:THR:O	41:CS:28:VAL:HG23	1.62	1.00
1:A2:16:A:H2'	1:A2:17:U:H5'	1.44	0.99
25:C3:75:C:O2'	25:C3:76:A:N7	1.92	0.99
29:CC:61:ARG:NH2	58:C1:2643:A:O2'	1.94	0.99
58:D1:2492:G:O2'	58:D1:2493:G:OP2	1.82	0.98
58:D1:1578:C:O2'	58:D1:1579:G:C2	2.17	0.98
58:C1:1377:G:N2	58:C1:1654:A:O2'	1.95	0.97
58:D1:2672:G:H2'	58:D1:2673:A:N3	1.79	0.97
35:CM:63:THR:OG1	58:C1:1185:U:OP2	1.81	0.96
58:D1:1331:A:O2'	58:D1:1333:U:OP2	1.83	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:D4:74:A:H5'	61:D4:75:C:H5'	1.45	0.95
55:D8:8:ASN:HD22	55:D8:8:ASN:C	1.68	0.95
4:BD:31:CYS:SG	4:BD:31:CYS:O	2.24	0.95
58:D1:2416:G:O2'	58:D1:2417:U:OP2	1.83	0.95
4:AD:9:CYS:SG	4:AD:31:CYS:O	2.26	0.94
44:CW:96:ILE:HD11	58:C1:2033:G:H4'	1.50	0.94
37:DO:59:LEU:HA	37:DO:61:ARG:NH1	1.83	0.94
58:C1:1346:A:O2'	58:C1:1347:A:H3'	1.68	0.92
56:C9:62:LEU:HD13	58:C1:230:G:H5''	1.52	0.90
39:DQ:11:ASN:OD1	39:DQ:12:ARG:N	2.06	0.89
35:DM:63:THR:OG1	58:D1:1185:U:OP2	1.90	0.89
58:D1:26:G:N2	58:D1:536:G:O2'	2.04	0.89
37:CO:50:ARG:NH1	58:C1:240:G:OP2	2.06	0.88
58:D1:2089:U:H3	58:D1:2441:A:H2	1.18	0.88
42:CT:58:ARG:NH1	58:C1:1200:A:OP2	2.06	0.88
58:C1:893:U:OP2	58:C1:973:G:O6	1.92	0.88
37:CO:58:THR:O	37:CO:61:ARG:CZ	2.23	0.87
58:D1:2666:G:O2'	58:D1:2667:U:OP2	1.91	0.87
56:D9:62:LEU:HD13	58:D1:230:G:H5''	1.53	0.87
58:D1:2475:C:O2'	58:D1:2476:C:O5'	1.93	0.87
45:DX:12:VAL:HG23	45:DX:13:LEU:H	1.40	0.86
25:C3:75:C:O3'	25:C3:76:A:H8	1.59	0.86
58:C1:2672:G:H2'	58:C1:2673:A:N3	1.90	0.85
29:CC:60:ASN:HB2	58:C1:2820:G:OP1	1.76	0.85
47:CZ:53:ILE:HG21	47:CZ:71:VAL:O	1.76	0.85
12:BL:60:LEU:HD23	12:BL:64:TYR:HB3	1.58	0.85
29:CC:132:HIS:ND1	58:C1:1704:C:OP1	2.10	0.85
39:CQ:11:ASN:OD1	39:CQ:12:ARG:N	2.08	0.85
31:CE:77:ILE:HG22	31:CE:80:PHE:H	1.38	0.85
46:CY:10:GLY:HA2	46:CY:27:VAL:HG13	1.58	0.85
42:DT:12:ARG:NH2	58:D1:1260:G:OP2	2.10	0.85
37:CO:58:THR:O	37:CO:61:ARG:NE	2.09	0.84
12:AL:32:PHE:HB3	12:AL:84:LEU:HD21	1.59	0.84
29:DC:132:HIS:CE1	58:D1:1704:C:OP1	2.28	0.84
41:DS:27:THR:O	41:DS:28:VAL:HG23	1.76	0.84
29:DC:132:HIS:HB3	58:D1:790:G:OP1	1.76	0.84
37:CO:63:PRO:HD2	58:C1:2405:C:OP1	1.78	0.84
37:CO:59:LEU:HA	37:CO:61:ARG:NH1	1.93	0.83
58:D1:2657:C:OP2	58:D1:2744:G:O2'	1.94	0.83
41:DS:50:ILE:HD11	41:DS:102:ILE:HD11	1.59	0.83
26:C4:5:G:O6	26:C4:69:C:N4	2.12	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:D1:1346:A:O2'	58:D1:1347:A:H2'	1.78	0.83
58:D1:2338:A:H2'	58:D1:2339:A:C8	2.12	0.83
42:DT:12:ARG:HH21	58:D1:1260:G:P	2.02	0.83
58:C1:2596:U:H5''	58:C1:2596:U:O2	1.78	0.83
58:D1:69:A:C8	58:D1:69:A:H5'	2.14	0.83
61:D4:17:C:H2'	61:D4:18:U:C6	2.13	0.83
30:CD:22:ALA:HB1	30:CD:26:ALA:HB2	1.61	0.83
58:D1:1377:G:N2	58:D1:1654:A:O2'	2.11	0.83
25:C3:75:C:O3'	25:C3:76:A:C8	2.32	0.82
35:DM:63:THR:HG21	58:D1:1185:U:H2'	1.58	0.82
58:D1:2492:G:HO2'	58:D1:2493:G:P	2.02	0.82
16:BP:53:VAL:HG12	16:BP:79:VAL:HG22	1.59	0.82
14:BN:48:ALA:HB2	14:BN:53:LEU:HD12	1.61	0.82
31:CE:109:VAL:O	31:CE:113:ARG:HG3	1.79	0.82
43:DU:19:LYS:HB3	43:DU:94:LEU:O	1.78	0.82
58:C1:2492:G:HO2'	58:C1:2493:G:P	2.02	0.82
30:CD:66:PRO:O	30:CD:67:GLN:HB3	1.78	0.82
58:D1:1346:A:O2'	58:D1:1347:A:C2'	2.28	0.82
58:C1:1875:G:H2'	58:C1:1876:G:H5'	1.61	0.82
25:C2:19:G:C6	58:C1:927:G:O2'	2.32	0.82
39:DQ:10:LEU:HB3	39:DQ:17:ARG:NE	1.94	0.82
37:DO:64:LYS:O	37:DO:66:GLY:N	2.12	0.82
12:BL:47:LYS:HB3	12:BL:48:PRO:HD3	1.61	0.82
58:C1:1424:A:O2'	58:C1:1425:G:OP1	1.97	0.82
46:DY:52:SER:O	46:DY:54:LYS:N	2.13	0.82
1:A2:16:A:C2'	1:A2:17:U:H5'	2.10	0.81
58:C1:1160:G:H2'	58:C1:1161:C:C6	2.15	0.81
56:D9:46:ARG:NH2	58:D1:655:A:OP2	2.11	0.81
58:C1:138:A:C8	58:C1:1453:C:O2'	2.33	0.81
28:DB:44:ASN:HB3	28:DB:49:ILE:HA	1.61	0.81
10:AJ:48:THR:HA	10:AJ:62:HIS:HB3	1.62	0.81
31:DE:113:ARG:NH1	52:D5:61:VAL:O	2.12	0.81
58:C1:1346:A:HO2'	58:C1:1347:A:H3'	1.45	0.81
25:C3:48:C:O2'	25:C3:49:C:P	2.39	0.81
37:DO:63:PRO:HD2	58:D1:2405:C:OP1	1.79	0.81
41:DS:3:ARG:NE	58:D1:2885:G:H4'	1.95	0.81
58:D1:1549:C:O2'	58:D1:1550:C:H5'	1.80	0.81
58:D1:1549:C:O2'	58:D1:1550:C:C5'	2.29	0.81
45:DX:44:GLU:OE1	58:D1:136:G:N2	2.13	0.80
58:D1:927:G:O2'	64:DV:19:G:O6	1.98	0.80
49:CH:29:GLY:O	49:CH:30:VAL:HG22	1.81	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:CQ:90:ARG:NH1	58:C1:2889:C:O2'	2.13	0.80
26:C4:35:C:O2'	26:C4:36:A:O5'	2.00	0.80
58:D1:2479:G:HO2'	58:D1:2487:A:H8	1.28	0.80
28:CB:35:LYS:HE2	28:CB:36:PRO:HB3	1.63	0.80
25:D3:34:G:C6	25:D3:35:A:C5	2.70	0.80
24:BC:50:ALA:HB1	24:BC:70:VAL:HG11	1.63	0.80
58:D1:1064:U:HO2'	58:D1:1066:A:H2	1.26	0.80
42:CT:90:VAL:O	42:CT:92:ARG:N	2.14	0.79
3:AC:37:GLN:NE2	14:AN:52:GLN:OE1	2.15	0.79
41:CS:88:ILE:HG22	41:CS:89:VAL:HG23	1.64	0.79
58:D1:1920:G:N2	58:D1:1923:C:H41	1.80	0.79
28:CB:35:LYS:HG2	28:CB:63:ARG:HG3	1.64	0.79
58:D1:1441:U:H2'	58:D1:1441:U:O2	1.79	0.79
25:D3:34:G:C6	25:D3:35:A:C6	2.70	0.79
30:CD:83:PHE:O	30:CD:85:GLY:N	2.15	0.79
43:DU:72:VAL:HG23	43:DU:85:LYS:HB3	1.63	0.79
61:D4:74:A:C5'	61:D4:75:C:H5'	2.13	0.79
42:DT:50:ARG:NH2	58:D1:1038:G:OP1	2.16	0.79
58:D1:1920:G:H22	58:D1:1923:C:H41	1.26	0.79
58:C1:2475:C:O2'	58:C1:2476:C:O5'	2.00	0.78
41:CS:119:LYS:HD2	58:C1:2873:G:OP1	1.83	0.78
42:DT:90:VAL:O	42:DT:92:ARG:N	2.17	0.78
58:D1:2084:C:H2'	58:D1:2085:C:H5'	1.65	0.78
54:C7:33:LYS:HA	54:C7:33:LYS:HE2	1.65	0.78
46:DY:76:CYS:HB3	46:DY:96:ILE:HD11	1.65	0.78
58:C1:1346:A:H4'	58:C1:1347:A:OP1	1.83	0.78
42:DT:15:LYS:NZ	58:D1:1261:C:OP2	2.15	0.78
61:D4:2:G:N1	61:D4:73:A:N3	2.14	0.78
58:C1:2492:G:O2'	58:C1:2493:G:P	2.41	0.78
58:C1:2672:G:H2'	58:C1:2673:A:C2	2.19	0.78
25:C3:8:U:H1'	25:C3:48:C:C2	2.18	0.78
42:CT:23:GLY:HA2	58:C1:17:C:O3'	1.84	0.78
41:DS:3:ARG:CD	58:D1:2885:G:H4'	2.14	0.78
58:D1:69:A:H5'	58:D1:69:A:H8	1.47	0.78
50:DK:7:ARG:NH2	58:D1:99:G:OP2	2.17	0.78
29:DC:61:ARG:NH2	58:D1:2643:A:O2'	2.17	0.78
41:DS:16:ARG:NH1	41:DS:19:LEU:HD21	1.99	0.78
11:BK:99:GLN:HG2	11:BK:105:VAL:HG21	1.65	0.77
35:CM:2:LYS:O	35:CM:4:TYR:CZ	2.37	0.77
40:DR:89:ARG:O	40:DR:92:TYR:HB3	1.84	0.77
58:C1:552:A:O2'	58:C1:553:A:H5'	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:DS:88:ILE:HG22	41:DS:89:VAL:HG23	1.65	0.77
12:BL:71:PRO:O	12:BL:102:ARG:NH1	2.17	0.77
28:CB:44:ASN:HB3	28:CB:49:ILE:HA	1.65	0.77
58:D1:2492:G:O2'	58:D1:2493:G:P	2.42	0.77
58:D1:1345:U:O2'	58:D1:1671:G:C2	2.37	0.77
58:D1:2120:U:O2	58:D1:2120:U:H2'	1.84	0.77
25:D3:34:G:O6	25:D3:35:A:C6	2.38	0.77
37:DO:107:LYS:O	37:DO:109:GLY:N	2.17	0.77
41:DS:13:ARG:HA	41:DS:13:ARG:CZ	2.15	0.77
41:DS:129:ARG:CZ	41:DS:131:ALA:HB3	2.15	0.77
57:C0:14:CYS:HG	57:C0:27:CYS:HG	1.30	0.77
25:D3:34:G:C2	25:D3:35:A:C4	2.72	0.77
30:DD:132:VAL:HG22	30:DD:133:ASN:H	1.49	0.77
37:DO:25:SER:HB2	58:D1:858:C:H5'	1.67	0.76
58:C1:1920:G:N2	58:C1:1923:C:H41	1.84	0.76
26:C4:61:U:H5''	26:C4:62:C:H5	1.50	0.76
32:DF:41:MET:HE2	32:DF:43:VAL:HG13	1.65	0.76
29:CC:132:HIS:HB3	58:C1:790:G:OP1	1.85	0.76
58:D1:276:G:O2'	58:D1:277:G:OP2	2.03	0.76
46:DY:17:SER:O	58:D1:333:A:OP1	2.04	0.76
13:BM:65:LYS:HA	13:BM:66:LEU:HB2	1.67	0.76
58:C1:2479:G:N2	58:C1:2492:G:O2'	2.19	0.76
53:D6:43:HIS:CD2	58:D1:2824:C:O2'	2.39	0.76
53:D6:3:LYS:O	53:D6:4:HIS:C	2.23	0.76
5:BE:100:VAL:HG12	5:BE:118:ILE:CG2	2.16	0.75
53:C6:13:LYS:HE2	58:C1:541:C:OP2	1.85	0.75
37:CO:16:ARG:HD3	37:CO:18:ARG:H	1.49	0.75
29:DC:130:GLY:O	29:DC:131:ALA:O	2.04	0.75
30:CD:169:ASN:HD21	58:C1:345:A:H3'	1.50	0.75
58:D1:1539:A:H2'	58:D1:1540:A:H5''	1.67	0.75
37:DO:23:PRO:HB2	37:DO:33:ARG:CD	2.16	0.75
30:CD:101:LEU:O	30:CD:106:ARG:NH1	2.20	0.75
38:CP:1:MET:O	38:CP:2:LEU:HB2	1.85	0.75
55:D8:8:ASN:ND2	55:D8:8:ASN:C	2.40	0.75
38:DP:16:ARG:NH2	58:D1:997:A:OP2	2.19	0.75
15:AO:23:GLY:O	15:AO:24:SER:HB3	1.86	0.75
58:D1:185:A:H5'	58:D1:185:A:C8	2.21	0.75
63:DW:64:MET:O	63:DW:65:LEU:HB3	1.84	0.75
37:CO:64:LYS:O	37:CO:66:GLY:N	2.18	0.75
25:D3:34:G:N1	25:D3:35:A:C4	2.54	0.75
58:D1:1346:A:HO2'	58:D1:1347:A:C2'	1.99	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AE:68:GLU:HG3	5:AE:68:GLU:O	1.86	0.75
19:BT:40:ILE:HG21	19:BT:62:ILE:HD11	1.69	0.75
41:CS:27:THR:OG1	41:CS:28:VAL:N	2.20	0.75
58:D1:1346:A:O2'	58:D1:1347:A:H3'	1.87	0.75
53:C6:41:PRO:O	53:C6:44:THR:OG1	2.00	0.74
58:C1:1908:C:H2'	58:C1:1909:G:H5'	1.69	0.74
58:D1:154:C:H3'	58:D1:157:U:P	2.27	0.74
39:DQ:9:LYS:O	39:DQ:10:LEU:HD23	1.87	0.74
37:DO:38:GLN:HG3	37:DO:39:LYS:H	1.53	0.74
4:BD:26:CYS:HA	4:BD:31:CYS:HB2	1.70	0.73
28:DB:259:THR:HG22	58:D1:1828:U:H5'	1.68	0.73
58:C1:659:C:O2'	58:C1:663:U:OP1	2.05	0.73
46:DY:76:CYS:SG	46:DY:77:PRO:CD	2.77	0.73
58:D1:158:U:H4'	58:D1:159:G:C8	2.22	0.73
31:DE:71:THR:HG21	58:D1:2323:U:O2'	1.88	0.73
16:BP:28:ARG:HG2	16:BP:29:ASP:OD2	1.88	0.73
33:CI:109:ILE:HG22	33:CI:130:TYR:CZ	2.22	0.73
53:D6:3:LYS:O	53:D6:4:HIS:O	2.06	0.73
28:DB:134:ARG:HG3	28:DB:135:PHE:CD1	2.23	0.73
39:DQ:117:VAL:O	39:DQ:118:GLU:HB2	1.88	0.73
58:D1:185:A:H5'	58:D1:185:A:H8	1.54	0.73
28:CB:11:PRO:O	28:CB:13:ARG:N	2.20	0.73
37:CO:48:PRO:O	37:CO:50:ARG:N	2.22	0.73
3:AC:73:PRO:O	3:AC:76:VAL:HG22	1.90	0.72
28:CB:242:ARG:NH2	58:C1:1856:G:H4'	2.04	0.72
58:C1:267:G:O2'	58:C1:268:G:OP2	2.06	0.72
41:CS:28:VAL:O	41:CS:29:ARG:HB2	1.87	0.72
58:D1:894:G:H2'	58:D1:895:A:C8	2.24	0.72
56:C9:61:LEU:HD12	56:C9:62:LEU:H	1.54	0.72
58:D1:1809:U:H5	58:D1:1814:A:N7	1.87	0.72
11:BK:54:ARG:O	11:BK:57:THR:HG22	1.87	0.72
54:C7:16:CYS:SG	54:C7:48:VAL:HG22	2.29	0.72
58:D1:1346:A:O2'	58:D1:1347:A:C3'	2.38	0.72
25:D3:66:U:H2'	25:D3:67:C:C6	2.25	0.72
29:DC:120:TRP:CD2	29:DC:155:LYS:HD3	2.24	0.72
41:CS:13:ARG:HA	41:CS:13:ARG:NH1	2.04	0.72
19:BT:22:LEU:O	19:BT:26:GLY:HA2	1.90	0.72
37:DO:23:PRO:HB2	37:DO:33:ARG:HD2	1.71	0.72
43:CU:62:LEU:HD21	43:CU:95:LEU:HB2	1.71	0.72
58:C1:1539:A:H2'	58:C1:1540:A:H5''	1.71	0.72
42:CT:83:LEU:HD12	42:CT:88:ILE:HD11	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:DM:62:VAL:HG22	35:DM:66:LYS:HD2	1.71	0.72
41:DS:16:ARG:HH12	41:DS:19:LEU:HD21	1.53	0.72
9:BI:104:ARG:O	9:BI:105:ASP:HB2	1.90	0.72
43:CU:19:LYS:HG3	43:CU:20:LEU:O	1.90	0.72
37:DO:33:ARG:HD3	58:D1:609:C:C5	2.25	0.72
58:D1:7:A:H2'	58:D1:8:U:C5	2.24	0.72
32:DF:156:ALA:O	32:DF:157:TYR:C	2.29	0.72
58:C1:138:A:H8	58:C1:1453:C:O2'	1.71	0.71
58:C1:1920:G:H22	58:C1:1923:C:H41	1.35	0.71
25:C3:48:C:O2'	25:C3:49:C:OP1	2.05	0.71
37:DO:6:LEU:HG	37:DO:8:PRO:O	1.90	0.71
28:DB:44:ASN:HB2	28:DB:48:ARG:O	1.90	0.71
46:DY:27:VAL:HG12	46:DY:29:GLU:OE1	1.88	0.71
1:A2:17:U:H2'	1:A2:18:G:C5'	2.18	0.71
30:DD:8:GLN:HB3	30:DD:126:VAL:HA	1.71	0.71
43:DU:46:VAL:HG13	43:DU:47:VAL:N	2.05	0.71
26:C4:12:G:H1'	58:C1:1944:U:O2'	1.89	0.71
43:CU:19:LYS:HB3	43:CU:94:LEU:O	1.91	0.71
58:D1:644:G:H5''	58:D1:644:G:N3	2.05	0.71
28:DB:238:GLY:O	28:DB:239:ARG:HB3	1.91	0.71
58:C1:2083:A:H5''	58:C1:2083:A:C4	2.25	0.71
58:D1:1539:A:N3	58:D1:1539:A:H5'	2.06	0.71
31:DE:86:MET:N	31:DE:87:PRO:HD2	2.06	0.71
4:AD:28:SER:HB3	4:AD:29:PRO:CD	2.21	0.71
46:DY:76:CYS:SG	46:DY:77:PRO:HD2	2.30	0.71
58:D1:2782:G:H5''	58:D1:2783:C:OP2	1.91	0.71
33:DI:94:ALA:CB	33:DI:114:LEU:HD11	2.20	0.71
35:DM:28:THR:HG21	58:D1:1057:U:O4	1.89	0.71
25:D3:64:A:H2'	25:D3:65:G:C8	2.26	0.71
28:CB:238:GLY:O	28:CB:239:ARG:HB3	1.91	0.70
58:D1:1171:A:OP1	58:D1:1171:A:H8	1.73	0.70
32:DF:156:ALA:O	32:DF:158:HIS:N	2.24	0.70
58:C1:2450:A:OP1	66:C1:3001:3V6:N	2.23	0.70
49:CH:44:PRO:O	49:CH:46:LEU:HD13	1.90	0.70
43:CU:19:LYS:HG3	43:CU:20:LEU:N	2.04	0.70
58:D1:2902:G:N3	58:D1:2902:G:H2'	2.04	0.70
4:BD:25:ARG:O	4:BD:27:TYR:N	2.24	0.70
58:C1:1254:A:H5''	58:C1:1256:G:O4'	1.90	0.70
46:DY:74:PRO:O	46:DY:80:GLY:HA2	1.90	0.70
4:AD:30:LYS:C	4:AD:32:ALA:H	1.92	0.70
58:C1:722:A:H8	58:C1:2090:G:H21	1.40	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:DO:62:LEU:HB3	58:D1:2404:A:H5'	1.74	0.70
41:CS:2:ASN:O	58:C1:2885:G:OP1	2.10	0.70
26:C4:4:G:O2'	26:C4:5:G:O5'	2.09	0.70
31:DE:71:THR:CG2	58:D1:2323:U:O2'	2.40	0.70
49:DH:90:ILE:HG22	49:DH:94:LEU:HD12	1.71	0.70
38:CP:14:ARG:NH1	58:C1:1002:U:OP2	2.24	0.70
25:C3:1:G:O6	25:C3:72:C:N4	2.25	0.70
58:D1:2802:A:N3	58:D1:2802:A:H2'	2.06	0.70
31:DE:47:LYS:HA	31:DE:88:ILE:HD13	1.74	0.70
53:C6:3:LYS:O	53:C6:4:HIS:O	2.09	0.70
28:CB:30:GLU:HB3	28:CB:35:LYS:HG3	1.74	0.70
56:D9:4:MET:HE2	58:D1:615:G:H1'	1.73	0.69
46:DY:88:LYS:O	46:DY:90:LEU:HD23	1.90	0.69
40:CR:97:ARG:HH21	40:CR:98:VAL:HA	1.57	0.69
56:D9:51:ALA:C	56:D9:53:PRO:HD2	2.12	0.69
35:DM:90:MET:O	35:DM:93:THR:O	2.09	0.69
56:C9:46:ARG:NH2	58:C1:655:A:OP2	2.25	0.69
25:C3:39:U:H4'	25:C3:39:U:OP1	1.91	0.69
28:CB:242:ARG:HH21	58:C1:1856:G:H4'	1.56	0.69
58:D1:8:U:C5	58:D1:2640:A:N6	2.60	0.69
40:CR:97:ARG:NH2	40:CR:98:VAL:HA	2.06	0.69
58:D1:138:A:H8	58:D1:1453:C:HO2'	1.41	0.69
58:D1:154:C:C3'	58:D1:157:U:P	2.80	0.69
38:DP:135:ASP:O	38:DP:138:ASP:OD2	2.09	0.69
58:C1:2323:U:H2'	58:C1:2324:C:H5'	1.73	0.69
46:DY:17:SER:OG	46:DY:18:GLY:N	2.20	0.69
37:DO:35:HIS:CE1	58:D1:1235:G:OP1	2.45	0.69
37:DO:47:ASP:HB3	37:DO:48:PRO:O	1.93	0.69
26:C4:17:C:N3	26:C4:18:U:C4	2.60	0.69
41:CS:80:SER:HB3	41:CS:81:PRO:HD3	1.75	0.69
58:D1:1498:C:N3	58:D1:1505:G:O6	2.26	0.69
28:DB:181:GLU:HA	28:DB:272:ALA:HB3	1.74	0.69
50:CK:13:ALA:HA	50:CK:16:LEU:HD12	1.75	0.69
46:DY:98:VAL:O	46:DY:99:CYS:SG	2.51	0.69
58:D1:1538:C:C4	58:D1:2226:G:O2'	2.46	0.68
61:D4:74:A:H5'	61:D4:75:C:C5'	2.21	0.68
37:DO:17:LYS:O	37:DO:19:VAL:N	2.26	0.68
36:CN:88:ASN:O	36:CN:91:LEU:N	2.25	0.68
58:D1:2692:C:H5	58:D1:2737:A:H62	1.41	0.68
2:BA:88:ALA:HB2	2:BA:219:VAL:HG13	1.75	0.68
58:C1:1908:C:C2'	58:C1:1909:G:H5'	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:CD:101:LEU:HD12	30:CD:102:PRO:HD2	1.73	0.68
41:DS:89:VAL:HG12	41:DS:91:ARG:HG3	1.76	0.68
23:B2:20:U:H2'	23:B2:21:C:C6	2.28	0.68
41:CS:50:ILE:HD11	41:CS:102:ILE:HD11	1.75	0.68
32:DF:20:ALA:HB1	32:DF:21:PRO:CD	2.24	0.68
4:BD:25:ARG:C	4:BD:27:TYR:H	1.97	0.68
4:BD:8:VAL:O	4:BD:10:ARG:N	2.27	0.68
19:BT:6:LYS:HG2	19:BT:7:LYS:HE3	1.76	0.68
56:C9:2:PRO:HA	58:C1:613:C:O2	1.92	0.68
38:CP:42:ILE:HD13	38:CP:97:VAL:CG2	2.24	0.68
33:CI:78:THR:HA	33:CI:141:LYS:O	1.94	0.68
58:D1:1336:C:H2'	58:D1:1337:U:C6	2.29	0.68
58:D1:1652:C:H4'	58:D1:1653:A:O5'	1.93	0.68
61:D4:17:C:C6	61:D4:18:U:C4	2.82	0.68
37:CO:33:ARG:HD3	58:C1:609:C:C5	2.29	0.68
47:CZ:54:HIS:HB3	47:CZ:101:PRO:HD3	1.76	0.68
58:D1:1850:U:H4'	58:D1:1851:A:OP2	1.94	0.68
41:DS:102:ILE:HB	41:DS:110:ILE:CD1	2.24	0.68
58:C1:1809:U:H5	58:C1:1814:A:N7	1.92	0.67
58:C1:2535:G:H5''	58:C1:2535:G:H8	1.59	0.67
58:C1:2782:G:H5''	58:C1:2783:C:OP2	1.93	0.67
37:CO:59:LEU:HA	37:CO:61:ARG:HH11	1.56	0.67
58:C1:644:G:N3	58:C1:644:G:H5''	2.10	0.67
26:C4:51:U:C2	26:C4:52:C:C5	2.82	0.67
58:D1:2192:A:O2'	58:D1:2193:U:O4'	2.11	0.67
58:D1:841:C:H2'	58:D1:842:C:H6	1.60	0.67
35:DM:55:VAL:HG22	35:DM:126:PRO:HA	1.76	0.67
4:AD:28:SER:HB3	4:AD:29:PRO:HD2	1.77	0.67
45:CX:12:VAL:HG13	45:CX:27:THR:O	1.94	0.67
10:BJ:40:LEU:HB2	10:BJ:69:ASN:HB2	1.76	0.67
29:CC:61:ARG:HD3	58:C1:2799:C:O2'	1.95	0.67
30:DD:67:GLN:HG3	30:DD:67:GLN:O	1.95	0.67
4:AD:30:LYS:C	4:AD:32:ALA:N	2.46	0.67
12:AL:90:VAL:O	12:AL:92:ASP:N	2.27	0.67
58:D1:2050:G:H2'	58:D1:2052:A:OP2	1.94	0.67
58:D1:1059:U:C2'	58:D1:1060:G:H5'	2.25	0.67
37:DO:16:ARG:O	58:D1:707:C:O2'	2.11	0.67
6:BF:50:TYR:OH	18:BS:74:ARG:O	2.10	0.67
66:C1:3001:3V6:C	66:C1:3001:3V6:CLI	2.79	0.67
28:CB:209:ALA:C	28:CB:210:GLY:O	2.29	0.67
37:CO:23:PRO:HB2	37:CO:33:ARG:HD2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:CO:58:THR:HG22	37:CO:58:THR:O	1.95	0.67
39:DQ:3:HIS:HB2	58:D1:1700:A:P	2.35	0.67
30:DD:9:ILE:HG23	30:DD:11:VAL:O	1.95	0.67
45:DX:18:TYR:O	45:DX:20:GLY:N	2.28	0.67
42:CT:92:ARG:NH2	58:C1:1041:A:OP2	2.27	0.67
58:C1:1549:C:O2'	58:C1:1550:C:O5'	2.13	0.67
35:CM:45:ASN:H	35:CM:45:ASN:HD22	1.43	0.67
58:D1:2089:U:N3	58:D1:2441:A:H2	1.91	0.67
41:DS:38:ASN:HD22	41:DS:40:THR:H	1.42	0.67
56:D9:4:MET:HE2	58:D1:615:G:C1'	2.25	0.67
41:DS:29:ARG:CB	41:DS:85:LYS:HA	2.25	0.67
4:AD:8:VAL:C	4:AD:10:ARG:H	1.98	0.67
16:BP:20:VAL:HG21	16:BP:32:TYR:CD1	2.30	0.67
26:C4:61:U:H5''	26:C4:62:C:C5	2.29	0.67
37:DO:81:GLN:HG2	37:DO:106:LEU:HA	1.77	0.67
41:DS:13:ARG:NH1	41:DS:13:ARG:HA	2.10	0.67
58:C1:2338:A:H2'	58:C1:2339:A:C8	2.30	0.66
36:CN:4:PRO:O	36:CN:5:GLN:HB2	1.94	0.66
58:D1:26:G:N2	58:D1:536:G:HO2'	1.93	0.66
11:BK:86:GLY:N	11:BK:112:THR:OG1	2.26	0.66
30:CD:66:PRO:O	30:CD:67:GLN:CB	2.42	0.66
58:D1:1059:U:H2'	58:D1:1060:G:H5'	1.78	0.66
58:D1:355:A:O2'	58:D1:357:C:OP2	2.12	0.66
40:DR:74:ALA:HB1	40:DR:103:GLU:HB3	1.77	0.66
58:D1:2001:G:O2'	58:D1:2003:C:OP2	2.12	0.66
58:D1:2671:A:H5'	58:D1:2672:G:C2	2.29	0.66
46:CY:66:PRO:O	46:CY:67:LEU:HB3	1.95	0.66
58:D1:2416:G:HO2'	58:D1:2417:U:P	2.15	0.66
39:DQ:10:LEU:HD22	39:DQ:17:ARG:HD2	1.77	0.66
28:CB:181:GLU:HA	28:CB:272:ALA:HB3	1.77	0.66
31:CE:32:PRO:HB3	31:CE:163:ALA:HB2	1.76	0.66
31:DE:128:ARG:O	31:DE:129:GLY:O	2.14	0.66
58:C1:906:U:H5	58:C1:962:A:N7	1.93	0.66
29:CC:77:ILE:HG22	29:CC:78:LEU:HD12	1.76	0.66
44:CW:65:LEU:HD23	44:CW:68:ARG:HD2	1.78	0.66
46:CY:42:VAL:HB	46:CY:65:ALA:HB3	1.78	0.66
58:D1:1538:C:N4	58:D1:2226:G:O2'	2.29	0.66
58:D1:1777:G:H2'	58:D1:1778:G:H5'	1.78	0.66
35:DM:2:LYS:O	35:DM:4:TYR:CZ	2.48	0.66
58:C1:2226:G:H21	58:C1:2227:G:H4'	1.60	0.66
58:C1:2319:G:N7	58:C1:2321:A:O5'	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:CD:24:LEU:HB3	30:CD:25:PRO:HD2	1.77	0.66
5:AE:10:MET:HB2	5:AE:32:VAL:HG22	1.77	0.66
10:BJ:48:THR:HA	10:BJ:62:HIS:HB3	1.78	0.66
25:C3:20:U:H2'	25:C3:21:A:H4'	1.77	0.66
54:C7:51:GLU:O	54:C7:52:VAL:HG23	1.94	0.66
30:CD:22:ALA:HB1	30:CD:26:ALA:CB	2.25	0.66
39:CQ:9:LYS:O	39:CQ:10:LEU:HD23	1.95	0.66
58:D1:2083:A:H2'	58:D1:2084:C:O5'	1.96	0.66
30:DD:9:ILE:CG2	30:DD:11:VAL:O	2.44	0.66
12:BL:24:VAL:O	12:BL:24:VAL:HG12	1.95	0.66
26:C4:51:U:H2'	26:C4:52:C:C6	2.31	0.66
37:CO:23:PRO:HB2	37:CO:33:ARG:CD	2.26	0.66
25:C3:25:C:H2'	25:C3:26:A:H8	1.61	0.66
41:CS:12:SER:O	41:CS:13:ARG:NH2	2.29	0.66
37:DO:63:PRO:CD	58:D1:2405:C:OP1	2.44	0.66
58:D1:2611:A:O3'	66:D1:3001:3V6:H19	1.95	0.66
40:DR:28:VAL:HB	40:DR:89:ARG:HD2	1.78	0.66
63:DW:9:TYR:H	63:DW:102:HIS:HD2	1.42	0.66
58:C1:2732:U:O2	58:C1:2732:U:H2'	1.96	0.65
37:DO:55:ARG:NH1	58:D1:879:U:O2	2.29	0.65
53:D6:41:PRO:O	53:D6:44:THR:OG1	2.12	0.65
28:DB:24:ILE:HA	28:DB:82:ILE:HG22	1.76	0.65
11:BK:73:MET:O	11:BK:76:GLY:N	2.29	0.65
19:BT:6:LYS:HG2	19:BT:7:LYS:CE	2.27	0.65
58:C1:2209:C:H2'	58:C1:2210:U:C1'	2.26	0.65
30:CD:53:THR:HG22	30:CD:56:GLU:OE2	1.96	0.65
28:DB:62:TYR:CE2	58:D1:1846:G:N7	2.65	0.65
61:D4:48:U:H3'	61:D4:49:C:H5'	1.78	0.65
49:DH:56:GLN:HA	49:DH:56:GLN:HE21	1.60	0.65
37:DO:106:LEU:HD13	37:DO:112:LEU:HD23	1.78	0.65
39:CQ:10:LEU:HB3	39:CQ:17:ARG:NE	2.12	0.65
35:DM:38:HIS:O	42:DT:67:ALA:HB1	1.96	0.65
42:DT:92:ARG:NE	58:D1:1041:A:H4'	2.11	0.65
58:D1:2057:C:H5'	58:D1:2057:C:H6	1.60	0.65
58:D1:629:U:H3	58:D1:645:A:H2	1.45	0.65
10:BJ:90:LEU:N	10:BJ:91:PRO:HD3	2.11	0.65
28:CB:65:ILE:HD11	28:CB:67:PHE:CE2	2.31	0.65
56:D9:2:PRO:HB3	58:D1:613:C:O2	1.95	0.65
42:DT:58:ARG:NH1	58:D1:1200:A:OP2	2.30	0.65
13:BM:32:GLU:O	13:BM:36:LYS:HG2	1.97	0.65
35:DM:43:THR:HB	35:DM:46:VAL:HG12	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:DO:146:VAL:HG22	37:DO:147:LEU:H	1.60	0.65
58:C1:1309:G:H3'	58:C1:1310:A:H5''	1.79	0.65
58:C1:2089:U:H3	58:C1:2441:A:H2	1.45	0.65
37:CO:18:ARG:HD2	58:C1:708:G:OP1	1.97	0.65
58:D1:1254:A:H8	58:D1:1254:A:H5'	1.61	0.65
58:D1:2479:G:O2'	58:D1:2487:A:C8	2.48	0.65
29:DC:144:ARG:CD	58:D1:2583:A:C8	2.80	0.65
28:DB:65:ILE:HD11	28:DB:67:PHE:CE2	2.32	0.65
8:BH:103:VAL:HG21	8:BH:110:ALA:HB2	1.78	0.65
58:C1:91:C:H5'	58:C1:92:G:OP2	1.97	0.65
25:C2:43:C:OP1	25:C2:43:C:H4'	1.97	0.65
28:DB:244:ARG:HG3	58:D1:1923:C:H1'	1.77	0.65
28:CB:44:ASN:HB2	28:CB:48:ARG:O	1.97	0.65
58:C1:139:A:C8	58:C1:1453:C:H1'	2.32	0.65
31:CE:73:ALA:N	31:CE:87:PRO:HG3	2.11	0.65
42:CT:112:ARG:O	42:CT:115:ALA:HB3	1.97	0.65
30:DD:51:THR:HB	30:DD:88:VAL:HG11	1.78	0.65
37:DO:35:HIS:CE1	58:D1:985:A:O2'	2.50	0.65
4:AD:49:ARG:HE	4:AD:49:ARG:HA	1.62	0.64
41:CS:28:VAL:O	41:CS:29:ARG:CB	2.45	0.64
58:C1:267:G:O2'	58:C1:268:G:P	2.55	0.64
37:CO:47:ASP:HB3	37:CO:48:PRO:O	1.97	0.64
46:CY:27:VAL:HG12	46:CY:29:GLU:OE1	1.98	0.64
58:D1:1336:C:H2'	58:D1:1337:U:H6	1.62	0.64
58:D1:2318:G:OP1	58:D1:2318:G:H4'	1.96	0.64
25:D3:39:U:OP1	25:D3:39:U:H4'	1.96	0.64
62:DA:56:GLN:HE22	62:DA:168:UNK:CB	2.11	0.64
58:C1:2412:U:H2'	58:C1:2413:C:H5''	1.78	0.64
58:D1:2083:A:C2'	58:D1:2084:C:O5'	2.45	0.64
32:DF:153:LYS:H	32:DF:153:LYS:HD3	1.62	0.64
4:AD:128:VAL:O	4:AD:130:GLY:N	2.31	0.64
5:AE:100:VAL:HG12	5:AE:118:ILE:HG22	1.78	0.64
26:C4:16:C:O2'	26:C4:61:U:O3'	2.14	0.64
28:CB:121:PRO:HB3	28:CB:135:PHE:CE2	2.33	0.64
37:CO:64:LYS:HD2	56:C9:25:MET:SD	2.38	0.64
39:CQ:10:LEU:HD22	39:CQ:17:ARG:CD	2.27	0.64
44:CW:9:TYR:H	44:CW:102:HIS:HD2	1.43	0.64
4:AD:12:CYS:SG	4:AD:19:LEU:O	2.56	0.64
24:BC:70:VAL:HG12	24:BC:72:LYS:H	1.62	0.64
37:CO:67:MET:N	58:C1:2426:G:H4'	2.13	0.64
13:BM:106:ASN:O	13:BM:107:ALA:HB3	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:C1:2722:A:OP1	58:C1:2724:A:OP1	2.16	0.64
53:D6:2:ALA:N	58:D1:2036:A:N3	2.46	0.64
39:DQ:2:ARG:NH2	58:D1:2736:C:OP2	2.30	0.64
58:D1:1625:A:H2'	58:D1:1626:A:C8	2.33	0.64
58:D1:2479:G:O2'	58:D1:2487:A:H8	1.80	0.64
36:DN:4:PRO:O	36:DN:5:GLN:HB2	1.96	0.64
37:DO:50:ARG:NH1	58:D1:240:G:OP2	2.31	0.64
54:D7:11:LEU:HD21	54:D7:51:GLU:HB2	1.80	0.64
30:DD:89:VAL:O	30:DD:91:GLY:N	2.29	0.64
58:C1:2613:A:H4'	58:C1:2613:A:OP2	1.97	0.64
38:CP:16:ARG:HH22	58:C1:996:G:P	2.21	0.64
32:DF:43:VAL:HG11	32:DF:52:VAL:HG22	1.78	0.64
35:DM:15:LEU:HD13	35:DM:16:ILE:N	2.12	0.64
13:AM:65:LYS:HA	13:AM:66:LEU:HB2	1.80	0.64
58:D1:1475:C:H2'	58:D1:1476:U:C6	2.33	0.64
58:D1:2054:A:H4'	58:D1:2055:U:OP1	1.98	0.64
58:D1:2054:A:O2'	58:D1:2056:G:OP2	2.16	0.64
56:D9:33:ASN:O	58:D1:2431:C:OP1	2.16	0.64
58:C1:2083:A:H5''	58:C1:2083:A:N3	2.13	0.63
58:D1:1895:G:H5'	58:D1:1896:C:OP2	1.98	0.63
6:BF:60:PHE:C	6:BF:61:LEU:HD12	2.17	0.63
58:C1:2269:C:H4'	58:C1:2270:G:OP2	1.97	0.63
39:DQ:3:HIS:HB2	58:D1:1700:A:OP2	1.98	0.63
41:DS:28:VAL:O	41:DS:29:ARG:HD3	1.97	0.63
58:C1:1984:U:H2'	58:C1:1984:U:O2	1.97	0.63
58:D1:154:C:O4'	58:D1:154:C:O2	2.13	0.63
58:D1:1765:G:C2	58:D1:1767:U:OP2	2.51	0.63
28:DB:134:ARG:HG3	28:DB:135:PHE:CE1	2.32	0.63
31:DE:20:ILE:HD13	31:DE:25:TYR:HB2	1.80	0.63
58:C1:154:C:O2	58:C1:154:C:O4'	2.16	0.63
46:CY:76:CYS:HB3	46:CY:96:ILE:HD11	1.80	0.63
58:D1:1920:G:H22	58:D1:1923:C:N4	1.96	0.63
45:DX:12:VAL:HG21	45:DX:17:ALA:HB1	1.80	0.63
1:A2:17:U:C2'	1:A2:18:G:H5''	2.20	0.63
58:C1:1826:U:H2'	58:C1:1827:C:C6	2.33	0.63
58:C1:2723:U:O2'	58:C1:2724:A:H5''	1.99	0.63
58:C1:355:A:O2'	58:C1:357:C:OP2	2.15	0.63
56:D9:33:ASN:O	58:D1:2431:C:P	2.57	0.63
2:BA:185:ILE:HG22	2:BA:199:TYR:HB2	1.80	0.63
41:CS:89:VAL:HG11	41:CS:91:ARG:HE	1.64	0.63
53:D6:35:GLU:O	53:D6:36:CYS:HB3	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:DO:45:LEU:HD23	37:DO:46:LYS:N	2.14	0.63
20:AU:73:HIS:HB3	20:AU:74:LYS:HG2	1.79	0.63
4:BD:30:LYS:C	4:BD:32:ALA:H	2.00	0.63
29:CC:61:ARG:CD	58:C1:2799:C:H1'	2.29	0.63
58:D1:353:A:O2'	58:D1:354:A:C8	2.52	0.63
20:AU:67:ALA:O	20:AU:73:HIS:CE1	2.52	0.63
31:CE:60:LEU:O	31:CE:64:THR:HG22	1.99	0.63
58:D1:1210:U:H2'	58:D1:1211:C:C6	2.34	0.63
58:D1:2083:A:H2'	58:D1:2084:C:C5'	2.29	0.63
58:D1:2462:A:H5''	58:D1:2463:C:OP2	1.99	0.63
54:D7:16:CYS:O	54:D7:17:LYS:HB2	1.99	0.63
9:AI:118:LYS:O	9:AI:119:ALA:HB3	1.98	0.62
58:C1:2084:C:H2'	58:C1:2085:C:H5'	1.81	0.62
58:D1:2543:G:O2'	58:D1:2668:A:N6	2.32	0.62
58:D1:893:U:OP2	58:D1:973:G:O6	2.17	0.62
25:D3:21:A:N6	25:D3:46:G:C4	2.67	0.62
31:DE:73:ALA:H	31:DE:87:PRO:HB2	1.64	0.62
33:DI:133:HIS:HB2	33:DI:134:PRO:CD	2.29	0.62
5:AE:102:ALA:HB1	5:AE:106:PRO:HG2	1.82	0.62
18:AS:43:PHE:HA	18:AS:51:LEU:HD12	1.81	0.62
13:BM:100:GLY:C	13:BM:101:GLN:HG2	2.20	0.62
58:D1:1097:C:H6	58:D1:1097:C:H3'	1.65	0.62
61:D4:2:G:N1	61:D4:73:A:C4	2.62	0.62
33:DI:72:LEU:HD13	33:DI:138:ILE:HD11	1.81	0.62
50:DK:22:GLU:OE2	50:DK:68:ARG:NH2	2.31	0.62
63:DW:64:MET:O	63:DW:65:LEU:CB	2.46	0.62
13:AM:106:ASN:O	13:AM:107:ALA:HB3	1.99	0.62
58:D1:1151:A:O2'	58:D1:1152:G:O4'	2.16	0.62
58:D1:1450:U:H2'	58:D1:1451:U:C6	2.33	0.62
46:DY:60:PHE:HA	46:DY:62:GLU:OE2	1.99	0.62
20:AU:104:LEU:HD23	20:AU:105:SER:N	2.14	0.62
24:BC:73:PRO:O	24:BC:76:VAL:HG22	1.99	0.62
58:C1:2449:U:O2'	58:C1:2451:C:OP1	2.16	0.62
58:C1:2817:U:O2	58:C1:2900:A:N6	2.32	0.62
43:CU:22:VAL:O	43:CU:23:GLU:HB2	1.99	0.62
45:CX:12:VAL:HG12	45:CX:17:ALA:HB1	1.81	0.62
58:D1:2842:G:H3'	58:D1:2843:G:C5'	2.28	0.62
37:DO:39:LYS:HG3	58:D1:853:U:OP2	1.98	0.62
38:DP:26:TYR:CE1	38:DP:28:ALA:HB2	2.34	0.62
41:DS:29:ARG:HG3	41:DS:30:VAL:HG13	1.81	0.62
13:BM:65:LYS:HD2	13:BM:69:GLU:O	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:D1:138:A:H8	58:D1:1453:C:O2'	1.82	0.62
31:DE:130:ASN:HB3	31:DE:160:VAL:HA	1.81	0.62
41:DS:96:ARG:NH1	58:D1:1784:C:OP1	2.32	0.62
26:C4:35:C:C2'	26:C4:36:A:O5'	2.48	0.62
30:DD:68:LYS:HE2	58:D1:2455:G:OP2	1.99	0.62
43:DU:22:VAL:O	43:DU:23:GLU:HB2	1.98	0.62
6:BF:30:LEU:O	6:BF:35:ALA:HB3	2.00	0.62
58:C1:570:A:N3	58:C1:570:A:H2'	2.13	0.62
24:BC:113:ALA:HB3	24:BC:114:PRO:HD3	1.81	0.62
58:D1:1920:G:O2'	58:D1:1921:A:OP2	2.16	0.62
28:DB:240:ALA:HA	58:D1:1992:A:C2	2.35	0.62
37:DO:7:ARG:HB2	37:DO:8:PRO:HD2	1.82	0.62
58:C1:2093:G:C2	58:C1:2449:U:O2	2.53	0.62
58:C1:2120:U:O2	58:C1:2120:U:H2'	1.99	0.62
51:CL:52:HIS:H	51:CL:52:HIS:CD2	2.16	0.62
28:DB:85:ASP:HB2	28:DB:92:ILE:HD12	1.82	0.62
43:DU:49:THR:HB	43:DU:50:PRO:HD2	1.82	0.62
12:BL:26:ALA:O	12:BL:27:LEU:O	2.17	0.62
52:C5:60:GLU:O	52:C5:61:VAL:HB	2.00	0.62
41:CS:10:VAL:O	41:CS:13:ARG:HG2	2.00	0.62
42:DT:25:TRP:CH2	58:D1:16:G:H4'	2.34	0.62
58:D1:1735:A:H62	58:D1:1744:A:H2	1.48	0.62
33:DI:94:ALA:HB2	33:DI:114:LEU:HD11	1.82	0.62
7:BG:79:ARG:NH2	25:D3:34:G:OP1	2.33	0.61
31:CE:57:ALA:HB2	31:CE:90:LEU:HD21	1.80	0.61
58:D1:2319:G:O6	58:D1:2321:A:H2'	2.00	0.61
56:D9:61:LEU:N	56:D9:63:PRO:HD2	2.14	0.61
31:DE:39:ILE:HD11	31:DE:60:LEU:HD21	1.81	0.61
38:DP:84:GLY:O	38:DP:85:LYS:HB2	2.00	0.61
39:DQ:24:GLN:NE2	39:DQ:36:THR:HG21	2.15	0.61
6:BF:91:VAL:HG11	18:BS:72:ARG:HH12	1.66	0.61
13:BM:65:LYS:HA	13:BM:66:LEU:CB	2.30	0.61
43:CU:28:GLU:HB3	43:CU:29:PRO:HD2	1.81	0.61
34:DJ:10:UNK:CB	58:D1:1091:A:H5''	2.31	0.61
29:DC:36:ARG:HH21	29:DC:88:GLY:HA3	1.64	0.61
41:DS:80:SER:HB3	41:DS:81:PRO:HD3	1.82	0.61
46:DY:2:ARG:C	46:DY:4:LYS:H	2.03	0.61
2:AA:185:ILE:HG22	2:AA:199:TYR:HB2	1.82	0.61
58:C1:2200:C:H4'	58:C1:2200:C:OP1	1.99	0.61
28:CB:44:ASN:CB	28:CB:49:ILE:HA	2.30	0.61
29:CC:16:ARG:O	29:CC:18:ASP:N	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:CH:11:ARG:HB2	49:CH:12:PRO:HD2	1.83	0.61
37:CO:77:ARG:HB2	37:CO:78:PRO:HD2	1.82	0.61
58:D1:2448:U:H2'	58:D1:2449:U:H5'	1.83	0.61
28:DB:35:LYS:O	28:DB:64:ILE:HG22	1.99	0.61
23:B2:20:U:H2'	23:B2:21:C:O4'	2.00	0.61
58:C1:1424:A:HO2'	58:C1:1425:G:P	2.23	0.61
25:C3:15:G:H2'	25:C3:15:G:N3	2.16	0.61
53:C6:33:CYS:SG	53:C6:40:LYS:HE3	2.41	0.61
55:C8:22:MET:O	55:C8:28:ARG:NH1	2.33	0.61
31:CE:46:ALA:HB2	31:CE:88:ILE:HG12	1.82	0.61
51:CL:43:ILE:O	51:CL:47:VAL:HG23	2.00	0.61
46:CY:8:LYS:HB2	46:CY:28:LYS:NZ	2.14	0.61
37:DO:115:LEU:HA	37:DO:134:ALA:HB2	1.81	0.61
5:BE:100:VAL:HG12	5:BE:118:ILE:HG22	1.81	0.61
16:BP:22:THR:HA	16:BP:33:ILE:HG12	1.80	0.61
58:C1:1578:C:O2'	58:C1:1579:G:C2	2.53	0.61
58:C1:1920:G:H22	58:C1:1923:C:N4	1.98	0.61
27:CA:64:LEU:HD22	27:CA:65:PRO:HD2	1.80	0.61
31:CE:96:ARG:O	31:CE:98:ARG:N	2.34	0.61
30:DD:81:PRO:HD2	58:D1:719:C:H5''	1.81	0.61
24:BC:68:VAL:HG12	24:BC:70:VAL:HG23	1.83	0.61
4:BD:11:LEU:O	4:BD:13:ARG:O	2.19	0.61
58:C1:1636:G:H5''	58:C1:1636:G:H8	1.65	0.61
58:C1:1698:A:H3'	58:C1:1699:G:C8	2.35	0.61
42:CT:49:HIS:HD2	58:C1:558:U:O2'	1.83	0.61
35:CM:18:ALA:HB1	35:CM:21:LYS:HB2	1.83	0.61
27:CA:169:UNK:O	27:CA:171:UNK:N	2.33	0.61
40:CR:89:ARG:HH11	40:CR:89:ARG:HG2	1.65	0.61
28:DB:30:GLU:HG3	28:DB:63:ARG:NH2	2.15	0.61
29:DC:144:ARG:HD2	58:D1:2583:A:C8	2.35	0.61
30:DD:185:ASP:OD1	30:DD:188:ARG:NH1	2.33	0.61
33:DI:94:ALA:HB1	33:DI:114:LEU:HD11	1.83	0.61
37:DO:64:LYS:HB3	56:D9:25:MET:HG3	1.83	0.61
53:C6:33:CYS:O	53:C6:36:CYS:O	2.18	0.61
58:D1:138:A:C8	58:D1:1453:C:O2'	2.52	0.61
66:D1:3001:3V6:OAG	66:D1:3001:3V6:OAE	2.15	0.61
16:AP:53:VAL:HG12	16:AP:79:VAL:HG22	1.83	0.61
58:C1:1908:C:C3'	58:C1:1909:G:H5'	2.31	0.61
58:C1:2802:A:H2'	58:C1:2802:A:N3	2.16	0.61
30:CD:181:LEU:HG	30:CD:186:ILE:HD11	1.81	0.61
31:CE:72:ARG:HA	31:CE:87:PRO:CG	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:CK:69:ARG:NH2	58:C1:108:A:H4'	2.16	0.61
46:CY:28:LYS:HB3	46:CY:37:VAL:HB	1.83	0.61
58:D1:722:A:H8	58:D1:2090:G:H21	1.49	0.61
46:DY:28:LYS:HB3	46:DY:37:VAL:HB	1.83	0.61
2:BA:233:SER:HB2	2:BA:234:PRO:HD2	1.83	0.60
58:C1:7:A:H2'	58:C1:8:U:C5	2.35	0.60
37:CO:17:LYS:CG	37:CO:17:LYS:O	2.49	0.60
43:CU:64:HIS:ND1	43:CU:92:THR:HG22	2.17	0.60
37:DO:7:ARG:HB2	37:DO:8:PRO:CD	2.31	0.60
63:DW:73:ALA:HB3	63:DW:106:ILE:HD11	1.82	0.60
46:DY:76:CYS:SG	46:DY:77:PRO:HD3	2.41	0.60
4:AD:30:LYS:HB3	4:AD:35:ARG:HD2	1.83	0.60
10:BJ:50:ILE:HA	10:BJ:60:ARG:HB2	1.83	0.60
58:C1:1286:A:H2'	58:C1:1287:A:O5'	2.01	0.60
58:C1:1625:A:H2'	58:C1:1626:A:C8	2.35	0.60
25:C3:25:C:H2'	25:C3:26:A:C8	2.35	0.60
56:C9:51:ALA:N	56:C9:53:PRO:HD2	2.16	0.60
41:CS:38:ASN:HD22	41:CS:40:THR:H	1.49	0.60
58:D1:1216:G:H5'	58:D1:1217:G:OP2	2.01	0.60
58:D1:2640:A:H2'	58:D1:2640:A:N3	2.16	0.60
61:D4:16:C:H3'	61:D4:17:C:H5'	1.83	0.60
29:DC:81:ILE:O	29:DC:81:ILE:HG22	2.01	0.60
38:DP:25:ASP:OD2	47:DZ:78:LYS:HD3	2.01	0.60
45:DX:35:THR:O	45:DX:39:ILE:HG12	2.01	0.60
18:BS:73:ALA:HB3	18:BS:79:LEU:HD12	1.82	0.60
39:CQ:10:LEU:HD22	39:CQ:17:ARG:HD2	1.81	0.60
58:D1:715:G:C8	58:D1:715:G:H5'	2.36	0.60
61:D4:17:C:H5'	61:D4:18:U:H5	1.66	0.60
28:DB:259:THR:HG22	58:D1:1828:U:C5'	2.30	0.60
42:DT:102:GLU:HG3	43:DU:2:PHE:CZ	2.36	0.60
5:AE:101:ILE:O	5:AE:120:THR:OG1	2.17	0.60
30:CD:178:PRO:HB2	30:CD:201:VAL:HG11	1.83	0.60
37:CO:35:HIS:CE1	58:C1:985:A:H4'	2.36	0.60
66:D1:3001:3V6:OAG	67:D1:3002:MG:MG	1.44	0.60
49:DH:93:GLU:C	49:DH:95:LEU:H	2.05	0.60
58:D1:2083:A:O2'	58:D1:2084:C:C5'	2.50	0.60
58:D1:2817:U:O2	58:D1:2900:A:N6	2.34	0.60
61:D4:17:C:C5	61:D4:18:U:N3	2.69	0.60
35:DM:58:ASP:O	35:DM:60:ILE:N	2.31	0.60
4:BD:92:VAL:O	4:BD:96:LEU:HD13	2.02	0.60
8:BH:109:ILE:HD11	8:BH:120:THR:CG2	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:C1:2298:A:H62	58:C1:2355:U:H3	1.48	0.60
40:CR:18:ILE:HD11	58:C1:2345:G:N3	2.15	0.60
35:DM:63:THR:CG2	58:D1:1185:U:H2'	2.31	0.60
53:D6:2:ALA:HA	58:D1:2036:A:H1'	1.83	0.60
36:CN:23:ARG:NH2	58:C1:2558:U:O2	2.34	0.60
30:CD:74:ARG:HD2	58:C1:720:G:H1'	1.82	0.60
37:CO:125:VAL:CG1	37:CO:138:LEU:HD21	2.32	0.60
29:DC:61:ARG:CD	58:D1:2799:C:H1'	2.32	0.60
5:AE:143:ARG:NH1	8:AH:77:GLU:OE1	2.35	0.60
5:BE:101:ILE:HD11	5:BE:119:LEU:HD23	1.81	0.60
20:BU:57:ARG:NH1	20:BU:102:GLY:HA3	2.16	0.60
39:CQ:53:HIS:CD2	58:C1:2849:C:H5''	2.36	0.60
41:CS:83:ILE:HG13	41:CS:84:GLN:H	1.67	0.60
58:D1:1636:G:H5''	58:D1:1636:G:H8	1.67	0.60
23:B2:19:U:O2	23:B2:19:U:H2'	2.02	0.60
28:CB:30:GLU:HG3	28:CB:63:ARG:NH2	2.17	0.60
30:CD:108:LYS:O	30:CD:112:MET:HG3	2.02	0.60
28:DB:144:ALA:HB3	28:DB:192:THR:HG23	1.84	0.60
41:DS:24:PRO:HA	41:DS:49:VAL:HG13	1.84	0.60
3:AC:58:GLU:HB2	3:AC:65:ALA:HB3	1.84	0.60
5:BE:10:MET:HB2	5:BE:32:VAL:HG22	1.82	0.60
12:BL:28:LYS:O	12:BL:29:GLY:C	2.40	0.60
28:CB:259:THR:HG21	58:C1:1833:A:O3'	2.02	0.60
58:D1:1088:C:H2'	58:D1:1089:G:C8	2.36	0.60
28:DB:49:ILE:HD11	28:DB:52:ARG:HA	1.82	0.60
28:DB:76:PRO:HB2	28:DB:116:GLN:HE21	1.67	0.60
8:BH:89:PRO:HA	8:BH:92:ARG:HH11	1.66	0.59
9:BI:53:VAL:O	9:BI:54:ASP:HB2	2.02	0.59
58:C1:260:A:H5''	58:C1:261:C:OP2	2.02	0.59
58:C1:2902:G:N3	58:C1:2902:G:H2'	2.16	0.59
25:D3:34:G:N1	25:D3:35:A:C5	2.69	0.59
31:DE:6:ALA:HB3	31:DE:104:GLU:OE2	2.02	0.59
10:AJ:49:VAL:HG21	14:AN:41:ARG:HB2	1.83	0.59
28:CB:30:GLU:HB2	28:CB:35:LYS:HE3	1.83	0.59
44:CW:24:ILE:HG21	44:CW:36:LEU:HD21	1.84	0.59
58:D1:2319:G:O2'	58:D1:2320:A:OP1	2.18	0.59
25:D3:39:U:H5''	25:D3:39:U:O2	2.01	0.59
28:DB:35:LYS:HD2	28:DB:36:PRO:CA	2.32	0.59
41:CS:23:ARG:NH2	58:C1:2858:U:O4	2.33	0.59
58:D1:1734:U:O2	58:D1:1746:A:H5''	2.03	0.59
61:D4:17:C:H2'	61:D4:18:U:C5	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:DF:41:MET:SD	32:DF:53:GLU:O	2.60	0.59
13:BM:90:LEU:HA	13:BM:93:ARG:HB2	1.82	0.59
29:CC:132:HIS:CD2	29:CC:135:HIS:CE1	2.90	0.59
45:CX:12:VAL:CG1	45:CX:17:ALA:HB1	2.32	0.59
25:D3:72:C:OP1	58:D1:1881:U:O2'	2.20	0.59
58:D1:2083:A:O2'	58:D1:2084:C:H5'	2.02	0.59
25:D3:20:U:H2'	25:D3:21:A:H4'	1.84	0.59
29:DC:119:ARG:HD2	29:DC:120:TRP:NE1	2.17	0.59
47:DZ:72:ARG:HG3	47:DZ:89:PHE:HB2	1.85	0.59
25:C3:8:U:C1'	25:C3:48:C:O2	2.51	0.59
26:C4:51:U:H3	26:C4:65:G:H1	1.48	0.59
30:CD:167:ALA:O	30:CD:169:ASN:N	2.35	0.59
33:CI:109:ILE:HG22	33:CI:130:TYR:CE1	2.36	0.59
35:CM:134:ARG:O	35:CM:136:GLU:N	2.35	0.59
30:CD:34:TRP:CE2	37:CO:12:ALA:HB2	2.37	0.59
43:DU:22:VAL:O	43:DU:23:GLU:CB	2.50	0.59
2:AA:77:ALA:HB2	2:AA:211:ILE:HD13	1.84	0.59
3:AC:76:VAL:HG21	3:AC:103:VAL:HG21	1.85	0.59
12:BL:25:PRO:C	12:BL:27:LEU:H	2.06	0.59
58:C1:1067:G:N2	58:C1:1187:A:C2	2.70	0.59
58:C1:1920:G:O2'	58:C1:1921:A:OP2	2.18	0.59
25:C2:64:A:H2'	25:C2:65:G:H8	1.66	0.59
29:CC:137:HIS:HB3	29:CC:138:PRO:HD2	1.85	0.59
37:CO:45:LEU:HD23	37:CO:46:LYS:H	1.67	0.59
38:CP:42:ILE:HD13	38:CP:97:VAL:HG21	1.83	0.59
38:CP:2:LEU:O	38:CP:70:PRO:HG2	2.01	0.59
31:DE:39:ILE:HG13	31:DE:92:VAL:HG12	1.85	0.59
12:AL:37:CYS:O	12:AL:79:GLU:O	2.20	0.59
58:C1:276:G:O2'	58:C1:277:G:P	2.59	0.59
40:CR:96:GLY:O	40:CR:98:VAL:N	2.30	0.59
58:D1:2325:C:O2'	58:D1:2326:G:H5'	2.02	0.59
28:DB:35:LYS:HG2	28:DB:63:ARG:HG3	1.84	0.59
51:DL:4:LEU:O	51:DL:36:VAL:HA	2.03	0.59
39:DQ:10:LEU:HD22	39:DQ:17:ARG:CD	2.33	0.59
58:C1:2209:C:H2'	58:C1:2210:U:O4'	2.03	0.59
57:D0:11:CYS:HB3	57:D0:14:CYS:SG	2.43	0.59
58:D1:2303:C:O2'	58:D1:2304:C:H5'	2.03	0.59
58:D1:567:C:HO2'	58:D1:570:A:P	2.25	0.59
58:D1:570:A:N3	58:D1:570:A:H2'	2.16	0.59
25:D3:39:U:O2	25:D3:39:U:C5'	2.51	0.59
29:DC:94:GLU:OE2	29:DC:177:PRO:HB3	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:DQ:38:VAL:HB	39:DQ:39:PRO:HD3	1.85	0.59
5:AE:6:PHE:HB2	5:AE:34:VAL:HG22	1.85	0.59
28:CB:34:VAL:O	28:CB:35:LYS:C	2.41	0.59
33:CI:109:ILE:HG22	33:CI:130:TYR:OH	2.03	0.59
47:CZ:93:ASP:HA	47:CZ:130:PRO:HD2	1.84	0.59
58:D1:935:C:O2	58:D1:935:C:O4'	2.20	0.59
33:DI:92:VAL:CG1	33:DI:120:ILE:HB	2.33	0.59
12:BL:90:VAL:O	12:BL:92:ASP:N	2.36	0.59
50:CK:7:ARG:NH2	58:C1:99:G:OP2	2.36	0.59
26:C4:3:C:O2	26:C4:3:C:H2'	2.01	0.59
29:CC:81:ILE:O	29:CC:81:ILE:HG22	2.02	0.59
46:CY:76:CYS:SG	46:CY:77:PRO:CD	2.91	0.59
58:D1:567:C:O2'	58:D1:570:A:P	2.61	0.59
58:D1:814:G:O2'	58:D1:1424:A:N6	2.35	0.59
56:D9:31:HIS:HE1	58:D1:2403:A:OP2	1.86	0.59
28:DB:238:GLY:O	28:DB:239:ARG:CB	2.50	0.59
37:DO:38:GLN:CD	58:D1:987:U:OP2	2.41	0.59
2:BA:47:THR:O	2:BA:51:LEU:HD12	2.03	0.58
4:BD:8:VAL:C	4:BD:10:ARG:H	2.05	0.58
15:BO:81:LEU:HD11	15:BO:85:LEU:HD13	1.85	0.58
16:BP:70:ALA:O	16:BP:74:LEU:HD12	2.03	0.58
26:C4:61:U:C5'	26:C4:62:C:H5	2.16	0.58
30:CD:24:LEU:O	30:CD:26:ALA:N	2.35	0.58
30:CD:4:VAL:HA	30:CD:19:GLU:HB3	1.85	0.58
58:D1:841:C:H2'	58:D1:842:C:C6	2.38	0.58
9:AI:48:GLU:N	9:AI:49:PRO:HD2	2.19	0.58
14:AN:27:CYS:C	14:AN:29:ARG:H	2.05	0.58
58:C1:2147:A:O2'	58:C1:2148:G:OP2	2.19	0.58
58:C1:552:A:C2	58:C1:2063:A:H2'	2.37	0.58
41:CS:54:ARG:HA	41:CS:59:THR:HB	1.86	0.58
42:DT:13:LYS:HD3	58:D1:1272:G:OP1	2.03	0.58
58:D1:1540:A:C2	58:D1:1541:A:C2	2.91	0.58
31:DE:104:GLU:OE1	52:D5:50:THR:HG22	2.03	0.58
31:DE:71:THR:HG22	31:DE:89:GLY:C	2.24	0.58
49:DH:52:ARG:O	49:DH:56:GLN:O	2.21	0.58
10:AJ:79:ARG:HA	10:AJ:79:ARG:HH11	1.68	0.58
19:BT:63:THR:O	19:BT:66:MET:HG2	2.03	0.58
58:C1:1540:A:OP1	58:C1:1540:A:O4'	2.21	0.58
58:C1:464:G:O2'	58:C1:465:G:H5'	2.03	0.58
40:CR:89:ARG:HH11	40:CR:89:ARG:CG	2.16	0.58
42:CT:92:ARG:O	42:CT:95:LEU:N	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:AP:20:VAL:HG21	16:AP:32:TYR:CG	2.38	0.58
42:CT:90:VAL:O	42:CT:91:ASP:C	2.40	0.58
45:CX:64:LYS:HE2	58:C1:1381:A:OP2	2.03	0.58
58:D1:1088:C:H2'	58:D1:1089:G:H8	1.66	0.58
58:D1:1152:G:H2'	58:D1:1153:U:O5'	2.04	0.58
62:DA:58:VAL:HG21	62:DA:166:UNK:N	2.19	0.58
31:DE:11:TYR:OH	31:DE:33:ARG:HB3	2.03	0.58
14:AN:29:ARG:HG2	14:AN:40:CYS:HB2	1.85	0.58
58:C1:1026:A:N1	58:C1:2048:G:O2'	2.31	0.58
58:C1:2487:A:C2	58:C1:2488:C:C6	2.91	0.58
41:CS:125:ARG:O	41:CS:128:GLU:HG3	2.04	0.58
58:D1:1441:U:C2'	58:D1:1441:U:O2	2.51	0.58
58:D1:2093:G:C2	58:D1:2449:U:O2	2.57	0.58
10:AJ:48:THR:HA	10:AJ:62:HIS:CB	2.34	0.58
30:CD:8:GLN:HB3	30:CD:126:VAL:HA	1.85	0.58
58:D1:842:C:H2'	58:D1:843:C:C6	2.39	0.58
29:DC:36:ARG:HH21	29:DC:88:GLY:CA	2.16	0.58
46:DY:50:ARG:HG2	46:DY:58:GLY:CA	2.33	0.58
2:AA:24:TRP:CZ3	2:AA:26:PRO:HA	2.39	0.58
12:AL:28:LYS:O	12:AL:29:GLY:C	2.42	0.58
3:AC:29:TYR:OH	14:AN:54:PRO:O	2.21	0.58
2:BA:88:ALA:HB2	2:BA:219:VAL:CG1	2.33	0.58
25:C2:1:G:H2'	25:C2:1:G:N3	2.18	0.58
49:CH:29:GLY:O	49:CH:30:VAL:CG2	2.51	0.58
58:D1:1035:A:OP2	58:D1:1036:C:OP2	2.20	0.58
46:DY:8:LYS:HB2	46:DY:28:LYS:CE	2.34	0.58
58:C1:1098:C:O3'	58:C1:1151:A:P	2.62	0.58
29:CC:131:ALA:HB2	58:C1:2590:C:O2'	2.03	0.58
56:C9:61:LEU:HD13	56:C9:62:LEU:HD12	1.85	0.58
28:CB:24:ILE:O	28:CB:25:THR:C	2.42	0.58
35:DM:18:ALA:HB1	35:DM:21:LYS:HB2	1.85	0.58
37:DO:23:PRO:HD2	37:DO:33:ARG:NH2	2.18	0.58
37:DO:7:ARG:HA	37:DO:7:ARG:NH1	2.19	0.58
26:C4:51:U:O2	26:C4:65:G:N2	2.35	0.58
46:CY:90:LEU:HG	46:CY:91:GLU:HG2	1.86	0.58
53:D6:42:PRO:HB2	53:D6:43:HIS:CD2	2.39	0.58
49:DH:56:GLN:HE21	49:DH:56:GLN:CA	2.17	0.58
40:DR:16:ASN:O	40:DR:19:LYS:HB3	2.04	0.58
3:AC:19:GLU:O	3:AC:40:ARG:NH2	2.36	0.57
4:AD:119:GLN:HG3	4:AD:123:HIS:CD2	2.39	0.57
23:B2:15:A:H2	25:D3:34:G:C6	2.21	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:C1:1359:C:H6	58:C1:1359:C:H5'	1.67	0.57
29:CC:70:ALA:O	29:CC:72:VAL:N	2.36	0.57
41:CS:96:ARG:NH1	58:C1:1784:C:OP1	2.37	0.57
42:DT:92:ARG:NH2	58:D1:1041:A:OP2	2.36	0.57
42:DT:2:PRO:HA	58:D1:470:C:OP1	2.03	0.57
46:DY:46:LYS:H	46:DY:62:GLU:HG2	1.68	0.57
5:AE:42:GLY:HA3	5:AE:66:MET:HG2	1.84	0.57
37:CO:17:LYS:O	37:CO:19:VAL:N	2.36	0.57
58:D1:1156:A:O2'	58:D1:1157:G:O4'	2.22	0.57
58:D1:2487:A:N1	58:D1:2488:C:C5	2.72	0.57
53:D6:43:HIS:HD2	58:D1:2824:C:O2'	1.85	0.57
32:DF:156:ALA:C	32:DF:158:HIS:N	2.57	0.57
32:DF:83:TYR:HB3	32:DF:134:SER:HA	1.85	0.57
41:DS:89:VAL:CG1	41:DS:91:ARG:HG3	2.34	0.57
58:C1:1574:A:N7	58:C1:1575:G:H8	2.02	0.57
58:C1:1875:G:H2'	58:C1:1876:G:C5'	2.32	0.57
58:C1:274:C:O2'	58:C1:275:C:H6	1.87	0.57
56:C9:30:ARG:O	56:C9:31:HIS:HB3	2.05	0.57
37:CO:146:VAL:HG22	37:CO:147:LEU:H	1.70	0.57
46:CY:17:SER:OG	46:CY:18:GLY:N	2.36	0.57
37:DO:27:HIS:ND1	58:D1:860:C:OP2	2.37	0.57
42:DT:91:ASP:OD1	42:DT:96:ALA:HB2	2.03	0.57
19:BT:9:VAL:O	19:BT:11:VAL:N	2.38	0.57
28:CB:210:GLY:O	28:CB:211:ARG:HB3	2.04	0.57
29:CC:132:HIS:CE1	58:C1:1704:C:OP1	2.57	0.57
31:DE:128:ARG:HD3	58:D1:2326:G:H21	1.69	0.57
43:DU:19:LYS:HG3	43:DU:20:LEU:N	2.18	0.57
57:C0:19:ARG:HA	58:C1:2769:A:OP1	2.03	0.57
58:C1:718:C:C2'	58:C1:719:C:H5'	2.34	0.57
33:CI:133:HIS:HB2	33:CI:134:PRO:CD	2.35	0.57
58:D1:1541:A:C8	58:D1:1623:C:O2'	2.57	0.57
31:DE:132:ASN:HB2	58:D1:2314:G:O2'	2.05	0.57
54:D7:28:ARG:O	54:D7:32:ASN:HB3	2.04	0.57
35:DM:106:MET:SD	58:D1:1182:G:N2	2.75	0.57
38:DP:9:TYR:OH	58:D1:956:A:H2'	2.04	0.57
45:DX:12:VAL:HG11	45:DX:27:THR:OG1	2.04	0.57
12:AL:89:ARG:HA	12:AL:97:ARG:HA	1.86	0.57
9:BI:118:LYS:O	9:BI:119:ALA:HB3	2.05	0.57
39:CQ:3:HIS:HB2	58:C1:1700:A:P	2.44	0.57
58:C1:2318:G:H5''	58:C1:2318:G:N3	2.20	0.57
58:C1:8:U:C5	58:C1:2640:A:N6	2.72	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:C1:247:G:H21	58:C1:645:A:H8	1.52	0.57
28:CB:9:TYR:CD1	28:CB:10:THR:HG22	2.39	0.57
29:CC:63:LEU:O	29:CC:64:LYS:C	2.42	0.57
32:CF:20:ALA:HB1	32:CF:21:PRO:HD2	1.85	0.57
62:DA:36:LYS:HE3	62:DA:36:LYS:HA	1.86	0.57
45:DX:18:TYR:C	45:DX:20:GLY:H	2.08	0.57
9:AI:28:VAL:HG22	9:AI:63:ILE:HB	1.86	0.57
17:BR:45:HIS:HB2	17:BR:65:ILE:HD13	1.86	0.57
58:C1:2332:G:N3	58:C1:2332:G:H2'	2.18	0.57
58:C1:2420:G:H2'	58:C1:2421:G:O4'	2.05	0.57
58:C1:2488:C:O2	58:C1:2492:G:O6	2.23	0.57
58:C1:2643:A:HO2'	58:C1:2820:G:HO2'	1.51	0.57
37:CO:39:LYS:HD3	58:C1:852:C:OP2	2.04	0.57
49:CH:67:ILE:N	49:CH:68:PRO:HD2	2.20	0.57
41:CS:28:VAL:HG22	41:CS:46:GLU:HG3	1.85	0.57
31:DE:137:GLU:HG2	31:DE:152:LEU:HD23	1.86	0.57
37:DO:101:VAL:C	37:DO:103:ALA:H	2.07	0.57
46:DY:17:SER:HA	46:DY:71:LYS:HE2	1.85	0.57
58:C1:2789:G:H5''	58:C1:2790:A:H5'	1.86	0.57
41:CS:66:VAL:HA	41:CS:71:GLY:HA2	1.85	0.57
43:CU:89:GLN:NE2	58:C1:1038:G:N3	2.52	0.57
58:D1:1540:A:N3	58:D1:1541:A:C2	2.73	0.57
45:DX:35:THR:HG22	58:D1:1643:C:O3'	2.05	0.57
4:BD:9:CYS:HA	4:BD:12:CYS:HB2	1.87	0.57
13:BM:82:MET:O	13:BM:82:MET:HG2	2.04	0.57
25:C3:21:A:N6	25:C3:46:G:C4	2.73	0.57
31:CE:32:PRO:HB2	31:CE:172:LEU:HD13	1.85	0.57
36:DN:31:LYS:HE2	58:D1:2017:C:OP1	2.05	0.57
38:DP:141:GLN:O	47:DZ:71:VAL:O	2.23	0.57
41:DS:32:TYR:HD2	41:DS:81:PRO:O	1.87	0.57
43:DU:34:GLU:O	43:DU:36:PRO:HD3	2.05	0.57
5:BE:76:ILE:HD11	5:BE:142:LEU:HD21	1.86	0.57
58:C1:1983:C:O5'	58:C1:1983:C:O2'	2.22	0.57
37:CO:16:ARG:HH12	58:C1:707:C:H4'	1.70	0.57
61:D4:12:G:C6	61:D4:13:C:C5	2.93	0.57
53:D6:46:CYS:SG	53:D6:48:GLU:HG2	2.45	0.57
46:DY:52:SER:C	46:DY:54:LYS:H	2.08	0.57
9:BI:50:LEU:O	9:BI:53:VAL:HG22	2.05	0.56
58:C1:1539:A:H3'	58:C1:1539:A:N3	2.20	0.56
58:D1:2744:G:H3'	58:D1:2745:A:C5'	2.34	0.56
36:DN:4:PRO:O	36:DN:5:GLN:CB	2.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:DS:54:ARG:HA	41:DS:59:THR:HB	1.86	0.56
13:AM:65:LYS:HA	13:AM:66:LEU:CB	2.34	0.56
15:AO:78:TYR:O	15:AO:82:ILE:HG22	2.05	0.56
58:C1:1087:G:H2'	58:C1:1087:G:N3	2.20	0.56
58:C1:2124:C:H3'	58:C1:2125:G:H5''	1.86	0.56
56:C9:51:ALA:C	56:C9:53:PRO:HD2	2.25	0.56
58:D1:1231:G:O5'	58:D1:1231:G:H8	1.88	0.56
58:D1:2475:C:O2'	58:D1:2476:C:P	2.63	0.56
29:DC:116:VAL:HG21	29:DC:122:PHE:CD2	2.40	0.56
33:DI:14:ASP:N	33:DI:17:GLN:OE1	2.37	0.56
35:DM:18:ALA:CB	35:DM:21:LYS:HB2	2.35	0.56
2:AA:167:PRO:HG3	2:AA:188:ALA:HB2	1.86	0.56
7:AG:116:ALA:O	7:AG:118:VAL:N	2.38	0.56
4:BD:25:ARG:C	4:BD:27:TYR:N	2.59	0.56
13:BM:67:GLU:OE2	13:BM:68:GLY:N	2.38	0.56
58:C1:1346:A:O2'	58:C1:1347:A:C3'	2.50	0.56
25:C2:72:C:O2	25:C2:72:C:H2'	2.05	0.56
41:CS:12:SER:O	41:CS:13:ARG:CZ	2.54	0.56
43:DU:49:THR:HB	43:DU:50:PRO:CD	2.36	0.56
5:AE:51:VAL:HB	5:AE:52:PRO:HD3	1.86	0.56
16:AP:20:VAL:HG21	16:AP:32:TYR:CD1	2.40	0.56
58:C1:669:C:O2	58:C1:669:C:O4'	2.22	0.56
50:CK:65:ASN:HB3	50:CK:69:ARG:NH2	2.20	0.56
42:CT:47:TYR:HA	42:CT:50:ARG:NH2	2.20	0.56
58:D1:1475:C:H2'	58:D1:1476:U:H6	1.68	0.56
58:D1:2732:U:O2	58:D1:2732:U:H2'	2.04	0.56
61:D4:18:U:H5''	61:D4:19:G:OP2	2.05	0.56
61:D4:4:G:H8	61:D4:4:G:H5''	1.71	0.56
28:DB:45:ASN:OD1	28:DB:46:GLN:N	2.38	0.56
31:DE:82:LEU:HD13	31:DE:87:PRO:HD3	1.87	0.56
2:AA:102:LEU:HD23	2:AA:182:ILE:HD12	1.88	0.56
3:AC:46:GLU:O	3:AC:47:LEU:HB2	2.05	0.56
15:AO:39:LEU:HD12	15:AO:56:LEU:HD13	1.86	0.56
20:AU:89:ARG:CZ	20:AU:104:LEU:HD21	2.35	0.56
10:BJ:49:VAL:HG22	14:BN:41:ARG:HB2	1.87	0.56
18:BS:53:ARG:C	18:BS:55:ARG:H	2.09	0.56
58:C1:1577:C:N4	58:C1:1579:G:OP1	2.38	0.56
26:C4:62:C:H2'	26:C4:63:C:H6	1.70	0.56
31:CE:16:ARG:HE	31:CE:31:VAL:HG11	1.70	0.56
35:CM:55:VAL:HG22	35:CM:126:PRO:HA	1.87	0.56
61:D4:67:C:H2'	61:D4:68:C:H6	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:D6:16:ARG:NH1	53:D6:17:ASP:OD1	2.39	0.56
30:DD:89:VAL:HG12	30:DD:90:PHE:N	2.21	0.56
32:DF:105:LEU:H	32:DF:105:LEU:HD23	1.70	0.56
26:C4:2:G:C2	26:C4:3:C:C5	2.93	0.56
26:C4:73:A:OP2	26:C4:73:A:H8	1.88	0.56
46:CY:76:CYS:SG	46:CY:77:PRO:HD2	2.45	0.56
25:D3:34:G:N1	25:D3:35:A:C2	2.73	0.56
29:DC:144:ARG:HD3	58:D1:2583:A:N7	2.20	0.56
33:DI:129:THR:HA	33:DI:137:PRO:HA	1.88	0.56
41:DS:28:VAL:HG13	41:DS:46:GLU:HB2	1.87	0.56
46:DY:7:VAL:HB	46:DY:8:LYS:CE	2.36	0.56
13:BM:115:LYS:O	13:BM:117:VAL:N	2.38	0.56
58:C1:1935:C:O4'	58:C1:1935:C:O2	2.23	0.56
58:D1:153:G:H3'	58:D1:154:C:O2	2.06	0.56
58:D1:2147:A:H4'	58:D1:2148:G:O5'	2.05	0.56
32:DF:20:ALA:HB1	32:DF:21:PRO:HD3	1.87	0.56
49:DH:45:ASN:C	49:DH:45:ASN:HD22	2.09	0.56
47:DZ:7:ALA:HB2	47:DZ:59:LEU:HD22	1.88	0.56
35:CM:63:THR:HG21	58:C1:1185:U:H2'	1.87	0.56
29:CC:131:ALA:CB	58:C1:2590:C:O2'	2.54	0.56
58:C1:906:U:O2	58:C1:906:U:O4'	2.22	0.56
25:C2:17:C:H4'	25:C2:17:C:OP2	2.05	0.56
58:D1:2083:A:H2'	58:D1:2084:C:H5'	1.87	0.56
49:DH:35:THR:HG21	58:D1:2101:G:OP1	2.05	0.56
9:AI:42:ARG:NH1	9:AI:71:SER:OG	2.39	0.56
42:DT:92:ARG:HE	58:D1:1041:A:H4'	1.70	0.56
58:D1:2890:C:C2	58:D1:2891:A:C8	2.93	0.56
37:DO:51:PHE:HB3	37:DO:52:GLU:HG2	1.86	0.56
41:DS:31:SER:HA	41:DS:32:TYR:CD2	2.40	0.56
58:C1:1336:C:H2'	58:C1:1337:U:C6	2.40	0.56
58:C1:2433:A:H4'	58:C1:2434:U:OP1	2.05	0.56
30:CD:167:ALA:HB1	30:CD:173:VAL:HG11	1.87	0.56
58:D1:1019:C:OP2	58:D1:1019:C:H4'	2.05	0.56
58:D1:1765:G:N1	58:D1:1767:U:OP2	2.39	0.56
58:D1:2346:A:C8	58:D1:2348:G:C5	2.94	0.56
61:D4:70:C:H2'	61:D4:71:G:O4'	2.06	0.56
28:DB:271:ILE:O	28:DB:272:ALA:HB2	2.05	0.56
29:DC:116:VAL:CG2	29:DC:122:PHE:CD2	2.89	0.56
5:BE:12:LEU:HD13	5:BE:31:LEU:HB3	1.88	0.56
24:BC:29:TYR:OH	14:BN:54:PRO:O	2.22	0.56
39:CQ:36:THR:HG22	58:C1:1323:A:OP1	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:C1:2051:A:H5''	58:C1:2052:A:OP1	2.06	0.56
58:D1:552:A:C2	58:D1:2064:C:H4'	2.41	0.56
37:DO:144:GLU:N	37:DO:145:PRO:HD3	2.21	0.56
37:DO:33:ARG:O	37:DO:34:GLY:C	2.44	0.56
41:DS:56:GLY:O	41:DS:59:THR:HG23	2.06	0.56
12:BL:32:PHE:HB3	12:BL:84:LEU:HD21	1.87	0.55
58:C1:935:C:O4'	58:C1:935:C:O2	2.22	0.55
28:CB:24:ILE:O	28:CB:25:THR:O	2.24	0.55
29:CC:65:GLY:HA2	29:CC:70:ALA:CB	2.36	0.55
30:CD:132:VAL:HG22	30:CD:133:ASN:H	1.69	0.55
41:CS:3:ARG:NE	58:C1:2885:G:H4'	2.22	0.55
35:DM:83:LYS:NZ	58:D1:2652:G:OP2	2.26	0.55
39:DQ:20:LEU:HD21	39:DQ:40:LYS:HD3	1.87	0.55
2:AA:233:SER:HB2	2:AA:234:PRO:CD	2.36	0.55
9:AI:82:ALA:HB1	9:AI:96:LEU:HD13	1.87	0.55
6:BF:62:TRP:CH2	6:BF:64:GLN:HB2	2.41	0.55
58:C1:1345:U:HO2'	58:C1:1671:G:N2	2.02	0.55
37:CO:16:ARG:NH1	58:C1:707:C:H4'	2.20	0.55
38:CP:87:LYS:NZ	58:C1:999:C:OP1	2.38	0.55
42:CT:12:ARG:NH2	58:C1:1260:G:OP2	2.38	0.55
46:CY:18:GLY:HA2	58:C1:332:G:O3'	2.07	0.55
25:D3:2:C:H2'	25:D3:3:C:C6	2.41	0.55
3:AC:134:ILE:HD11	3:AC:153:VAL:HG23	1.88	0.55
12:AL:40:VAL:HG11	12:AL:77:LEU:O	2.07	0.55
58:C1:68:G:H2'	58:C1:110:G:O2'	2.05	0.55
27:CA:47:LEU:N	27:CA:47:LEU:HD23	2.22	0.55
37:CO:47:ASP:HB3	37:CO:48:PRO:CA	2.36	0.55
58:D1:1472:A:H4'	58:D1:1473:C:O5'	2.06	0.55
58:D1:2671:A:H5'	58:D1:2672:G:N3	2.21	0.55
28:DB:62:TYR:CZ	58:D1:1846:G:C8	2.95	0.55
31:DE:116:ASP:O	31:DE:117:PHE:CB	2.53	0.55
9:AI:53:VAL:HG23	9:AI:55:ALA:H	1.71	0.55
14:AN:27:CYS:O	14:AN:29:ARG:N	2.34	0.55
35:CM:25:ARG:NH2	58:C1:1188:A:OP1	2.39	0.55
26:C4:62:C:H2'	26:C4:63:C:C6	2.41	0.55
58:D1:1596:C:OP1	58:D1:1764:U:O2'	2.24	0.55
30:DD:24:LEU:O	30:DD:26:ALA:N	2.39	0.55
4:AD:11:LEU:C	4:AD:13:ARG:N	2.60	0.55
6:BF:89:MET:SD	18:BS:76:LEU:HD21	2.46	0.55
20:BU:50:GLU:HG3	20:BU:100:ILE:HB	1.87	0.55
56:C9:52:LYS:N	56:C9:53:PRO:HD2	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:CD:7:TYR:HD2	30:CD:16:GLY:HA3	1.71	0.55
46:CY:17:SER:HB2	46:CY:71:LYS:HE2	1.88	0.55
30:DD:22:ALA:HB1	30:DD:26:ALA:HB2	1.87	0.55
31:DE:47:LYS:HB2	31:DE:82:LEU:HD12	1.88	0.55
4:BD:25:ARG:O	4:BD:28:SER:N	2.31	0.55
39:CQ:96:ARG:NE	58:C1:2891:A:OP1	2.35	0.55
58:C1:670:A:H2'	58:C1:671:G:O4'	2.06	0.55
29:CC:111:ARG:HA	39:CQ:2:ARG:HB3	1.89	0.55
37:CO:48:PRO:O	37:CO:49:ARG:C	2.44	0.55
42:CT:92:ARG:O	42:CT:94:ASN:N	2.39	0.55
46:CY:8:LYS:HB2	46:CY:28:LYS:CE	2.37	0.55
58:D1:1539:A:H2'	58:D1:1540:A:C5'	2.36	0.55
36:DN:22:ILE:HD12	58:D1:1973:A:C6	2.41	0.55
58:D1:2203:G:H2'	58:D1:2204:C:C6	2.41	0.55
36:DN:23:ARG:NH1	58:D1:2573:U:O2'	2.37	0.55
54:D7:46:HIS:CB	54:D7:47:THR:HG21	2.36	0.55
28:DB:209:ALA:C	28:DB:210:GLY:O	2.43	0.55
33:DI:133:HIS:HB2	33:DI:134:PRO:HD2	1.89	0.55
42:DT:92:ARG:O	42:DT:95:LEU:N	2.40	0.55
45:DX:80:ILE:O	45:DX:80:ILE:HD13	2.05	0.55
46:DY:10:GLY:CA	46:DY:27:VAL:HG13	2.37	0.55
46:DY:44:ILE:HG22	46:DY:45:VAL:N	2.21	0.55
2:BA:183:PRO:HA	2:BA:198:ASP:OD1	2.06	0.55
7:BG:113:GLU:CG	7:BG:119:ARG:HG2	2.36	0.55
29:CC:119:ARG:HD2	29:CC:120:TRP:NE1	2.21	0.55
35:CM:133:GLN:O	35:CM:134:ARG:HB3	2.07	0.55
58:D1:353:A:C2	58:D1:1254:A:H2'	2.41	0.55
58:D1:388:G:H2'	58:D1:388:G:N3	2.21	0.55
58:D1:509:C:H2'	58:D1:510:C:C6	2.42	0.55
61:D4:48:U:O4'	61:D4:48:U:OP1	2.25	0.55
37:DO:63:PRO:HB3	56:D9:13:ARG:HB3	1.88	0.55
37:DO:7:ARG:CB	37:DO:8:PRO:CD	2.85	0.55
36:DN:104:ARG:HH21	41:DS:33:LYS:HE2	1.71	0.55
46:DY:42:VAL:CG1	46:DY:65:ALA:HB3	2.37	0.55
16:AP:28:ARG:HG2	16:AP:29:ASP:OD2	2.06	0.55
24:BC:7:PRO:O	24:BC:11:ARG:NH1	2.40	0.55
19:BT:31:ILE:HG23	19:BT:49:ILE:HA	1.89	0.55
58:C1:967:U:H2'	58:C1:968:C:C6	2.42	0.55
29:CC:128:SER:OG	29:CC:129:HIS:N	2.36	0.55
36:CN:64:ARG:NH1	41:CS:70:VAL:HG21	2.22	0.55
36:CN:87:ILE:CG2	36:CN:91:LEU:HA	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:CS:12:SER:O	41:CS:13:ARG:NE	2.40	0.55
58:D1:67:C:O2	58:D1:71:A:O2'	2.22	0.55
40:DR:34:HIS:NE2	40:DR:54:LEU:HB3	2.22	0.55
13:AM:7:VAL:HG12	13:AM:7:VAL:O	2.07	0.55
19:AT:40:ILE:HG21	19:AT:62:ILE:HD11	1.87	0.55
19:AT:58:VAL:O	19:AT:58:VAL:HG23	2.07	0.55
58:C1:1652:C:H4'	58:C1:1653:A:O5'	2.07	0.55
58:C1:2516:G:O2'	58:C1:2517:U:O5'	2.23	0.55
25:C3:8:U:H1'	25:C3:48:C:O2	2.07	0.55
28:CB:35:LYS:HB3	28:CB:36:PRO:HD3	1.88	0.55
2:AA:80:ILE:HD12	2:AA:80:ILE:H	1.71	0.55
4:AD:9:CYS:HB2	4:AD:22:LYS:HD2	1.89	0.55
2:BA:77:ALA:HB2	2:BA:211:ILE:HD13	1.87	0.55
58:D1:2200:C:OP1	58:D1:2200:C:H4'	2.06	0.55
58:D1:353:A:O2'	58:D1:354:A:H8	1.90	0.55
58:D1:862:C:O2'	58:D1:976:G:O6	2.25	0.55
61:D4:35:C:H2'	61:D4:35:C:O2	2.07	0.55
37:DO:41:ARG:NH1	37:DO:45:LEU:HD13	2.22	0.55
37:DO:7:ARG:HH11	37:DO:7:ARG:HA	1.72	0.55
19:BT:18:LYS:O	19:BT:22:LEU:HD23	2.07	0.54
31:CE:95:ARG:O	31:CE:96:ARG:O	2.25	0.54
40:CR:89:ARG:HB3	40:CR:92:TYR:HB3	1.89	0.54
41:CS:23:ARG:O	41:CS:25:GLY:N	2.41	0.54
44:CW:60:ASN:ND2	58:C1:511:C:O2'	2.39	0.54
58:D1:431:U:O4'	58:D1:431:U:O2	2.25	0.54
28:DB:30:GLU:HB2	28:DB:35:LYS:HE3	1.88	0.54
31:DE:47:LYS:CB	31:DE:82:LEU:HD12	2.37	0.54
32:DF:153:LYS:HD3	32:DF:153:LYS:N	2.22	0.54
46:DY:7:VAL:HB	46:DY:8:LYS:CD	2.37	0.54
12:AL:50:SER:O	12:AL:51:ALA:HB2	2.07	0.54
18:AS:52:PRO:O	18:AS:56:THR:HG23	2.08	0.54
2:BA:24:TRP:CZ3	2:BA:26:PRO:HA	2.41	0.54
19:BT:50:ALA:HB1	19:BT:57:HIS:HB3	1.89	0.54
58:C1:2222:C:O2'	58:C1:2223:C:H5'	2.07	0.54
58:C1:274:C:O2'	58:C1:275:C:C6	2.56	0.54
58:C1:566:C:C2'	58:C1:567:C:OP1	2.55	0.54
58:D1:1009:C:H5''	58:D1:1009:C:H6	1.72	0.54
58:D1:1309:G:H3'	58:D1:1310:A:H5''	1.90	0.54
58:D1:439:C:H4'	58:D1:1901:C:O2'	2.07	0.54
58:D1:2789:G:H5''	58:D1:2790:A:H5'	1.89	0.54
32:DF:85:LYS:HD2	32:DF:145:ALA:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:BI:53:VAL:HG23	9:BI:55:ALA:H	1.72	0.54
10:BJ:34:VAL:HG22	10:BJ:74:ILE:HG22	1.89	0.54
26:C4:17:C:C4	26:C4:18:U:O4	2.60	0.54
28:CB:30:GLU:HG3	28:CB:63:ARG:CZ	2.36	0.54
28:CB:34:VAL:HG23	28:CB:35:LYS:H	1.71	0.54
51:CL:19:GLN:HE22	51:CL:52:HIS:CE1	2.24	0.54
35:CM:128:HIS:O	35:CM:130:HIS:N	2.40	0.54
44:CW:5:ALA:HB2	44:CW:54:ALA:HB2	1.88	0.54
58:D1:1792:A:O5'	58:D1:1792:A:H8	1.90	0.54
61:D4:33:C:H2'	61:D4:33:C:O2	2.07	0.54
41:DS:104:ASN:HB3	41:DS:105:LEU:HG	1.89	0.54
9:AI:50:LEU:HD21	9:AI:81:ILE:CG2	2.38	0.54
13:AM:3:ARG:HG2	13:AM:9:ILE:CG1	2.37	0.54
26:C4:76:C:H4'	66:C1:3001:3V6:H14	1.90	0.54
28:CB:34:VAL:HG23	28:CB:35:LYS:N	2.22	0.54
30:CD:65:TRP:CZ3	30:CD:75:HIS:HD2	2.25	0.54
40:CR:89:ARG:HG2	40:CR:92:TYR:HA	1.88	0.54
58:D1:113:C:O2'	58:D1:123:A:N3	2.35	0.54
58:D1:1346:A:HO2'	58:D1:1347:A:H2'	1.63	0.54
4:AD:117:ALA:O	4:AD:121:VAL:HG23	2.07	0.54
4:AD:92:VAL:O	4:AD:96:LEU:HD13	2.08	0.54
11:AK:111:ASP:HA	18:AS:84:LYS:HE2	1.90	0.54
58:C1:1066:A:H8	58:C1:1066:A:H3'	1.73	0.54
58:C1:1286:A:C2'	58:C1:1287:A:O5'	2.55	0.54
53:C6:2:ALA:HA	58:C1:2036:A:H1'	1.89	0.54
37:CO:17:LYS:O	37:CO:17:LYS:HG2	2.08	0.54
58:D1:1097:C:H3'	58:D1:1097:C:C6	2.42	0.54
58:D1:2120:U:O2	58:D1:2120:U:C2'	2.55	0.54
31:DE:63:ILE:HD12	31:DE:141:PHE:CG	2.42	0.54
41:DS:29:ARG:HB3	41:DS:85:LYS:HA	1.88	0.54
2:AA:185:ILE:HG22	2:AA:199:TYR:CD1	2.42	0.54
15:BO:23:GLY:O	15:BO:24:SER:HB3	2.08	0.54
56:C9:61:LEU:CD1	56:C9:62:LEU:HD12	2.36	0.54
31:CE:36:LYS:HD2	31:CE:160:VAL:HG21	1.88	0.54
31:CE:72:ARG:HA	31:CE:87:PRO:HG2	1.87	0.54
35:CM:56:ASN:HA	35:CM:125:GLY:H	1.72	0.54
29:DC:132:HIS:CD2	29:DC:135:HIS:NE2	2.76	0.54
31:DE:42:GLY:HA2	58:D1:2323:U:O2	2.06	0.54
41:DS:57:PHE:O	41:DS:59:THR:N	2.40	0.54
42:DT:106:PHE:O	42:DT:109:LEU:HB2	2.07	0.54
4:BD:168:ARG:N	4:BD:168:ARG:HD2	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:C1:1574:A:N7	58:C1:1575:G:C8	2.76	0.54
30:CD:63:LYS:HE2	58:C1:721:A:OP1	2.07	0.54
30:CD:9:ILE:HA	30:CD:13:SER:O	2.08	0.54
32:CF:20:ALA:HB1	32:CF:21:PRO:CD	2.38	0.54
46:CY:10:GLY:CA	46:CY:27:VAL:HG13	2.36	0.54
58:D1:1538:C:O2	58:D1:1538:C:C2'	2.56	0.54
61:D4:2:G:N2	61:D4:73:A:N3	2.45	0.54
41:DS:102:ILE:O	41:DS:106:SER:HB3	2.07	0.54
7:AG:116:ALA:O	7:AG:119:ARG:N	2.36	0.54
14:AN:44:LEU:HD12	14:AN:44:LEU:C	2.28	0.54
4:BD:12:CYS:SG	4:BD:19:LEU:O	2.65	0.54
58:C1:1333:U:H4'	58:C1:1334:C:OP2	2.07	0.54
58:C1:154:C:C3'	58:C1:157:U:P	2.95	0.54
58:C1:2672:G:H2'	58:C1:2673:A:C4	2.43	0.54
30:CD:22:ALA:O	30:CD:26:ALA:HB2	2.08	0.54
31:CE:39:ILE:HG13	31:CE:92:VAL:HG13	1.90	0.54
35:CM:2:LYS:O	35:CM:4:TYR:CE1	2.61	0.54
41:CS:129:ARG:HH12	41:CS:131:ALA:HB2	1.72	0.54
41:CS:28:VAL:HG21	41:CS:88:ILE:HG13	1.90	0.54
58:D1:47:A:H5''	58:D1:49:G:O4'	2.07	0.54
61:D4:17:C:O2'	61:D4:18:U:OP1	2.24	0.54
62:DA:72:VAL:HG21	62:DA:161:UNK:HA	1.90	0.54
29:DC:16:ARG:O	29:DC:18:ASP:N	2.41	0.54
45:DX:27:THR:HB	45:DX:80:ILE:HB	1.89	0.54
58:C1:1067:G:O2'	58:C1:1068:U:OP2	2.17	0.54
27:CA:18:LYS:HB2	27:CA:22:ILE:HD12	1.88	0.54
30:CD:122:LYS:HB3	30:CD:191:ARG:HG3	1.89	0.54
35:CM:42:TRP:CD1	42:CT:63:VAL:HG11	2.43	0.54
46:CY:98:VAL:O	46:CY:99:CYS:SG	2.65	0.54
58:D1:1154:C:C5	58:D1:1155:G:C6	2.96	0.54
35:DM:23:LEU:HD23	58:D1:1184:C:OP1	2.08	0.54
58:D1:2155:A:H2'	58:D1:2155:A:N3	2.23	0.54
28:DB:47:GLY:HA3	58:D1:819:U:H4'	1.90	0.54
43:DU:17:GLY:HA2	43:DU:96:ILE:HB	1.90	0.54
15:AO:82:ILE:HG12	15:AO:87:ILE:HG13	1.89	0.54
58:C1:2416:G:O2'	58:C1:2422:A:N6	2.40	0.54
51:CL:49:LYS:NZ	58:C1:897:U:OP1	2.39	0.54
49:CH:41:ARG:HD3	49:CH:43:TYR:OH	2.07	0.54
47:CZ:151:HIS:HA	47:CZ:171:ILE:HG12	1.90	0.54
38:DP:56:ARG:NH2	58:D1:2481:G:OP1	2.40	0.54
62:DA:58:VAL:HG21	62:DA:166:UNK:H	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:DB:30:GLU:HB3	28:DB:35:LYS:HG3	1.89	0.54
4:AD:43:HIS:O	4:AD:45:GLN:N	2.40	0.53
15:AO:82:ILE:HD13	15:AO:82:ILE:C	2.29	0.53
10:BJ:32:ALA:H	10:BJ:78:ASN:HD21	1.55	0.53
13:BM:112:GLY:O	13:BM:113:PRO:O	2.26	0.53
58:C1:154:C:O3'	58:C1:157:U:P	2.66	0.53
58:C1:2403:A:H2	58:C1:2435:C:H42	1.55	0.53
37:CO:38:GLN:CD	58:C1:987:U:OP2	2.47	0.53
38:CP:16:ARG:NH2	58:C1:996:G:OP1	2.41	0.53
25:C3:30:G:H2'	25:C3:31:A:C8	2.43	0.53
49:CH:51:VAL:O	49:CH:57:GLU:O	2.26	0.53
35:CM:42:TRP:O	42:CT:64:ARG:NH1	2.23	0.53
41:CS:13:ARG:HA	41:CS:13:ARG:NE	2.20	0.53
44:CW:64:MET:O	44:CW:65:LEU:HB3	2.08	0.53
58:D1:659:C:O2'	58:D1:663:U:OP1	2.26	0.53
34:DJ:5:UNK:O	58:D1:1089:G:OP2	2.27	0.53
42:DT:31:SER:C	42:DT:33:ARG:H	2.11	0.53
42:DT:90:VAL:HG21	43:DU:47:VAL:HG21	1.90	0.53
13:AM:112:GLY:O	13:AM:113:PRO:O	2.27	0.53
7:BG:101:LEU:O	7:BG:105:VAL:HG23	2.08	0.53
7:BG:113:GLU:HG2	7:BG:119:ARG:HG2	1.90	0.53
58:C1:2475:C:O2'	58:C1:2476:C:O4'	2.26	0.53
26:C4:17:C:C2	26:C4:18:U:C4	2.96	0.53
37:CO:21:ARG:O	37:CO:23:PRO:HD3	2.08	0.53
40:CR:35:ILE:H	40:CR:53:SER:HB2	1.71	0.53
43:CU:38:LEU:HD23	43:CU:39:LEU:N	2.24	0.53
61:D4:17:C:C6	61:D4:18:U:N3	2.77	0.53
30:DD:116:ASP:OD2	37:DO:5:ASP:N	2.42	0.53
46:DY:10:GLY:HA2	46:DY:27:VAL:HG13	1.90	0.53
10:BJ:58:ASP:O	10:BJ:59:SER:C	2.47	0.53
58:C1:1393:G:H2'	58:C1:1394:A:H5''	1.90	0.53
26:C4:16:C:O2'	26:C4:62:C:P	2.67	0.53
28:CB:10:THR:C	28:CB:11:PRO:O	2.47	0.53
28:CB:49:ILE:HG23	58:C1:825:U:OP1	2.08	0.53
37:CO:85:LEU:H	37:CO:85:LEU:HD23	1.72	0.53
43:CU:22:VAL:O	43:CU:23:GLU:CB	2.55	0.53
47:CZ:53:ILE:HG23	47:CZ:71:VAL:HB	1.90	0.53
58:D1:2331:A:H2'	58:D1:2331:A:N3	2.24	0.53
58:D1:2529:A:C8	58:D1:2529:A:H5'	2.43	0.53
29:DC:4:ILE:HG12	29:DC:5:LEU:O	2.08	0.53
31:DE:26:GLN:HE21	31:DE:26:GLN:N	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:DP:43:THR:HB	38:DP:45:GLN:HE21	1.73	0.53
39:DQ:87:TYR:O	39:DQ:89:ASP:N	2.38	0.53
41:DS:23:ARG:O	41:DS:25:GLY:N	2.42	0.53
41:DS:27:THR:O	41:DS:28:VAL:CG2	2.53	0.53
47:DZ:101:PRO:HA	47:DZ:123:ASP:HB3	1.90	0.53
58:C1:1377:G:H5''	58:C1:1377:G:H8	1.73	0.53
58:C1:2548:U:H2'	58:C1:2549:C:C6	2.44	0.53
28:CB:240:ALA:HB1	28:CB:241:PRO:HD2	1.90	0.53
31:CE:57:ALA:CB	31:CE:90:LEU:HD21	2.38	0.53
58:D1:1403:G:O2'	58:D1:1404:A:H5''	2.07	0.53
38:DP:56:ARG:NE	58:D1:2480:A:O2'	2.40	0.53
4:BD:161:ASN:O	4:BD:165:MET:HG2	2.08	0.53
13:BM:3:ARG:HG2	13:BM:9:ILE:HG12	1.90	0.53
53:C6:3:LYS:O	53:C6:4:HIS:C	2.46	0.53
56:C9:30:ARG:O	56:C9:30:ARG:HD3	2.08	0.53
44:CW:91:GLY:HA2	58:C1:1659:A:N1	2.24	0.53
58:D1:1740:C:O2'	58:D1:1741:G:C4	2.60	0.53
58:D1:2302:U:H2'	58:D1:2303:C:C6	2.44	0.53
62:DA:197:UNK:O	62:DA:199:UNK:N	2.41	0.53
28:DB:30:GLU:HG3	28:DB:63:ARG:CZ	2.38	0.53
30:DD:34:TRP:CZ2	37:DO:12:ALA:HB2	2.44	0.53
37:DO:144:GLU:N	37:DO:145:PRO:CD	2.71	0.53
37:DO:18:ARG:CZ	37:DO:18:ARG:HB3	2.38	0.53
20:AU:96:GLY:O	20:AU:97:ALA:O	2.27	0.53
7:BG:112:PRO:HD2	7:BG:113:GLU:OE2	2.09	0.53
9:BI:15:ALA:HB2	9:BI:65:VAL:HG23	1.90	0.53
11:BK:21:ILE:HB	11:BK:84:VAL:HG12	1.90	0.53
58:C1:1549:C:O2'	58:C1:1550:C:C5'	2.56	0.53
58:C1:1565:U:H2'	58:C1:1566:G:O4'	2.08	0.53
58:C1:191:C:H3'	58:C1:192:A:H5''	1.90	0.53
58:C1:2692:C:H5	58:C1:2737:A:H62	1.55	0.53
28:CB:165:ILE:HD13	28:CB:175:LEU:HD21	1.90	0.53
37:CO:46:LYS:HE2	58:C1:183:A:OP1	2.08	0.53
58:C1:144:G:C2'	58:C1:145:G:H5'	2.38	0.53
30:CD:90:PHE:CD1	58:C1:610:U:H1'	2.44	0.53
55:C8:8:ASN:HD22	55:C8:9:ARG:N	2.05	0.53
29:CC:119:ARG:HG2	29:CC:160:TYR:HB2	1.90	0.53
37:CO:56:SER:O	37:CO:58:THR:N	2.42	0.53
58:D1:1152:G:C2'	58:D1:1153:U:O5'	2.57	0.53
58:D1:2671:A:H5'	58:D1:2672:G:N2	2.24	0.53
29:DC:197:ILE:HD11	29:DC:199:ARG:HE	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:DF:148:ILE:O	32:DF:162:ILE:HD11	2.09	0.53
39:DQ:96:ARG:HB2	39:DQ:117:VAL:HG23	1.91	0.53
46:DY:46:LYS:N	46:DY:62:GLU:HG2	2.23	0.53
3:AC:164:ARG:NH1	3:AC:166:GLU:OE1	2.41	0.53
24:BC:113:ALA:HB3	24:BC:114:PRO:CD	2.39	0.53
58:C1:2054:A:O2'	58:C1:2056:G:OP2	2.23	0.53
37:DO:18:ARG:HD2	58:D1:708:G:OP1	2.09	0.53
63:DW:29:LEU:HD21	63:DW:33:ARG:NH2	2.24	0.53
14:AN:23:ARG:HD2	14:AN:28:GLY:O	2.09	0.53
13:BM:15:VAL:O	13:BM:19:LEU:HD23	2.09	0.53
58:C1:1066:A:C8	58:C1:1066:A:H3'	2.44	0.53
49:CH:46:LEU:HD23	49:CH:61:ARG:HD3	1.91	0.53
47:CZ:51:ALA:O	47:CZ:52:SER:HB3	2.09	0.53
58:D1:2553:A:N3	58:D1:2553:A:O4'	2.42	0.53
58:D1:2854:G:O2'	58:D1:2855:G:H5'	2.09	0.53
38:DP:6:ARG:NH2	58:D1:915:G:O3'	2.37	0.53
61:D4:48:U:H3'	61:D4:49:C:C5'	2.39	0.53
37:DO:62:LEU:H	37:DO:62:LEU:HD23	1.74	0.53
37:DO:6:LEU:CG	37:DO:8:PRO:O	2.56	0.53
42:DT:92:ARG:CZ	58:D1:1041:A:OP2	2.57	0.53
43:DU:15:GLU:O	43:DU:16:PRO:C	2.47	0.53
6:AF:100:ASN:HD21	18:AS:23:LYS:HG2	1.74	0.53
19:AT:49:ILE:O	19:AT:60:VAL:HG12	2.08	0.53
10:BJ:90:LEU:N	10:BJ:91:PRO:CD	2.72	0.53
30:CD:95:ARG:NH2	58:C1:1292:A:OP1	2.42	0.53
56:C9:62:LEU:HD13	58:C1:230:G:C5'	2.33	0.53
29:CC:137:HIS:HB3	29:CC:138:PRO:CD	2.38	0.53
40:CR:69:VAL:O	40:CR:72:ALA:HB3	2.09	0.53
46:CY:8:LYS:HD3	46:CY:72:VAL:HG23	1.90	0.53
58:D1:1450:U:H2'	58:D1:1451:U:H6	1.73	0.53
58:D1:1685:U:O2'	58:D1:1686:C:H5''	2.09	0.53
49:DH:90:ILE:O	49:DH:94:LEU:N	2.39	0.53
41:DS:60:THR:HG22	41:DS:77:PRO:HA	1.90	0.53
6:AF:60:PHE:C	6:AF:61:LEU:HD12	2.30	0.52
4:BD:10:ARG:HG2	4:BD:11:LEU:HD23	1.92	0.52
58:C1:2604:U:H2'	58:C1:2605:C:C6	2.44	0.52
28:CB:24:ILE:HG12	28:CB:25:THR:N	2.23	0.52
37:CO:114:ILE:HD12	37:CO:115:LEU:N	2.24	0.52
58:D1:1895:G:H5'	58:D1:1896:C:P	2.49	0.52
28:DB:238:GLY:O	58:D1:2602:C:OP2	2.27	0.52
29:DC:134:ILE:HD12	29:DC:134:ILE:C	2.28	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:DC:188:VAL:O	29:DC:189:PRO:O	2.27	0.52
29:DC:24:THR:CG2	29:DC:184:VAL:HG23	2.40	0.52
31:DE:166:ASP:HA	31:DE:169:ALA:HB3	1.90	0.52
38:DP:1:MET:O	38:DP:2:LEU:HB2	2.10	0.52
41:DS:92:GLY:O	41:DS:93:ARG:C	2.47	0.52
3:AC:50:ALA:HB2	3:AC:75:VAL:HB	1.91	0.52
5:AE:76:ILE:HG12	5:AE:77:PRO:HD2	1.91	0.52
13:AM:100:GLY:C	13:AM:101:GLN:HG2	2.29	0.52
14:BN:15:LYS:O	14:BN:16:PHE:O	2.27	0.52
26:C4:1:C:H2'	26:C4:1:C:O2	2.08	0.52
28:CB:10:THR:HG23	28:CB:13:ARG:HB3	1.92	0.52
36:CN:111:PHE:HB3	36:CN:114:ILE:HD13	1.89	0.52
46:CY:7:VAL:HB	46:CY:8:LYS:HD2	1.92	0.52
58:D1:1064:U:O2'	58:D1:1066:A:H2	1.91	0.52
58:D1:2228:A:H1'	58:D1:2230:G:C4	2.43	0.52
54:D7:46:HIS:HA	54:D7:47:THR:HG21	1.90	0.52
30:DD:202:PHE:O	30:DD:206:ILE:HG12	2.09	0.52
37:DO:58:THR:O	37:DO:61:ARG:NH2	2.41	0.52
5:BE:9:LYS:HB3	5:BE:112:LEU:HD11	1.92	0.52
13:BM:106:ASN:O	13:BM:107:ALA:CB	2.57	0.52
1:A2:19:U:N3	25:C2:37:A:C2	2.77	0.52
56:C9:16:ILE:HD12	56:C9:57:ARG:HG2	1.91	0.52
38:CP:34:LEU:HD11	38:CP:129:THR:HB	1.91	0.52
42:CT:91:ASP:OD1	42:CT:96:ALA:HB2	2.10	0.52
45:CX:35:THR:O	45:CX:39:ILE:HG12	2.09	0.52
58:D1:1628:C:O2'	58:D1:1631:A:C8	2.60	0.52
58:D1:2667:U:H2'	58:D1:2668:A:H5''	1.91	0.52
25:D3:34:G:O6	25:D3:35:A:N6	2.41	0.52
25:D3:61:C:H2'	25:D3:62:C:C6	2.44	0.52
29:DC:144:ARG:HD3	58:D1:2583:A:C8	2.43	0.52
32:DF:41:MET:CE	32:DF:43:VAL:HG13	2.35	0.52
45:DX:29:TRP:CZ3	45:DX:78:LYS:HB3	2.44	0.52
6:BF:10:LEU:HD13	6:BF:61:LEU:HD13	1.91	0.52
20:BU:83:ARG:HA	20:BU:86:ARG:HD3	1.91	0.52
58:C1:1628:C:O2'	58:C1:1631:A:C8	2.61	0.52
58:C1:2147:A:H4'	58:C1:2148:G:O5'	2.10	0.52
25:C3:30:G:H2'	25:C3:31:A:H8	1.74	0.52
31:CE:51:ARG:NE	31:CE:51:ARG:HA	2.24	0.52
32:CF:124:GLU:HB2	32:CF:132:ARG:HG2	1.92	0.52
46:CY:79:CYS:HG	46:CY:80:GLY:H	1.49	0.52
47:CZ:17:ALA:HA	47:CZ:20:ARG:HD2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:D1:1463:G:OP1	58:D1:1633:C:O2'	2.24	0.52
58:D1:669:C:O2	58:D1:669:C:O4'	2.26	0.52
33:DI:127:VAL:HG22	33:DI:139:GLN:HA	1.91	0.52
37:DO:33:ARG:NH2	58:D1:609:C:H2'	2.24	0.52
37:DO:85:LEU:HB3	37:DO:114:ILE:HD11	1.92	0.52
4:BD:11:LEU:C	4:BD:13:ARG:N	2.59	0.52
4:BD:170:VAL:HG12	4:BD:174:LEU:HB2	1.91	0.52
6:BF:5:GLU:HG3	6:BF:93:SER:OG	2.10	0.52
17:BR:50:LYS:HE3	17:BR:51:TYR:CE1	2.45	0.52
58:C1:2554:G:H2'	58:C1:2555:G:C8	2.44	0.52
42:CT:92:ARG:HB2	43:CU:11:GLN:NE2	2.25	0.52
37:DO:64:LYS:HD2	56:D9:25:MET:SD	2.50	0.52
39:DQ:10:LEU:HB3	39:DQ:17:ARG:CD	2.39	0.52
10:AJ:61:GLU:OE2	14:AN:45:ARG:HD2	2.10	0.52
12:AL:32:PHE:HB3	12:AL:84:LEU:CD2	2.36	0.52
2:BA:135:GLN:O	2:BA:139:LYS:HG2	2.10	0.52
58:C1:154:C:H3'	58:C1:157:U:P	2.49	0.52
58:C1:1812:C:C4	58:C1:2598:A:N1	2.77	0.52
46:CY:2:ARG:C	46:CY:4:LYS:H	2.13	0.52
58:D1:1984:U:H4'	58:D1:1985:G:OP1	2.09	0.52
39:DQ:53:HIS:CD2	58:D1:2849:C:H5''	2.44	0.52
25:D3:67:C:H2'	25:D3:68:C:C6	2.45	0.52
61:D4:17:C:HO2'	61:D4:18:U:P	2.32	0.52
35:DM:42:TRP:CD1	42:DT:63:VAL:HG11	2.44	0.52
45:DX:12:VAL:CG1	45:DX:27:THR:OG1	2.57	0.52
46:DY:8:LYS:HB2	46:DY:28:LYS:NZ	2.24	0.52
10:AJ:6:ILE:HD11	10:AJ:72:VAL:HB	1.92	0.52
5:BE:131:ILE:O	5:BE:134:ALA:HB3	2.09	0.52
8:BH:103:VAL:CG2	8:BH:110:ALA:HB2	2.39	0.52
12:BL:38:THR:CG2	12:BL:57:LYS:HB3	2.39	0.52
14:BN:44:LEU:HD12	14:BN:44:LEU:C	2.30	0.52
58:C1:2412:U:C2'	58:C1:2413:C:H5''	2.38	0.52
58:C1:676:C:C6	58:C1:676:C:OP2	2.63	0.52
58:D1:1920:G:C2'	58:D1:1921:A:OP2	2.58	0.52
58:D1:2284:A:H2'	58:D1:2285:A:C8	2.44	0.52
58:D1:2554:G:H2'	58:D1:2555:G:C8	2.45	0.52
50:DK:63:VAL:HA	50:DK:66:GLU:HG2	1.92	0.52
36:DN:43:VAL:HG21	36:DN:52:VAL:CG1	2.40	0.52
41:DS:106:SER:C	41:DS:107:ASP:OD1	2.48	0.52
46:DY:26:LYS:HG2	46:DY:27:VAL:H	1.74	0.52
3:AC:134:ILE:HD11	3:AC:153:VAL:CG2	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:AL:91:LYS:O	12:AL:91:LYS:HG3	2.10	0.52
58:C1:2052:A:C6	58:C1:2509:C:H1'	2.44	0.52
58:C1:2810:A:O2'	58:C1:2903:U:H5'	2.10	0.52
28:CB:121:PRO:HB3	28:CB:135:PHE:HE2	1.72	0.52
28:CB:58:HIS:HD2	28:CB:59:LYS:O	1.93	0.52
32:CF:156:ALA:O	32:CF:157:TYR:C	2.48	0.52
37:CO:66:GLY:O	37:CO:67:MET:HB3	2.09	0.52
58:D1:1326:G:H5''	58:D1:1326:G:H8	1.74	0.52
39:DQ:77:ARG:NH1	58:D1:1500:U:OP1	2.42	0.52
58:D1:2487:A:C2	58:D1:2488:C:C6	2.98	0.52
28:DB:239:ARG:HB3	58:D1:2602:C:OP2	2.09	0.52
25:D3:25:C:H2'	25:D3:26:A:H8	1.75	0.52
42:DT:15:LYS:HZ1	58:D1:1261:C:P	2.30	0.52
14:AN:21:TYR:HD2	14:AN:22:THR:O	1.93	0.52
4:BD:30:LYS:C	4:BD:32:ALA:N	2.63	0.52
12:BL:75:HIS:HD2	12:BL:77:LEU:H	1.58	0.52
19:BT:29:ARG:O	19:BT:31:ILE:HG22	2.10	0.52
42:CT:14:HIS:CD2	42:CT:32:ALA:HB1	2.45	0.52
42:CT:70:ARG:HA	42:CT:74:LEU:O	2.10	0.52
25:D3:25:C:H2'	25:D3:26:A:C8	2.45	0.52
36:DN:24:VAL:CG2	36:DN:30:ALA:HB3	2.40	0.52
37:DO:16:ARG:HD3	37:DO:17:LYS:N	2.25	0.52
43:DU:38:LEU:HD23	43:DU:39:LEU:N	2.24	0.52
46:DY:81:LYS:HD3	46:DY:97:ARG:O	2.10	0.52
2:AA:84:GLU:HB3	2:AA:219:VAL:HG21	1.91	0.52
21:AW:5:ASP:O	21:AW:11:GLY:HA3	2.10	0.52
4:BD:26:CYS:CA	4:BD:31:CYS:HB2	2.39	0.52
10:BJ:61:GLU:OE2	14:BN:45:ARG:NH1	2.43	0.52
11:BK:21:ILE:HD12	11:BK:21:ILE:N	2.25	0.52
58:C1:552:A:C2	58:C1:2064:C:H4'	2.45	0.52
41:CS:46:GLU:O	41:CS:65:LYS:HD2	2.10	0.52
46:CY:17:SER:O	58:C1:333:A:OP1	2.28	0.52
58:D1:1066:A:H3'	58:D1:1066:A:C8	2.45	0.52
30:DD:167:ALA:O	30:DD:169:ASN:N	2.43	0.52
37:DO:30:THR:HG22	37:DO:31:ALA:H	1.75	0.52
37:DO:84:ASN:HA	37:DO:115:LEU:O	2.09	0.52
40:DR:83:LYS:HE2	40:DR:105:ALA:HB3	1.92	0.52
14:AN:40:CYS:SG	14:AN:43:CYS:N	2.77	0.51
16:BP:28:ARG:HH11	16:BP:28:ARG:HG2	1.76	0.51
42:CT:59:ARG:HD2	58:C1:1054:A:O4'	2.10	0.51
26:C4:49:C:C2	26:C4:60:A:H1'	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:CB:24:ILE:HA	28:CB:82:ILE:HG22	1.92	0.51
49:CH:90:ILE:O	49:CH:94:LEU:HB2	2.11	0.51
37:CO:114:ILE:O	37:CO:130:PHE:HA	2.10	0.51
40:CR:101:LEU:HD12	40:CR:102:ALA:O	2.10	0.51
41:CS:30:VAL:HG21	41:CS:83:ILE:HG13	1.92	0.51
44:CW:18:ARG:HG2	44:CW:76:VAL:HG13	1.92	0.51
29:DC:77:ILE:HG22	29:DC:78:LEU:HD12	1.92	0.51
37:DO:13:ASN:HD22	37:DO:13:ASN:C	2.12	0.51
37:DO:48:PRO:O	37:DO:50:ARG:N	2.43	0.51
4:AD:86:LYS:HE3	4:AD:86:LYS:HA	1.91	0.51
58:C1:1766:A:C2	58:C1:1768:G:H8	2.28	0.51
58:C1:2487:A:N3	58:C1:2488:C:H5'	2.26	0.51
44:CW:60:ASN:HD21	58:C1:511:C:H4'	1.73	0.51
58:C1:718:C:O2'	58:C1:719:C:H5'	2.09	0.51
31:CE:161:THR:HG22	31:CE:163:ALA:H	1.75	0.51
37:CO:84:ASN:HA	37:CO:115:LEU:O	2.10	0.51
43:CU:52:VAL:HG13	43:CU:55:ALA:HB3	1.93	0.51
58:D1:1777:G:C2'	58:D1:1778:G:H5'	2.38	0.51
58:D1:2147:A:O2'	58:D1:2148:G:OP2	2.27	0.51
58:D1:2666:G:HO2'	58:D1:2667:U:P	2.27	0.51
58:D1:634:C:C2'	58:D1:635:G:H5'	2.41	0.51
36:DN:98:VAL:CG1	36:DN:117:LEU:HB3	2.41	0.51
46:DY:38:ILE:HD12	46:DY:66:PRO:HA	1.91	0.51
3:AC:11:ARG:O	3:AC:13:GLY:N	2.44	0.51
13:AM:15:VAL:O	13:AM:19:LEU:HD23	2.11	0.51
18:BS:56:THR:HB	18:BS:58:LEU:HD13	1.91	0.51
58:C1:636:U:O4'	58:C1:636:U:O2	2.25	0.51
37:CO:16:ARG:CZ	37:CO:18:ARG:HG2	2.41	0.51
43:CU:91:TYR:C	43:CU:91:TYR:HD1	2.14	0.51
46:CY:26:LYS:O	46:CY:27:VAL:O	2.28	0.51
58:D1:1724:G:N2	58:D1:2010:G:H22	2.07	0.51
58:D1:2168:G:H2'	58:D1:2169:G:O4'	2.11	0.51
58:D1:2542:A:N7	58:D1:2671:A:N6	2.58	0.51
61:D4:76:C:O2'	66:D1:3001:3V6:H8	2.09	0.51
28:DB:45:ASN:CG	28:DB:46:GLN:H	2.13	0.51
29:DC:24:THR:HG21	29:DC:188:VAL:CG1	2.40	0.51
31:DE:45:GLU:CD	31:DE:45:GLU:H	2.14	0.51
31:DE:47:LYS:CA	31:DE:88:ILE:HD13	2.40	0.51
37:DO:83:VAL:CG1	37:DO:112:LEU:HD21	2.40	0.51
41:DS:25:GLY:O	41:DS:26:ASP:HB2	2.10	0.51
13:AM:90:LEU:C	13:AM:92:HIS:H	2.14	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:C1:2192:A:O2'	58:C1:2193:U:O4'	2.26	0.51
27:CA:58:VAL:HG21	27:CA:166:UNK:N	2.25	0.51
36:CN:96:THR:O	36:CN:97:ARG:HG2	2.11	0.51
47:CZ:38:TYR:O	47:CZ:38:TYR:HD1	1.93	0.51
58:D1:2612:C:H6	58:D1:2612:C:O5'	1.93	0.51
31:DE:45:GLU:O	31:DE:46:ALA:HB3	2.10	0.51
50:DK:48:HIS:O	50:DK:52:ASP:HB2	2.11	0.51
63:DW:24:ILE:HG21	63:DW:36:LEU:HD21	1.93	0.51
47:DZ:129:SER:HB3	47:DZ:132:ASN:HD22	1.76	0.51
10:AJ:54:PHE:CE2	10:AJ:55:LYS:HE3	2.45	0.51
19:BT:5:LEU:HD12	19:BT:8:GLY:C	2.31	0.51
58:C1:2808:U:O4'	58:C1:2808:U:O2	2.28	0.51
37:CO:64:LYS:HB3	56:C9:25:MET:HG3	1.92	0.51
39:CQ:73:VAL:O	39:CQ:76:VAL:HG12	2.10	0.51
58:D1:1530:G:H1'	58:D1:1550:C:N4	2.25	0.51
58:D1:2904:C:C6	58:D1:2904:C:H3'	2.44	0.51
60:D2:55:U:H3'	60:D2:55:U:O2	2.11	0.51
53:D6:40:LYS:CE	53:D6:46:CYS:HB3	2.41	0.51
29:DC:30:PRO:O	29:DC:32:PRO:HD3	2.10	0.51
30:DD:169:ASN:HD21	58:D1:345:A:H3'	1.76	0.51
37:DO:85:LEU:H	37:DO:85:LEU:HD23	1.74	0.51
43:DU:28:GLU:HB3	43:DU:29:PRO:HD2	1.92	0.51
10:AJ:61:GLU:OE1	14:AN:58:LYS:NZ	2.33	0.51
4:BD:134:ASP:OD2	4:BD:134:ASP:N	2.44	0.51
6:BF:91:VAL:HG11	18:BS:72:ARG:NH1	2.26	0.51
29:CC:132:HIS:O	58:C1:1704:C:OP1	2.27	0.51
31:CE:29:TRP:O	31:CE:33:ARG:NH1	2.44	0.51
41:CS:128:GLU:O	41:CS:130:ALA:N	2.43	0.51
41:CS:92:GLY:O	41:CS:93:ARG:C	2.49	0.51
58:D1:2042:C:H4'	58:D1:2043:U:OP2	2.10	0.51
42:DT:31:SER:O	42:DT:33:ARG:N	2.40	0.51
58:C1:1390:C:O2'	58:C1:1391:G:H5'	2.10	0.51
29:CC:60:ASN:CB	58:C1:2820:G:OP1	2.54	0.51
58:C1:663:U:H2'	58:C1:664:C:C6	2.45	0.51
26:C4:10:G:H8	26:C4:10:G:C5'	2.23	0.51
32:CF:43:VAL:HG11	32:CF:52:VAL:HG22	1.93	0.51
58:D1:1249:U:H4'	58:D1:1250:G:OP2	2.11	0.51
58:D1:1377:G:H22	58:D1:1654:A:C2'	2.24	0.51
58:D1:2083:A:C2'	58:D1:2084:C:C5'	2.88	0.51
56:D9:52:LYS:N	56:D9:53:PRO:CD	2.73	0.51
30:DD:108:LYS:O	30:DD:112:MET:HG3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:DT:92:ARG:HD3	42:DT:94:ASN:HB3	1.92	0.51
4:AD:110:PHE:CD1	4:AD:110:PHE:N	2.78	0.51
58:C1:1479:A:H61	58:C1:1604:A:N6	2.09	0.51
29:CC:203:LYS:O	29:CC:204:ALA:HB2	2.10	0.51
39:CQ:85:PRO:O	39:CQ:87:TYR:N	2.44	0.51
43:CU:89:GLN:OE1	43:CU:90:PRO:HD2	2.10	0.51
47:CZ:57:ILE:HD12	47:CZ:57:ILE:N	2.26	0.51
58:D1:2239:G:C6	58:D1:2240:C:C4	2.99	0.51
62:DA:212:UNK:O	62:DA:213:UNK:CB	2.58	0.51
37:DO:59:LEU:HA	37:DO:61:ARG:CZ	2.41	0.51
40:DR:96:GLY:O	40:DR:98:VAL:N	2.36	0.51
43:DU:38:LEU:C	43:DU:39:LEU:HD13	2.31	0.51
9:AI:40:LEU:O	9:AI:42:ARG:N	2.44	0.51
18:AS:56:THR:HB	18:AS:58:LEU:HD13	1.92	0.51
19:AT:9:VAL:O	19:AT:9:VAL:HG12	2.11	0.51
18:BS:44:LEU:O	18:BS:45:SER:O	2.29	0.51
58:C1:2226:G:N2	58:C1:2227:G:H4'	2.26	0.51
49:CH:29:GLY:HA3	58:C1:2407:G:O2'	2.11	0.51
39:CQ:90:ARG:NH1	58:C1:2889:C:O3'	2.42	0.51
29:CC:36:ARG:NH1	29:CC:85:ASN:OD1	2.44	0.51
32:CF:144:VAL:O	32:CF:148:ILE:HG12	2.11	0.51
35:CM:58:ASP:O	35:CM:60:ILE:N	2.44	0.51
40:CR:16:ASN:OD1	40:CR:17:ARG:N	2.44	0.51
44:CW:18:ARG:NH1	44:CW:76:VAL:O	2.44	0.51
45:CX:11:PRO:HB2	45:CX:12:VAL:HG22	1.93	0.51
47:CZ:151:HIS:CB	47:CZ:170:THR:HA	2.41	0.51
47:CZ:24:LEU:HD21	47:CZ:86:VAL:HG23	1.91	0.51
58:D1:1538:C:O2	58:D1:1538:C:H2'	2.11	0.51
58:D1:2450:A:OP1	66:D1:3001:3V6:N	2.43	0.51
58:D1:69:A:H5"	58:D1:71:A:C8	2.46	0.51
30:DD:24:LEU:HB3	30:DD:25:PRO:HD2	1.93	0.51
30:DD:66:PRO:O	30:DD:67:GLN:CB	2.59	0.51
41:DS:3:ARG:O	41:DS:4:GLY:C	2.49	0.51
5:AE:76:ILE:CG1	5:AE:77:PRO:HD2	2.40	0.51
12:AL:70:ILE:HG12	12:AL:100:ILE:HD12	1.92	0.51
7:BG:16:LEU:CD1	9:BI:42:ARG:HA	2.40	0.51
58:C1:2154:G:C6	58:C1:2178:G:O6	2.64	0.51
42:CT:92:ARG:NE	58:C1:1041:A:H4'	2.26	0.51
58:D1:2309:A:H2'	58:D1:2310:G:O4'	2.10	0.51
58:D1:2535:G:H8	58:D1:2535:G:C5'	2.24	0.51
32:DF:117:PRO:HB3	32:DF:123:PHE:CE1	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:DI:9:LEU:H	33:DI:13:GLY:HA2	1.76	0.51
63:DW:80:PRO:HB3	58:D1:25:G:OP1	2.10	0.51
45:DX:18:TYR:C	45:DX:20:GLY:N	2.65	0.51
4:BD:117:ALA:O	4:BD:121:VAL:HG23	2.11	0.50
5:BE:91:LEU:CD1	5:BE:120:THR:HG22	2.40	0.50
7:BG:143:ARG:O	7:BG:145:ALA:O	2.29	0.50
58:C1:1697:G:N2	58:C1:2028:C:C2	2.79	0.50
58:C1:559:C:O2'	58:C1:560:A:H5'	2.10	0.50
30:CD:34:TRP:CZ2	37:CO:12:ALA:HB2	2.47	0.50
28:DB:62:TYR:OH	58:D1:1846:G:H8	1.93	0.50
58:D1:2786:C:H2'	58:D1:2787:A:O4'	2.11	0.50
31:DE:64:THR:HG23	31:DE:66:GLN:H	1.75	0.50
32:DF:92:ILE:O	32:DF:94:TYR:N	2.44	0.50
35:DM:15:LEU:HB2	35:DM:134:ARG:HB2	1.93	0.50
35:DM:41:ASP:N	35:DM:41:ASP:OD1	2.43	0.50
47:DZ:52:SER:OG	47:DZ:53:ILE:N	2.43	0.50
9:AI:53:VAL:O	9:AI:54:ASP:HB2	2.12	0.50
4:BD:80:GLU:O	4:BD:84:LYS:HG2	2.10	0.50
26:C4:12:G:H2'	26:C4:13:C:O5'	2.12	0.50
27:CA:78:ALA:HB1	27:CA:82:LYS:HB2	1.94	0.50
51:CL:59:VAL:OXT	51:CL:59:VAL:HG12	2.11	0.50
44:CW:64:MET:O	44:CW:65:LEU:CB	2.58	0.50
58:D1:579:U:H2'	58:D1:580:G:H8	1.76	0.50
2:AA:20:GLU:HG3	2:AA:191:ASP:HB2	1.93	0.50
10:AJ:6:ILE:HG13	10:AJ:72:VAL:O	2.11	0.50
58:C1:1216:G:H5'	58:C1:1217:G:OP2	2.11	0.50
54:C7:22:ALA:HB2	54:C7:39:TYR:CE2	2.47	0.50
28:CB:237:GLU:OE1	58:C1:2611:A:OP2	2.29	0.50
30:CD:132:VAL:HG13	30:CD:133:ASN:CG	2.31	0.50
35:CM:65:LYS:O	35:CM:69:GLN:HG3	2.11	0.50
37:CO:107:LYS:O	37:CO:109:GLY:N	2.39	0.50
41:CS:106:SER:HA	41:CS:110:ILE:HG12	1.94	0.50
43:CU:72:VAL:HG23	43:CU:85:LYS:HB3	1.92	0.50
58:D1:2738:U:O4'	58:D1:2738:U:O2	2.29	0.50
56:D9:51:ALA:N	56:D9:53:PRO:HD2	2.25	0.50
28:DB:259:THR:HG21	58:D1:1833:A:O2'	2.12	0.50
24:BC:52:LEU:H	24:BC:52:LEU:HD23	1.75	0.50
24:BC:86:VAL:O	24:BC:90:GLU:HG2	2.10	0.50
7:BG:118:VAL:O	7:BG:121:ALA:HB3	2.12	0.50
58:C1:2226:G:N2	58:C1:2227:G:H5'	2.26	0.50
58:C1:275:C:C2'	58:C1:276:G:H5'	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:C1:88:U:O2'	58:C1:89:A:H5''	2.11	0.50
25:C2:27:G:H2'	25:C2:28:G:C8	2.46	0.50
36:CN:114:ILE:H	36:CN:114:ILE:HD12	1.76	0.50
40:CR:89:ARG:CG	40:CR:92:TYR:HA	2.41	0.50
41:CS:90:GLN:NE2	41:CS:124:ASP:OD2	2.44	0.50
43:CU:91:TYR:C	43:CU:91:TYR:CD1	2.85	0.50
58:D1:2057:C:H5'	58:D1:2057:C:C6	2.44	0.50
58:D1:2448:U:H2'	58:D1:2449:U:C5'	2.41	0.50
29:DC:77:ILE:HG21	58:D1:2646:C:OP1	2.10	0.50
58:D1:648:C:O2	58:D1:703:U:H5'	2.10	0.50
58:D1:715:G:H4'	58:D1:716:A:OP2	2.11	0.50
58:D1:7:A:H2'	58:D1:8:U:C6	2.46	0.50
31:DE:10:LYS:O	31:DE:15:VAL:HG23	2.12	0.50
50:DK:46:GLN:HA	50:DK:46:GLN:OE1	2.11	0.50
50:DK:71:ASN:O	50:DK:71:ASN:OD1	2.30	0.50
37:DO:47:ASP:HB3	37:DO:48:PRO:C	2.32	0.50
64:DV:43:G:H2'	64:DV:44:A:C8	2.47	0.50
3:AC:11:ARG:O	3:AC:12:LEU:C	2.49	0.50
15:AO:25:THR:HG21	15:AO:70:LEU:HB2	1.93	0.50
2:BA:124:SER:OG	2:BA:125:PRO:HD2	2.10	0.50
58:C1:2209:C:H2'	58:C1:2210:U:C6	2.47	0.50
58:C1:2596:U:O4'	58:C1:2596:U:O2	2.28	0.50
35:CM:46:VAL:O	35:CM:47:ALA:HB3	2.11	0.50
46:CY:31:LEU:HB2	46:CY:32:PRO:HA	1.93	0.50
35:DM:130:HIS:HB3	58:D1:5:A:O2'	2.12	0.50
55:D8:10:ARG:HG3	58:D1:122:G:C6	2.46	0.50
46:DY:7:VAL:HG21	46:DY:8:LYS:HZ1	1.76	0.50
3:AC:139:GLN:O	3:AC:143:GLU:HB2	2.12	0.50
5:AE:51:VAL:O	5:AE:55:VAL:HG23	2.11	0.50
10:BJ:49:VAL:CG2	14:BN:41:ARG:HB2	2.41	0.50
25:C2:21:A:N6	25:C2:46:G:C2	2.79	0.50
25:C3:56:C:C5	25:C3:57:G:N7	2.78	0.50
43:CU:21:ARG:HG2	43:CU:91:TYR:CD2	2.47	0.50
28:DB:266:SER:OG	58:D1:1830:C:OP1	2.29	0.50
58:D1:516:A:C2'	58:D1:517:G:O5'	2.59	0.50
23:B2:15:A:C2	25:D3:34:G:C6	2.98	0.50
62:DA:78:ALA:HB1	62:DA:82:LYS:HB2	1.93	0.50
32:DF:137:ASP:O	32:DF:138:LYS:HB2	2.12	0.50
41:DS:3:ARG:HB3	41:DS:6:LEU:H	1.77	0.50
46:DY:8:LYS:HB2	46:DY:28:LYS:HZ3	1.76	0.50
46:DY:35:TYR:CD2	46:DY:69:ALA:HB3	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:AL:30:ALA:HB1	12:AL:31:PRO:HD2	1.92	0.50
20:AU:16:HIS:O	20:AU:19:SER:HB3	2.12	0.50
35:CM:63:THR:CG2	58:C1:1185:U:H2'	2.40	0.50
58:C1:1268:G:H5''	58:C1:1269:C:OP2	2.11	0.50
30:CD:81:PRO:HD2	58:C1:719:C:H5''	1.94	0.50
47:CZ:17:ALA:O	47:CZ:20:ARG:HG2	2.11	0.50
57:D0:19:ARG:HA	58:D1:2769:A:OP1	2.11	0.50
58:D1:1703:C:H2'	58:D1:1704:C:C6	2.47	0.50
66:D1:3001:3V6:H5	67:D1:3002:MG:MG	1.19	0.50
54:D7:30:THR:O	54:D7:31:PRO:C	2.49	0.50
29:DC:3:GLY:HA3	29:DC:81:ILE:HG21	1.92	0.50
30:DD:175:THR:O	30:DD:176:LEU:HB2	2.12	0.50
31:DE:63:ILE:HD12	31:DE:141:PHE:CD2	2.47	0.50
63:DW:88:ARG:HB2	63:DW:92:ARG:HB3	1.93	0.50
47:DZ:113:ALA:CB	47:DZ:146:ILE:HD13	2.40	0.50
12:BL:38:THR:HG21	12:BL:65:GLU:OE2	2.11	0.50
58:C1:1085:C:O2'	58:C1:1086:C:P	2.70	0.50
58:C1:2602:C:H2'	58:C1:2603:G:C8	2.47	0.50
26:C4:17:C:H5'	26:C4:62:C:OP1	2.12	0.50
28:CB:127:VAL:HA	28:CB:193:VAL:HG13	1.94	0.50
30:CD:68:LYS:HE2	58:C1:2455:G:OP2	2.11	0.50
36:CN:111:PHE:O	36:CN:115:VAL:HG23	2.11	0.50
39:CQ:38:VAL:HB	39:CQ:39:PRO:HD3	1.93	0.50
57:D0:14:CYS:HA	57:D0:27:CYS:HA	1.94	0.50
58:D1:1703:C:H2'	58:D1:1704:C:H6	1.76	0.50
58:D1:1766:A:C6	58:D1:1769:A:N1	2.80	0.50
58:D1:2534:G:H2'	58:D1:2535:G:H5''	1.94	0.50
25:D3:16:U:C2	25:D3:19:G:OP2	2.64	0.50
52:D5:42:CYS:SG	52:D5:62:CYS:HB3	2.52	0.50
28:DB:11:PRO:O	28:DB:13:ARG:N	2.43	0.50
28:DB:211:ARG:O	28:DB:215:LEU:HG	2.11	0.50
31:DE:113:ARG:NE	31:DE:113:ARG:HA	2.27	0.50
37:DO:91:PHE:CE2	37:DO:95:VAL:HG12	2.47	0.50
24:BC:13:GLY:HA3	14:BN:57:ARG:HE	1.77	0.50
12:BL:60:LEU:HD21	12:BL:66:VAL:HG22	1.92	0.50
58:C1:2228:A:H1'	58:C1:2230:G:C4	2.47	0.50
58:C1:2421:G:C2	58:C1:2422:A:H1'	2.47	0.50
58:C1:551:C:O4'	58:C1:551:C:O2	2.28	0.50
58:C1:715:G:H4'	58:C1:716:A:OP2	2.10	0.50
58:C1:820:A:O2'	58:C1:821:G:P	2.69	0.50
47:CZ:127:LYS:HE2	47:CZ:164:ALA:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:D1:1067:G:H22	58:D1:1187:A:H2	1.55	0.50
58:D1:1875:G:H2'	58:D1:1876:G:H5''	1.93	0.50
28:DB:22:SER:O	28:DB:23:GLU:C	2.50	0.50
29:DC:70:ALA:O	29:DC:72:VAL:N	2.45	0.50
45:DX:12:VAL:HG23	45:DX:13:LEU:N	2.20	0.50
58:C1:267:G:O2'	58:C1:268:G:H8	1.95	0.49
58:C1:2702:C:O2'	58:C1:2703:C:H5'	2.11	0.49
58:C1:516:A:H2'	58:C1:517:G:O4'	2.12	0.49
56:C9:33:ASN:O	56:C9:34:TRP:HB3	2.11	0.49
28:CB:79:VAL:HG21	28:CB:111:LEU:HD11	1.94	0.49
28:CB:218:ARG:HB3	28:CB:219:PRO:HD2	1.94	0.49
28:CB:24:ILE:CG1	28:CB:25:THR:N	2.75	0.49
28:CB:70:TRP:CD1	28:CB:70:TRP:C	2.85	0.49
41:CS:67:SER:N	41:CS:70:VAL:O	2.45	0.49
58:D1:8:U:C4	58:D1:2640:A:N6	2.80	0.49
28:DB:210:GLY:O	28:DB:211:ARG:CB	2.60	0.49
28:DB:35:LYS:HD3	28:DB:63:ARG:HD2	1.94	0.49
29:DC:44:TYR:O	29:DC:45:THR:HB	2.11	0.49
30:DD:74:ARG:HD2	58:D1:720:G:H1'	1.94	0.49
36:DN:35:VAL:HG11	36:DN:103:ALA:HB3	1.94	0.49
37:DO:32:THR:HG21	37:DO:37:GLY:HA2	1.93	0.49
17:AR:48:GLU:O	17:AR:49:GLU:C	2.50	0.49
2:BA:61:LEU:HD23	2:BA:68:ILE:HD11	1.93	0.49
20:BU:93:GLU:OE1	20:BU:94:ALA:N	2.45	0.49
58:C1:1540:A:N3	58:C1:1541:A:C2	2.80	0.49
58:C1:2535:G:C5'	58:C1:2535:G:H8	2.24	0.49
31:CE:120:LEU:N	31:CE:179:PRO:O	2.34	0.49
31:CE:53:LEU:HD22	31:CE:53:LEU:N	2.26	0.49
58:D1:1067:G:N2	58:D1:1187:A:C2	2.78	0.49
58:D1:2371:A:H2'	58:D1:2372:A:O4'	2.11	0.49
58:D1:2612:C:P	66:D1:3001:3V6:H19	2.51	0.49
58:D1:567:C:O2'	58:D1:570:A:OP2	2.28	0.49
58:D1:826:G:H21	58:D1:829:A:H62	1.60	0.49
25:D3:34:G:N2	25:D3:35:A:N3	2.60	0.49
53:D6:35:GLU:O	53:D6:36:CYS:CB	2.60	0.49
35:DM:1:MET:HG2	35:DM:2:LYS:N	2.27	0.49
37:DO:38:GLN:HG3	37:DO:39:LYS:N	2.26	0.49
38:DP:1:MET:HE1	38:DP:45:GLN:HB3	1.94	0.49
41:DS:32:TYR:CD2	41:DS:81:PRO:HB2	2.48	0.49
4:AD:31:CYS:C	4:AD:33:MET:H	2.16	0.49
2:BA:19:HIS:HD2	2:BA:189:ASP:OD2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:BS:37:VAL:O	18:BS:41:LYS:HB2	2.12	0.49
58:C1:1475:C:H2'	58:C1:1476:U:C6	2.47	0.49
58:C1:2469:G:O2'	58:C1:2471:U:O4	2.26	0.49
58:C1:2799:C:O2	58:C1:2799:C:H2'	2.11	0.49
58:C1:55:C:H2'	58:C1:56:G:O4'	2.11	0.49
28:CB:4:LYS:HE3	28:CB:20:ASP:HA	1.94	0.49
45:CX:10:ALA:HB1	45:CX:11:PRO:CD	2.41	0.49
58:D1:1405:A:H5''	58:D1:1406:G:OP2	2.12	0.49
58:D1:1541:A:H8	58:D1:1623:C:O2'	1.95	0.49
58:D1:1556:A:H2'	58:D1:1557:G:O4'	2.12	0.49
58:D1:2535:G:H8	58:D1:2535:G:H5''	1.77	0.49
25:D3:16:U:O2	25:D3:19:G:H5''	2.11	0.49
25:D3:47:U:O2	25:D3:47:U:O4'	2.30	0.49
54:D7:15:GLU:OE2	54:D7:41:PRO:CG	2.60	0.49
31:DE:2:PRO:HD2	52:D5:51:TYR:CZ	2.48	0.49
2:AA:88:ALA:HB2	2:AA:219:VAL:HG13	1.94	0.49
14:AN:24:CYS:HB3	14:AN:29:ARG:HB3	1.94	0.49
4:BD:18:LYS:HE2	4:BD:31:CYS:HB3	1.94	0.49
4:BD:8:VAL:C	4:BD:10:ARG:N	2.64	0.49
17:BR:7:THR:CG2	17:BR:58:GLU:HG2	2.42	0.49
58:C1:2291:G:O2'	58:C1:2399:A:N1	2.40	0.49
29:CC:61:ARG:NH1	58:C1:2819:A:O2'	2.45	0.49
58:C1:324:G:C4	58:C1:325:C:C5	3.00	0.49
55:C8:16:HIS:ND1	58:C1:730:G:OP1	2.44	0.49
43:CU:28:GLU:CB	43:CU:29:PRO:HD2	2.42	0.49
46:CY:29:GLU:N	46:CY:29:GLU:OE1	2.46	0.49
58:D1:2492:G:C2'	58:D1:2493:G:OP2	2.61	0.49
25:D3:21:A:C6	25:D3:46:G:C4	3.00	0.49
61:D4:56:U:O4	61:D4:59:A:OP2	2.30	0.49
61:D4:74:A:C5'	61:D4:75:C:C5'	2.84	0.49
56:D9:62:LEU:N	56:D9:63:PRO:CD	2.75	0.49
28:DB:13:ARG:NH1	28:DB:16:MET:SD	2.86	0.49
28:DB:43:ARG:HD2	28:DB:44:ASN:OD1	2.12	0.49
32:DF:41:MET:HE2	32:DF:43:VAL:CG1	2.39	0.49
9:BI:48:GLU:N	9:BI:49:PRO:HD2	2.27	0.49
9:BI:16:ARG:O	9:BI:63:ILE:HG23	2.12	0.49
58:C1:1920:G:O2'	58:C1:1921:A:H5''	2.11	0.49
38:CP:80:GLU:HA	58:C1:2505:G:O2'	2.12	0.49
58:C1:2845:U:H2'	58:C1:2846:G:C8	2.48	0.49
58:C1:7:A:H2'	58:C1:8:U:C6	2.46	0.49
58:C1:879:U:H2'	58:C1:880:C:H6	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:C9:50:LEU:C	56:C9:53:PRO:HD2	2.33	0.49
56:C9:62:LEU:N	56:C9:63:PRO:CD	2.75	0.49
28:CB:118:VAL:HG22	28:CB:119:ALA:H	1.77	0.49
28:CB:242:ARG:HD2	28:CB:242:ARG:N	2.27	0.49
28:CB:267:SER:HA	28:CB:270:ILE:HG13	1.93	0.49
29:CC:9:VAL:HG13	29:CC:25:VAL:O	2.13	0.49
31:CE:27:ASN:HB2	31:CE:30:GLU:HB2	1.93	0.49
25:D3:21:A:N6	25:D3:46:G:N3	2.60	0.49
42:DT:91:ASP:CG	42:DT:96:ALA:HB2	2.33	0.49
4:BD:127:THR:HG23	4:BD:147:ALA:HB3	1.94	0.49
58:C1:1306:C:C2'	58:C1:1307:A:O5'	2.61	0.49
58:C1:2488:C:C2	58:C1:2492:G:O6	2.66	0.49
58:C1:534:C:OP1	58:C1:535:U:OP2	2.30	0.49
28:CB:2:ALA:O	28:CB:3:VAL:HB	2.13	0.49
50:CK:47:ASN:HD22	58:C1:92:G:H21	1.61	0.49
36:CN:17:ARG:HB2	36:CN:45:GLU:HG3	1.94	0.49
38:CP:84:GLY:O	38:CP:85:LYS:HB2	2.13	0.49
46:CY:28:LYS:O	46:CY:38:ILE:HB	2.13	0.49
36:DN:22:ILE:HD12	58:D1:1973:A:C5	2.48	0.49
58:D1:2083:A:O2'	58:D1:2084:C:P	2.71	0.49
58:D1:217:A:H3'	58:D1:218:U:H5'	1.95	0.49
25:D3:44:G:H2'	25:D3:45:U:O4'	2.13	0.49
28:DB:70:TRP:CH2	28:DB:150:LYS:HA	2.48	0.49
28:DB:62:TYR:OH	58:D1:1846:G:C8	2.66	0.49
30:DD:89:VAL:HG12	30:DD:90:PHE:H	1.78	0.49
24:BC:37:GLN:NE2	14:BN:52:GLN:OE1	2.46	0.49
7:BG:148:ASN:HD22	7:BG:148:ASN:N	2.09	0.49
9:BI:13:ALA:HB2	9:BI:68:GLY:HA3	1.95	0.49
16:BP:3:LYS:O	16:BP:21:VAL:HA	2.12	0.49
58:C1:1777:G:H2'	58:C1:1778:G:H5'	1.94	0.49
29:CC:77:ILE:HG22	29:CC:78:LEU:H	1.77	0.49
30:CD:74:ARG:HD3	58:C1:720:G:O2'	2.12	0.49
33:CI:93:THR:HG22	33:CI:96:ASP:OD2	2.12	0.49
37:CO:47:ASP:HB3	37:CO:48:PRO:C	2.33	0.49
66:D1:3001:3V6:CLI	66:D1:3001:3V6:C	2.98	0.49
54:D7:13:CYS:O	54:D7:21:TYR:HA	2.13	0.49
28:DB:65:ILE:O	28:DB:65:ILE:HD13	2.13	0.49
32:DF:158:HIS:NE2	32:DF:170:ARG:O	2.46	0.49
49:DH:15:ALA:O	49:DH:40:ARG:HG3	2.12	0.49
38:DP:75:THR:HA	38:DP:89:ASN:O	2.13	0.49
39:DQ:4:LEU:O	39:DQ:5:LYS:HD3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:DS:31:SER:CA	41:DS:32:TYR:CD2	2.96	0.49
41:DS:3:ARG:C	41:DS:5:ALA:N	2.66	0.49
47:DZ:105:VAL:O	47:DZ:141:VAL:HG13	2.12	0.49
10:AJ:32:ALA:HB3	10:AJ:76:ASN:HB3	1.94	0.49
18:AS:58:LEU:HD23	18:AS:62:GLU:HB3	1.95	0.49
5:BE:81:GLU:HG2	5:BE:90:VAL:HG22	1.95	0.49
13:BM:108:ARG:O	13:BM:111:LYS:O	2.31	0.49
26:C4:2:G:C2	26:C4:3:C:C6	3.01	0.49
28:CB:20:ASP:C	28:CB:20:ASP:OD1	2.51	0.49
29:CC:36:ARG:HH21	29:CC:88:GLY:HA2	1.78	0.49
36:CN:101:PRO:HG3	41:CS:67:SER:HB3	1.94	0.49
41:CS:29:ARG:HB3	41:CS:85:LYS:HA	1.94	0.49
58:D1:2083:A:C2'	58:D1:2084:C:H5'	2.42	0.49
58:D1:491:A:N3	58:D1:729:C:H1'	2.28	0.49
37:DO:146:VAL:HG13	37:DO:147:LEU:N	2.28	0.49
40:DR:16:ASN:O	40:DR:19:LYS:N	2.45	0.49
40:DR:83:LYS:CE	40:DR:105:ALA:HB3	2.43	0.49
43:DU:21:ARG:HG2	43:DU:91:TYR:CD2	2.48	0.49
13:AM:106:ASN:O	13:AM:107:ALA:CB	2.60	0.49
7:BG:73:MET:HG2	7:BG:90:GLU:HA	1.95	0.49
9:BI:33:PHE:CZ	9:BI:47:LEU:HD11	2.48	0.49
58:C1:2107:U:H2'	58:C1:2108:G:C8	2.47	0.49
26:C4:7:G:O5'	26:C4:7:G:H8	1.96	0.49
40:CR:66:ALA:O	40:CR:69:VAL:HG12	2.13	0.49
58:D1:1801:C:H1'	58:D1:1816:A:C8	2.47	0.49
58:D1:276:G:HO2'	58:D1:277:G:P	2.30	0.49
58:D1:996:G:C6	58:D1:997:A:N7	2.81	0.49
29:DC:95:ILE:HD13	29:DC:95:ILE:N	2.27	0.49
2:BA:32:ILE:HD11	2:BA:40:HIS:HB3	1.95	0.49
24:BC:3:ASN:OD1	24:BC:3:ASN:N	2.45	0.49
11:BK:34:ASP:HB2	11:BK:35:PRO:CD	2.43	0.49
20:BU:26:ASN:HB2	20:BU:71:THR:HG23	1.94	0.49
58:C1:2178:G:O2'	58:C1:2179:A:O5'	2.28	0.49
58:C1:2535:G:C8	58:C1:2535:G:C5'	2.96	0.49
58:C1:879:U:H2'	58:C1:880:C:C6	2.48	0.49
26:C4:10:G:C8	26:C4:10:G:H5'	2.47	0.49
28:CB:10:THR:HG23	28:CB:13:ARG:CB	2.42	0.49
31:CE:95:ARG:O	31:CE:96:ARG:HG2	2.13	0.49
43:CU:39:LEU:HD12	43:CU:50:PRO:O	2.13	0.49
58:D1:1095:A:O2'	58:D1:2764:C:H1'	2.13	0.49
58:D1:1097:C:C3'	58:D1:1097:C:C6	2.96	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:DB:254:THR:OG1	58:D1:1854:G:N3	2.45	0.49
58:D1:296:C:O2'	58:D1:297:G:OP1	2.28	0.49
58:D1:516:A:H2'	58:D1:517:G:O5'	2.13	0.49
28:DB:49:ILE:HG22	58:D1:825:U:OP1	2.13	0.49
31:DE:25:TYR:OH	31:DE:168:GLU:OE1	2.31	0.49
51:DL:45:GLY:HA3	58:D1:897:U:O2'	2.13	0.49
38:DP:21:THR:HG22	38:DP:21:THR:O	2.12	0.49
9:AI:50:LEU:O	9:AI:53:VAL:HG22	2.13	0.48
19:AT:19:VAL:O	19:AT:23:ASN:N	2.45	0.48
58:C1:1231:G:H8	58:C1:1231:G:O5'	1.96	0.48
58:C1:1685:U:C2'	58:C1:1686:C:H5''	2.43	0.48
58:C1:1920:G:C2'	58:C1:1921:A:OP2	2.60	0.48
58:C1:173:U:H4'	58:C1:206:A:H4'	1.95	0.48
58:C1:2402:G:O2'	58:C1:2435:C:N4	2.40	0.48
58:C1:2089:U:N3	58:C1:2441:A:H2	2.10	0.48
58:C1:935:C:H1'	58:C1:936:A:O4'	2.13	0.48
33:CI:5:LEU:HD22	33:CI:9:LEU:CD1	2.43	0.48
41:CS:61:PHE:CE2	41:CS:76:PHE:HB2	2.48	0.48
42:CT:92:ARG:O	42:CT:93:LYS:C	2.51	0.48
43:DU:79:VAL:HG22	58:D1:1232:U:H4'	1.95	0.48
32:DF:17:VAL:O	32:DF:45:VAL:HG22	2.13	0.48
32:DF:54:ARG:NH1	32:DF:65:HIS:HD2	2.11	0.48
2:AA:118:LEU:HB2	2:AA:142:LEU:HD12	1.95	0.48
3:AC:50:ALA:HB1	3:AC:70:VAL:HG11	1.95	0.48
58:C1:139:A:H5''	58:C1:140:C:OP2	2.12	0.48
58:C1:1902:C:O2	58:C1:1902:C:H2'	2.13	0.48
29:CC:61:ARG:NH2	58:C1:2643:A:C2'	2.76	0.48
42:CT:102:GLU:HG3	43:CU:2:PHE:CZ	2.47	0.48
58:D1:1624:U:H2'	58:D1:1625:A:H5'	1.94	0.48
58:D1:2124:C:H3'	58:D1:2125:G:H5''	1.95	0.48
28:DB:35:LYS:HB3	28:DB:36:PRO:HD3	1.95	0.48
28:DB:43:ARG:NH1	28:DB:44:ASN:OD1	2.43	0.48
38:DP:28:ALA:O	38:DP:29:PHE:CD1	2.66	0.48
42:DT:90:VAL:O	42:DT:91:ASP:C	2.51	0.48
4:AD:9:CYS:CB	4:AD:22:LYS:HD2	2.43	0.48
12:AL:25:PRO:O	12:AL:27:LEU:HD22	2.13	0.48
19:AT:6:LYS:HG2	19:AT:7:LYS:HE3	1.93	0.48
2:BA:84:GLU:HG3	2:BA:215:LEU:HB3	1.95	0.48
12:BL:47:LYS:HB3	12:BL:48:PRO:CD	2.36	0.48
25:C3:28:G:C2	25:C3:29:G:C5	3.01	0.48
26:C4:6:G:C2	26:C4:69:C:N3	2.82	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:CB:10:THR:O	28:CB:11:PRO:O	2.31	0.48
29:CC:188:VAL:HG22	29:CC:189:PRO:HD2	1.94	0.48
37:CO:68:GLN:HE22	56:C9:12:LYS:CB	2.26	0.48
38:CP:55:VAL:O	38:CP:56:ARG:C	2.52	0.48
42:CT:66:ASN:ND2	42:CT:70:ARG:HE	2.11	0.48
35:DM:25:ARG:NH2	58:D1:1188:A:OP1	2.46	0.48
58:D1:2611:A:H5''	66:D1:3001:3V6:CB	2.43	0.48
58:D1:721:A:C8	58:D1:850:A:C6	3.01	0.48
58:D1:91:C:H2'	58:D1:91:C:O2	2.13	0.48
60:D2:42:C:H3'	60:D2:43:C:H5''	1.95	0.48
28:DB:118:VAL:HG22	28:DB:119:ALA:N	2.28	0.48
28:DB:186:HIS:HD2	28:DB:188:GLU:H	1.60	0.48
29:DC:120:TRP:CE3	29:DC:155:LYS:HD3	2.47	0.48
33:DI:72:LEU:CD1	33:DI:138:ILE:HD11	2.43	0.48
41:DS:85:LYS:HB3	41:DS:85:LYS:NZ	2.28	0.48
10:AJ:34:VAL:HG22	10:AJ:74:ILE:HG22	1.95	0.48
11:AK:73:MET:O	11:AK:76:GLY:N	2.45	0.48
11:BK:59:TYR:O	11:BK:62:GLN:HB3	2.14	0.48
28:CB:49:ILE:CG2	58:C1:825:U:OP1	2.61	0.48
32:CF:85:LYS:HG3	32:CF:145:ALA:HB2	1.95	0.48
36:CN:2:ILE:HD11	36:CN:82:ASN:HD22	1.78	0.48
29:CC:111:ARG:HG3	39:CQ:2:ARG:HG2	1.94	0.48
44:CW:59:VAL:HG12	44:CW:60:ASN:N	2.27	0.48
53:D6:4:HIS:HB2	53:D6:5:PRO:HD3	1.96	0.48
28:DB:4:LYS:HE3	28:DB:20:ASP:HA	1.96	0.48
30:DD:74:ARG:HD3	58:D1:720:G:O2'	2.14	0.48
31:DE:127:GLY:O	31:DE:129:GLY:N	2.46	0.48
35:DM:128:HIS:CG	35:DM:128:HIS:O	2.66	0.48
35:DM:24:GLY:O	35:DM:28:THR:HG22	2.13	0.48
13:AM:9:ILE:HD13	31:CE:146:TYR:CE1	2.49	0.48
20:AU:75:ASN:O	20:AU:79:ARG:N	2.46	0.48
6:BF:84:ASN:O	6:BF:86:ARG:HG3	2.13	0.48
8:BH:86:ILE:HG21	8:BH:133:LEU:HD22	1.94	0.48
58:C1:1344:G:H5''	58:C1:1345:U:OP1	2.14	0.48
58:C1:1441:U:O2	58:C1:1441:U:H2'	2.13	0.48
58:C1:1479:A:H61	58:C1:1604:A:H62	1.61	0.48
58:C1:8:U:O2'	58:C1:9:G:P	2.72	0.48
1:A2:19:U:C2	25:C2:37:A:C2	3.02	0.48
28:CB:58:HIS:CD2	58:C1:1613:A:H5'	2.48	0.48
41:CS:89:VAL:HG11	41:CS:91:ARG:NE	2.29	0.48
43:CU:40:LEU:HD22	43:CU:46:VAL:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:D1:1156:A:O2'	58:D1:1157:G:C1'	2.62	0.48
58:D1:31:C:O2'	58:D1:32:U:H5'	2.14	0.48
31:DE:5:VAL:HG22	31:DE:8:LYS:HB2	1.96	0.48
37:DO:30:THR:HG22	37:DO:31:ALA:N	2.28	0.48
41:DS:30:VAL:HG21	41:DS:84:GLN:H	1.77	0.48
8:AH:109:ILE:HG23	8:AH:137:VAL:HB	1.96	0.48
13:AM:49:THR:HG22	13:AM:51:ALA:H	1.78	0.48
15:BO:32:LEU:O	15:BO:33:THR:C	2.51	0.48
58:C1:232:A:C2	58:C1:243:A:C4	3.01	0.48
58:C1:2753:A:H2'	58:C1:2754:C:O4'	2.14	0.48
32:CF:137:ASP:OD1	32:CF:138:LYS:N	2.47	0.48
35:CM:15:LEU:HB2	35:CM:134:ARG:HB2	1.95	0.48
35:CM:94:HIS:O	35:CM:97:ARG:HB2	2.13	0.48
37:CO:9:ASN:C	37:CO:11:GLY:N	2.67	0.48
39:CQ:23:ASN:ND2	58:C1:1339:U:O2'	2.47	0.48
58:D1:2450:A:C8	58:D1:2450:A:C5'	2.95	0.48
58:D1:2723:U:C5'	58:D1:2723:U:O2	2.61	0.48
58:D1:2807:G:N3	58:D1:2807:G:H2'	2.27	0.48
58:D1:2890:C:N3	58:D1:2891:A:N7	2.61	0.48
29:DC:69:LYS:C	29:DC:71:GLY:H	2.16	0.48
50:DK:16:LEU:HD13	50:DK:20:GLU:HG3	1.95	0.48
51:DL:52:HIS:CD2	51:DL:52:HIS:H	2.30	0.48
41:DS:82:LEU:N	41:DS:82:LEU:HD12	2.28	0.48
3:AC:154:SER:OG	3:AC:155:GLY:N	2.47	0.48
4:BD:4:TYR:O	4:BD:5:ILE:HB	2.13	0.48
19:BT:20:LEU:HD23	19:BT:23:ASN:HD22	1.78	0.48
58:C1:2535:G:C8	58:C1:2535:G:H5'	2.45	0.48
29:CC:111:ARG:CZ	39:CQ:2:ARG:HH21	2.27	0.48
29:CC:96:PHE:HA	29:CC:100:GLU:OE1	2.13	0.48
30:CD:24:LEU:HB3	30:CD:25:PRO:CD	2.44	0.48
38:CP:31:ASP:O	38:CP:133:ARG:O	2.31	0.48
41:CS:65:LYS:O	41:CS:72:VAL:N	2.37	0.48
43:CU:4:ILE:O	43:CU:4:ILE:HG22	2.14	0.48
58:D1:217:A:H3'	58:D1:218:U:C5'	2.43	0.48
37:DO:33:ARG:CZ	58:D1:609:C:H2'	2.43	0.48
61:D4:14:A:C5	61:D4:23:G:C6	3.02	0.48
32:DF:137:ASP:O	32:DF:138:LYS:CB	2.62	0.48
33:DI:94:ALA:HB2	33:DI:114:LEU:CD1	2.43	0.48
46:DY:37:VAL:O	46:DY:66:PRO:O	2.32	0.48
46:DY:98:VAL:O	46:DY:98:VAL:HG12	2.13	0.48
2:AA:67:THR:HG21	2:AA:155:LEU:HD21	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AE:92:LYS:HB3	5:AE:119:LEU:HB2	1.96	0.48
24:BC:23:TYR:CD2	24:BC:24:ALA:N	2.81	0.48
8:BH:109:ILE:HD11	8:BH:120:THR:HG21	1.95	0.48
30:CD:160:ASN:OD1	30:CD:163:VAL:HG23	2.14	0.48
40:CR:97:ARG:C	40:CR:97:ARG:NE	2.67	0.48
56:D9:30:ARG:NH1	58:D1:2430:U:O4	2.47	0.48
56:D9:33:ASN:O	58:D1:2431:C:OP2	2.31	0.48
58:D1:2449:U:H6	58:D1:2449:U:H3'	1.78	0.48
58:D1:2666:G:O2'	58:D1:2675:G:N1	2.43	0.48
56:D9:61:LEU:HD12	56:D9:62:LEU:H	1.78	0.48
39:DQ:117:VAL:HG13	39:DQ:118:GLU:N	2.28	0.48
41:DS:36:GLU:O	41:DS:36:GLU:HG2	2.13	0.48
2:AA:100:GLY:O	2:AA:101:MET:C	2.51	0.48
2:AA:80:ILE:HG22	2:AA:80:ILE:O	2.13	0.48
9:AI:9:ARG:HG2	9:AI:14:VAL:HG13	1.95	0.48
13:AM:3:ARG:HG2	13:AM:9:ILE:HG13	1.95	0.48
14:BN:13:THR:N	14:BN:14:PRO:HD3	2.29	0.48
19:BT:58:VAL:O	19:BT:58:VAL:HG23	2.13	0.48
58:C1:1345:U:O2'	58:C1:1671:G:N2	2.47	0.48
58:C1:2085:C:H2'	58:C1:2086:C:C6	2.49	0.48
25:C2:42:C:H3'	25:C2:43:C:H5''	1.96	0.48
26:C4:4:G:O2'	26:C4:5:G:P	2.72	0.48
50:CK:45:SER:O	50:CK:46:GLN:NE2	2.46	0.48
41:CS:117:ASP:O	41:CS:118:ARG:C	2.52	0.48
46:CY:87:LYS:O	46:CY:88:LYS:HB2	2.14	0.48
58:D1:1540:A:H2'	58:D1:1540:A:N3	2.28	0.48
58:D1:2346:A:C8	58:D1:2348:G:N7	2.82	0.48
58:D1:247:G:H21	58:D1:645:A:H8	1.62	0.48
29:DC:7:VAL:HG11	41:DS:1:MET:SD	2.54	0.48
40:DR:19:LYS:O	40:DR:19:LYS:HG2	2.14	0.48
40:DR:95:HIS:CG	40:DR:96:GLY:N	2.81	0.48
13:AM:66:LEU:H	13:AM:70:LEU:HD12	1.78	0.48
17:BR:7:THR:HG22	17:BR:58:GLU:HG2	1.96	0.48
58:C1:1366:A:H2'	58:C1:1367:A:O4'	2.14	0.48
58:C1:2085:C:C5'	58:C1:2085:C:H6	2.27	0.48
28:CB:13:ARG:NH1	58:C1:775:G:OP2	2.45	0.48
27:CA:212:UNK:O	27:CA:213:UNK:CB	2.61	0.48
32:CF:106:THR:HG22	32:CF:112:PRO:HB3	1.96	0.48
43:CU:76:LYS:O	43:CU:79:VAL:HG12	2.14	0.48
58:D1:1319:A:N3	58:D1:1342:C:H1'	2.28	0.48
58:D1:2555:G:O5'	58:D1:2555:G:H8	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:DQ:90:ARG:NH1	58:D1:2889:C:O2'	2.38	0.48
58:D1:2612:C:H5''	66:D1:3001:3V6:CLJ	2.50	0.48
25:D3:53:G:O2'	25:D3:54:U:H5'	2.13	0.48
30:DD:117:ARG:HA	30:DD:120:GLU:HG3	1.95	0.48
33:DI:2:LYS:O	33:DI:39:ALA:HB3	2.14	0.48
39:DQ:71:GLN:HA	39:DQ:71:GLN:HE21	1.78	0.48
40:DR:30:ARG:HD2	40:DR:31:SER:O	2.14	0.48
41:DS:57:PHE:O	41:DS:58:ASN:C	2.53	0.48
46:DY:28:LYS:O	46:DY:29:GLU:C	2.51	0.48
47:DZ:119:GLU:OE1	47:DZ:122:ARG:HD2	2.14	0.48
49:CH:61:ARG:NH2	58:C1:1409:G:OP2	2.47	0.47
58:C1:1538:C:C2'	58:C1:1538:C:O2	2.60	0.47
58:C1:1345:U:O2'	58:C1:1671:G:C2	2.60	0.47
28:CB:165:ILE:HD13	28:CB:175:LEU:CD2	2.44	0.47
28:CB:24:ILE:C	28:CB:25:THR:O	2.53	0.47
46:CY:77:PRO:O	46:CY:78:ALA:HB2	2.14	0.47
47:CZ:38:TYR:O	47:CZ:38:TYR:CD1	2.66	0.47
58:D1:1066:A:H3'	58:D1:1066:A:H8	1.79	0.47
58:D1:2155:A:C2	58:D1:2180:G:H1'	2.49	0.47
58:D1:2401:U:O5'	58:D1:2401:U:H6	1.95	0.47
54:D7:12:GLU:HA	54:D7:23:THR:HA	1.96	0.47
29:DC:11:MET:HB3	29:DC:24:THR:HA	1.96	0.47
33:DI:127:VAL:HG13	33:DI:138:ILE:O	2.14	0.47
4:AD:18:LYS:HE2	4:AD:31:CYS:HB2	1.96	0.47
10:AJ:40:LEU:HB2	10:AJ:69:ASN:HB2	1.94	0.47
7:BG:74:GLU:HG2	7:BG:91:VAL:HG22	1.96	0.47
10:BJ:55:LYS:O	10:BJ:56:HIS:CG	2.67	0.47
58:C1:1538:C:C5	58:C1:2226:G:O2'	2.66	0.47
58:C1:257:U:O2	58:C1:257:U:H2'	2.15	0.47
58:C1:2830:A:OP2	58:C1:2831:G:OP2	2.32	0.47
28:CB:27:THR:HG23	28:CB:83:GLU:HB3	1.95	0.47
31:CE:43:LEU:HB3	31:CE:45:GLU:HG2	1.94	0.47
37:CO:38:GLN:OE1	58:C1:987:U:OP2	2.32	0.47
42:DT:77:SER:OG	58:D1:1056:G:H5''	2.14	0.47
42:DT:13:LYS:CD	58:D1:1272:G:OP1	2.61	0.47
28:DB:259:THR:CG2	58:D1:1828:U:H5'	2.41	0.47
58:D1:2752:A:H2'	58:D1:2753:A:C8	2.49	0.47
11:BK:54:ARG:NH2	25:D3:39:U:O2'	2.47	0.47
37:DO:107:LYS:HB2	37:DO:108:LYS:CE	2.44	0.47
4:AD:189:PRO:HB2	4:AD:194:LEU:HD21	1.95	0.47
17:AR:56:VAL:O	17:AR:77:VAL:HB	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BD:126:ILE:N	4:BD:126:ILE:HD12	2.29	0.47
17:BR:27:PHE:CZ	17:BR:36:ILE:HD11	2.49	0.47
19:BT:6:LYS:HG2	19:BT:7:LYS:HE2	1.96	0.47
46:CY:2:ARG:NH2	58:C1:103:C:O2'	2.39	0.47
58:C1:1540:A:H2'	58:C1:1541:A:C2	2.49	0.47
58:C1:859:U:H2'	58:C1:860:C:C6	2.49	0.47
54:C7:17:LYS:HB2	54:C7:18:ARG:HH12	1.80	0.47
30:CD:53:THR:HG23	30:CD:55:GLY:H	1.80	0.47
49:CH:23:LYS:HD3	49:CH:28:GLY:HA3	1.95	0.47
37:CO:144:GLU:N	37:CO:145:PRO:CD	2.77	0.47
40:CR:15:ARG:O	40:CR:18:ILE:HB	2.14	0.47
40:CR:26:LEU:HD23	40:CR:26:LEU:O	2.14	0.47
58:D1:2611:A:C6	58:D1:2612:C:N4	2.83	0.47
58:D1:2778:G:H2'	58:D1:2778:G:N3	2.29	0.47
58:D1:509:C:H2'	58:D1:510:C:H6	1.78	0.47
58:D1:555:C:C5	58:D1:2056:G:C2	3.03	0.47
58:D1:636:U:O2	58:D1:636:U:O4'	2.30	0.47
58:D1:663:U:H2'	58:D1:664:C:C6	2.50	0.47
29:DC:63:LEU:O	29:DC:64:LYS:C	2.51	0.47
29:DC:36:ARG:NH1	29:DC:85:ASN:OD1	2.46	0.47
30:DD:9:ILE:HG22	30:DD:11:VAL:O	2.14	0.47
49:DH:90:ILE:CG2	49:DH:94:LEU:HD12	2.43	0.47
37:DO:35:HIS:C	37:DO:36:LYS:HG3	2.33	0.47
37:DO:64:LYS:C	37:DO:66:GLY:N	2.67	0.47
38:DP:29:PHE:N	38:DP:105:GLU:OE2	2.47	0.47
47:DZ:91:LEU:HD23	47:DZ:96:VAL:HG11	1.96	0.47
3:AC:58:GLU:O	3:AC:59:ARG:HG3	2.14	0.47
5:AE:61:TYR:O	5:AE:64:ARG:HB3	2.13	0.47
58:C1:1064:U:O2'	58:C1:1066:A:C2	2.60	0.47
58:C1:1875:G:C2'	58:C1:1876:G:H5'	2.39	0.47
26:C4:3:C:N4	26:C4:4:G:N7	2.63	0.47
26:C4:52:C:H2'	26:C4:52:C:O2	2.14	0.47
56:C9:6:THR:HG21	58:C1:231:U:OP1	2.14	0.47
41:CS:89:VAL:CG1	41:CS:91:ARG:HG3	2.45	0.47
58:D1:863:C:O2'	58:D1:885:U:OP1	2.25	0.47
61:D4:68:C:H2'	61:D4:68:C:O2	2.12	0.47
28:DB:35:LYS:HD2	28:DB:36:PRO:N	2.30	0.47
29:DC:24:THR:HG21	29:DC:188:VAL:HG12	1.96	0.47
38:DP:66:ILE:HG13	38:DP:66:ILE:O	2.14	0.47
47:DZ:31:ARG:HH22	47:DZ:94:GLU:HG3	1.78	0.47
17:AR:57:VAL:HG12	17:AR:76:LEU:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:BK:48:ILE:HD11	11:BK:64:ALA:HA	1.97	0.47
58:C1:179:A:H2'	58:C1:180:C:C6	2.49	0.47
58:C1:2168:G:H2'	58:C1:2169:G:O4'	2.14	0.47
58:C1:820:A:O2'	58:C1:821:G:OP2	2.26	0.47
25:C3:9:A:O4'	25:C3:46:G:N2	2.47	0.47
29:CC:11:MET:HB2	29:CC:23:VAL:O	2.14	0.47
38:CP:58:PHE:HD1	38:CP:58:PHE:O	1.98	0.47
42:CT:66:ASN:HD21	42:CT:70:ARG:NE	2.13	0.47
58:D1:1578:C:O2'	58:D1:1579:G:N2	2.44	0.47
58:D1:193:G:O2'	58:D1:194:U:OP2	2.33	0.47
58:D1:505:A:H3'	58:D1:506:G:H5''	1.96	0.47
35:DM:3:THR:O	35:DM:5:VAL:N	2.47	0.47
36:DN:87:ILE:HG21	36:DN:91:LEU:HD13	1.96	0.47
37:DO:13:ASN:O	37:DO:15:ARG:N	2.47	0.47
8:AH:87:SER:HA	8:AH:93:VAL:HG23	1.96	0.47
10:AJ:49:VAL:HG21	14:AN:41:ARG:CB	2.45	0.47
16:AP:19:ILE:HG22	16:AP:36:ILE:HG13	1.95	0.47
23:B2:20:U:C6	23:B2:21:C:C5	3.02	0.47
11:BK:22:HIS:HB3	11:BK:29:ILE:HG23	1.96	0.47
58:C1:1377:G:H5''	58:C1:1377:G:C8	2.49	0.47
58:C1:2375:C:H2'	58:C1:2376:G:O4'	2.14	0.47
26:C4:3:C:O2	26:C4:3:C:C2'	2.62	0.47
29:CC:23:VAL:HG12	29:CC:173:VAL:HG21	1.97	0.47
37:CO:85:LEU:HB3	37:CO:114:ILE:HD11	1.97	0.47
40:CR:13:ARG:O	40:CR:15:ARG:HG3	2.14	0.47
41:CS:85:LYS:NZ	41:CS:85:LYS:HB3	2.30	0.47
58:D1:1905:A:H2'	58:D1:1906:A:H5''	1.95	0.47
61:D4:16:C:O2	61:D4:61:U:H4'	2.14	0.47
29:DC:68:ALA:C	29:DC:70:ALA:H	2.18	0.47
38:DP:134:ARG:HA	38:DP:137:TYR:CD1	2.49	0.47
38:DP:26:TYR:HE1	38:DP:28:ALA:HB2	1.76	0.47
43:DU:15:GLU:O	43:DU:96:ILE:HG21	2.15	0.47
47:DZ:146:ILE:HD12	58:D1:941:A:C1'	2.44	0.47
3:AC:23:TYR:C	3:AC:23:TYR:CD2	2.88	0.47
9:AI:15:ALA:HB2	9:AI:65:VAL:HG23	1.96	0.47
9:AI:47:LEU:C	9:AI:49:PRO:HD2	2.34	0.47
13:AM:19:LEU:O	13:AM:22:ILE:CD1	2.63	0.47
13:AM:94:ARG:NE	19:AT:81:ARG:HG2	2.29	0.47
58:C1:1448:C:H5''	58:C1:1517:A:H1'	1.97	0.47
58:C1:1647:U:H3'	58:C1:1648:A:C5'	2.45	0.47
39:CQ:3:HIS:HB2	58:C1:1700:A:OP1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:CA:77:ILE:O	27:CA:77:ILE:HG23	2.15	0.47
27:CA:82:LYS:HB3	27:CA:86:ALA:HB2	1.97	0.47
31:CE:110:ALA:HB1	31:CE:140:ILE:CD1	2.44	0.47
37:CO:33:ARG:O	37:CO:34:GLY:C	2.53	0.47
58:D1:1898:A:H5''	58:D1:1899:G:OP2	2.14	0.47
61:D4:4:G:H8	61:D4:4:G:C5'	2.27	0.47
28:DB:242:ARG:HD2	28:DB:242:ARG:N	2.29	0.47
31:DE:126:ASP:O	31:DE:128:ARG:N	2.48	0.47
37:DO:41:ARG:HH11	37:DO:45:LEU:HD13	1.80	0.47
40:DR:54:LEU:HD22	40:DR:57:LYS:HA	1.96	0.47
2:AA:11:LEU:HD12	2:AA:217:ARG:NH2	2.30	0.47
2:AA:233:SER:CB	2:AA:234:PRO:CD	2.93	0.47
2:AA:69:LEU:HD12	2:AA:70:PHE:N	2.29	0.47
4:AD:110:PHE:N	4:AD:110:PHE:HD1	2.11	0.47
10:AJ:23:ILE:HG23	10:AJ:85:LEU:HD22	1.96	0.47
4:AD:195:ALA:O	6:BF:16:GLN:HG3	2.15	0.47
6:BF:97:PHE:O	18:BS:31:LEU:HD23	2.14	0.47
17:BR:33:GLY:O	17:BR:34:LYS:O	2.33	0.47
58:C1:2890:C:C2	58:C1:2891:A:C8	3.03	0.47
58:C1:565:C:H2'	58:C1:566:C:C6	2.50	0.47
53:C6:33:CYS:SG	53:C6:40:LYS:CE	3.03	0.47
54:C7:19:ARG:NH1	54:C7:43:CYS:SG	2.88	0.47
54:C7:46:HIS:HB2	54:C7:47:THR:HB	1.97	0.47
29:CC:6:GLY:HA2	29:CC:51:PHE:CZ	2.49	0.47
51:CL:6:VAL:O	51:CL:34:GLU:HA	2.14	0.47
37:CO:39:LYS:HG3	58:C1:853:U:OP2	2.14	0.47
37:CO:57:THR:O	37:CO:58:THR:HB	2.14	0.47
38:CP:133:ARG:O	38:CP:134:ARG:HG2	2.14	0.47
41:CS:27:THR:HG1	41:CS:28:VAL:H	1.60	0.47
44:CW:9:TYR:H	44:CW:102:HIS:CD2	2.28	0.47
47:CZ:127:LYS:HB2	47:CZ:162:GLU:HG3	1.96	0.47
58:D1:1069:G:H3'	58:D1:1070:G:H5''	1.96	0.47
58:D1:13:A:H8	58:D1:13:A:O5'	1.97	0.47
58:D1:1727:G:O2'	58:D1:1792:A:H2'	2.13	0.47
58:D1:2450:A:C8	58:D1:2450:A:H5''	2.49	0.47
58:D1:2672:G:H2'	58:D1:2673:A:C4	2.47	0.47
28:DB:127:VAL:HA	28:DB:193:VAL:HG13	1.96	0.47
29:DC:44:TYR:O	29:DC:45:THR:CB	2.62	0.47
32:DF:116:GLU:HG2	32:DF:117:PRO:HD2	1.96	0.47
32:DF:125:VAL:HG12	32:DF:127:GLU:O	2.15	0.47
51:DL:8:LEU:HD13	51:DL:31:LEU:HD23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:DP:118:LEU:HD12	38:DP:131:ILE:CG2	2.44	0.47
41:DS:27:THR:OG1	41:DS:28:VAL:N	2.45	0.47
18:AS:50:ILE:CD1	18:AS:70:ILE:HG21	2.45	0.47
16:BP:20:VAL:HG23	16:BP:35:LYS:HA	1.96	0.47
58:C1:1540:A:H2'	58:C1:1540:A:N3	2.30	0.47
26:C4:10:G:C8	26:C4:10:G:C5'	2.97	0.47
54:C7:33:LYS:HA	54:C7:33:LYS:CE	2.40	0.47
28:CB:45:ASN:CG	28:CB:46:GLN:H	2.18	0.47
30:CD:116:ASP:OD2	37:CO:5:ASP:N	2.47	0.47
51:CL:19:GLN:HE22	51:CL:52:HIS:HE1	1.62	0.47
58:D1:2269:C:H4'	58:D1:2270:G:OP2	2.15	0.47
56:D9:30:ARG:CZ	58:D1:2430:U:O4	2.63	0.47
58:D1:551:C:O4'	58:D1:551:C:O2	2.32	0.47
61:D4:76:C:H5''	61:D4:76:C:H6	1.79	0.47
28:DB:108:PRO:HB3	28:DB:143:HIS:CE1	2.50	0.47
30:DD:179:GLU:N	30:DD:179:GLU:OE1	2.48	0.47
30:DD:66:PRO:O	30:DD:67:GLN:HB3	2.13	0.47
32:DF:137:ASP:HB3	32:DF:140:LYS:HB2	1.97	0.47
50:DK:25:VAL:HG21	50:DK:61:LEU:CD1	2.45	0.47
42:DT:92:ARG:HD2	42:DT:95:LEU:HD12	1.97	0.47
43:DU:19:LYS:HG3	43:DU:20:LEU:O	2.14	0.47
43:DU:39:LEU:HB3	43:DU:47:VAL:HG11	1.96	0.47
3:AC:53:ALA:HB2	3:AC:115:LEU:HD21	1.96	0.47
3:AC:23:TYR:CD2	3:AC:24:ALA:N	2.83	0.47
10:AJ:50:ILE:HA	10:AJ:60:ARG:CB	2.45	0.47
20:AU:69:GLY:O	20:AU:73:HIS:NE2	2.48	0.47
23:B2:20:U:O2'	23:B2:21:C:H5'	2.15	0.47
4:BD:24:GLU:O	4:BD:27:TYR:HB2	2.14	0.47
4:BD:25:ARG:HA	4:BD:28:SER:OG	2.15	0.47
5:BE:102:ALA:HB1	5:BE:106:PRO:HG2	1.96	0.47
5:BE:151:LEU:HD11	8:BH:77:GLU:OE2	2.15	0.47
58:C1:2450:A:C5'	58:C1:2450:A:C8	2.98	0.47
37:CO:105:LEU:O	37:CO:106:LEU:HB3	2.15	0.47
46:CY:47:LYS:HG2	46:CY:60:PHE:HE2	1.79	0.47
39:DQ:16:HIS:CE1	58:D1:1320:A:C4	3.03	0.47
58:D1:1884:A:H2'	58:D1:1885:G:O4'	2.15	0.47
58:D1:2904:C:C3'	58:D1:2904:C:C6	2.97	0.47
32:DF:106:THR:HG22	32:DF:112:PRO:HB3	1.97	0.47
34:DJ:86:UNK:O	34:DJ:87:UNK:CB	2.63	0.47
51:DL:17:LYS:HG2	58:D1:1013:U:OP1	2.15	0.47
42:DT:102:GLU:HG3	43:DU:2:PHE:CE1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AF:8:ILE:HG22	6:AF:10:LEU:CD1	2.44	0.47
9:AI:103:THR:HG22	9:AI:104:ARG:H	1.80	0.47
15:AO:39:LEU:HD12	15:AO:56:LEU:HB2	1.96	0.47
19:AT:42:PRO:O	19:AT:43:GLU:HB3	2.15	0.47
2:BA:69:LEU:HD13	2:BA:91:PRO:HB2	1.97	0.47
24:BC:83:ARG:O	24:BC:86:VAL:HG22	2.14	0.47
58:C1:1346:A:C4'	58:C1:1347:A:OP1	2.59	0.47
58:C1:2487:A:C2	58:C1:2488:C:H6	2.33	0.47
58:C1:2044:G:H5'	58:C1:2628:C:H4'	1.97	0.47
46:CY:47:LYS:HB3	58:C1:508:A:O4'	2.15	0.47
31:CE:60:LEU:O	31:CE:60:LEU:HD13	2.15	0.47
35:CM:41:ASP:O	35:CM:42:TRP:C	2.53	0.47
38:CP:16:ARG:NH2	58:C1:996:G:P	2.88	0.47
43:CU:18:LEU:N	43:CU:18:LEU:CD1	2.78	0.47
58:D1:1423:A:O2'	58:D1:1424:A:H5''	2.15	0.47
58:D1:894:G:O6	58:D1:973:G:H2'	2.14	0.47
60:D2:42:C:H42	64:DV:28:G:H1	1.61	0.47
2:AA:104:ASN:OD1	2:AA:107:THR:OG1	2.33	0.46
2:AA:235:SER:HG	2:AA:236:TYR:HD1	1.63	0.46
5:AE:106:PRO:O	5:AE:110:LEU:HG	2.15	0.46
8:BH:89:PRO:HA	8:BH:92:ARG:NH1	2.30	0.46
15:BO:62:GLN:HA	15:BO:65:ARG:NH1	2.30	0.46
20:BU:73:HIS:O	20:BU:76:ALA:HB3	2.15	0.46
55:C8:8:ASN:HD22	55:C8:8:ASN:C	2.18	0.46
38:CP:71:ASP:OD2	58:C1:953:C:O2'	2.29	0.46
36:CN:104:ARG:NE	41:CS:33:LYS:HE3	2.31	0.46
45:CX:38:GLU:OE2	58:C1:142:C:H4'	2.15	0.46
39:DQ:36:THR:HG22	58:D1:1323:A:OP1	2.15	0.46
58:D1:98:G:HO2'	58:D1:98:G:H8	1.60	0.46
33:DI:81:VAL:HG21	33:DI:88:ILE:CG2	2.45	0.46
37:DO:117:GLU:OE2	58:D1:661:A:H2'	2.15	0.46
38:DP:76:LYS:HB3	38:DP:91:GLU:HG3	1.97	0.46
3:AC:76:VAL:HG23	3:AC:77:ILE:HG13	1.96	0.46
7:AG:116:ALA:O	7:AG:117:ALA:C	2.54	0.46
16:AP:74:LEU:O	16:AP:79:VAL:HG23	2.15	0.46
10:BJ:50:ILE:HG22	10:BJ:60:ARG:HB3	1.97	0.46
17:BR:48:GLU:O	17:BR:49:GLU:C	2.53	0.46
58:C1:2480:A:H2	58:C1:2492:G:H21	1.62	0.46
58:C1:321:G:H5'	58:C1:322:A:OP1	2.15	0.46
54:C7:18:ARG:HD2	54:C7:43:CYS:SG	2.55	0.46
29:CC:120:TRP:O	29:CC:121:ASN:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:CE:71:THR:HG22	31:CE:89:GLY:C	2.35	0.46
33:CI:110:ASP:C	33:CI:112:LYS:H	2.19	0.46
33:CI:114:LEU:O	33:CI:115:ALA:HB2	2.16	0.46
41:CS:56:GLY:O	41:CS:59:THR:CG2	2.63	0.46
43:CU:2:PHE:O	43:CU:3:ALA:HB3	2.16	0.46
58:D1:157:U:H6	58:D1:157:U:OP2	1.98	0.46
58:D1:1895:G:C5'	58:D1:1896:C:OP2	2.63	0.46
58:D1:2551:C:H2'	58:D1:2552:A:O4'	2.15	0.46
58:D1:579:U:H2'	58:D1:580:G:C8	2.49	0.46
54:D7:22:ALA:O	54:D7:23:THR:OG1	2.24	0.46
54:D7:37:ARG:O	54:D7:48:VAL:O	2.33	0.46
30:DD:28:ILE:HG21	30:DD:116:ASP:HB2	1.97	0.46
37:DO:16:ARG:HG3	37:DO:17:LYS:H	1.80	0.46
13:BM:120:LYS:HE3	13:BM:121:LYS:O	2.16	0.46
21:BW:5:ASP:O	21:BW:11:GLY:HA3	2.15	0.46
58:C1:1336:C:H2'	58:C1:1337:U:H6	1.81	0.46
58:C1:1538:C:O2	58:C1:1538:C:H2'	2.15	0.46
58:C1:2323:U:C2'	58:C1:2324:C:H5'	2.44	0.46
38:CP:123:HIS:CG	58:C1:2478:C:H4'	2.51	0.46
58:C1:47:A:H5''	58:C1:49:G:O4'	2.15	0.46
58:C1:996:G:C6	58:C1:1010:G:C6	3.04	0.46
56:C9:61:LEU:HG	56:C9:61:LEU:H	1.27	0.46
30:CD:89:VAL:HG12	30:CD:90:PHE:N	2.30	0.46
32:CF:158:HIS:NE2	32:CF:170:ARG:O	2.48	0.46
33:CI:123:LEU:HD23	33:CI:124:GLY:N	2.30	0.46
35:CM:133:GLN:O	35:CM:134:ARG:CB	2.62	0.46
58:D1:1766:A:O2'	58:D1:1767:U:H5'	2.16	0.46
25:D3:19:G:O2'	58:D1:2133:G:H1'	2.15	0.46
58:D1:2144:G:H2'	58:D1:2145:G:O4'	2.16	0.46
58:D1:2612:C:P	66:D1:3001:3V6:CB	3.04	0.46
58:D1:2859:A:OP2	58:D1:2875:U:C5	2.68	0.46
28:DB:142:VAL:HG23	28:DB:192:THR:O	2.14	0.46
47:DZ:26:GLY:HA2	47:DZ:85:HIS:CD2	2.51	0.46
5:AE:10:MET:CB	5:AE:32:VAL:HG22	2.45	0.46
14:AN:44:LEU:HD12	14:AN:44:LEU:O	2.16	0.46
16:AP:55:ARG:O	16:AP:58:TYR:N	2.48	0.46
4:BD:43:HIS:O	4:BD:45:GLN:N	2.48	0.46
15:BO:3:ILE:HG22	15:BO:38:ARG:HE	1.79	0.46
58:C1:1405:A:H5''	58:C1:1406:G:OP2	2.15	0.46
58:C1:1698:A:O3'	58:C1:1699:G:C8	2.69	0.46
58:C1:2020:C:H2'	58:C1:2021:G:O4'	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:C9:31:HIS:HE1	58:C1:2403:A:OP2	1.98	0.46
58:C1:2502:U:H4'	58:C1:2581:G:OP1	2.16	0.46
56:C9:43:GLN:C	56:C9:44:LYS:HD2	2.35	0.46
27:CA:40:THR:HB	58:C1:2146:G:H5'	1.98	0.46
28:CB:242:ARG:HD2	28:CB:242:ARG:H	1.80	0.46
30:CD:20:LEU:HD22	30:CD:23:ASP:OD2	2.15	0.46
37:CO:50:ARG:HH11	58:C1:240:G:P	2.38	0.46
40:CR:74:ALA:HB1	40:CR:103:GLU:CB	2.46	0.46
40:CR:74:ALA:HB1	40:CR:103:GLU:HB2	1.97	0.46
40:CR:97:ARG:HH21	40:CR:98:VAL:HG22	1.81	0.46
47:CZ:151:HIS:HB3	47:CZ:170:THR:HA	1.98	0.46
47:CZ:52:SER:OG	47:CZ:53:ILE:N	2.48	0.46
58:D1:2710:C:H2'	58:D1:2711:C:O4'	2.16	0.46
58:D1:2723:U:O2'	58:D1:2724:A:OP2	2.26	0.46
58:D1:2799:C:O2	58:D1:2799:C:H2'	2.14	0.46
29:DC:183:LEU:N	29:DC:183:LEU:HD12	2.30	0.46
43:DU:81:TYR:CE2	58:D1:1231:G:H5''	2.51	0.46
63:DW:82:LEU:HB2	63:DW:98:LYS:HB2	1.96	0.46
2:AA:144:ARG:HA	2:AA:147:LYS:HB3	1.97	0.46
3:AC:64:VAL:O	3:AC:100:ALA:HB3	2.15	0.46
5:AE:20:GLN:O	5:AE:23:GLY:O	2.34	0.46
12:AL:27:LEU:HD21	12:AL:64:TYR:CE1	2.50	0.46
13:AM:3:ARG:HG2	13:AM:9:ILE:HG12	1.98	0.46
19:AT:50:ALA:HB1	19:AT:57:HIS:HB3	1.96	0.46
2:BA:167:PRO:HD3	2:BA:188:ALA:HB2	1.97	0.46
5:BE:20:GLN:O	5:BE:21:ALA:C	2.53	0.46
10:BJ:6:ILE:HG13	10:BJ:72:VAL:O	2.16	0.46
40:CR:18:ILE:HD11	58:C1:2345:G:H21	1.81	0.46
58:C1:918:A:C6	58:C1:951:G:C2	3.04	0.46
30:CD:183:VAL:O	30:CD:187:VAL:HG23	2.15	0.46
38:CP:21:THR:CG2	38:CP:101:ARG:HB2	2.46	0.46
43:CU:38:LEU:C	43:CU:39:LEU:HD13	2.35	0.46
58:D1:2801:C:OP1	58:D1:2801:C:H4'	2.15	0.46
56:D9:4:MET:CE	56:D9:61:LEU:HD22	2.46	0.46
29:DC:110:GLY:O	39:DQ:5:LYS:NZ	2.46	0.46
31:DE:47:LYS:HG3	31:DE:48:GLU:H	1.80	0.46
13:AM:65:LYS:HA	13:AM:66:LEU:CG	2.46	0.46
18:AS:43:PHE:CA	18:AS:51:LEU:HD12	2.44	0.46
6:BF:67:MET:CE	6:BF:75:LEU:HD22	2.46	0.46
58:C1:179:A:H2'	58:C1:180:C:H6	1.81	0.46
58:C1:2487:A:N1	58:C1:2488:C:C5	2.84	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:C1:552:A:N1	58:C1:2064:C:O5'	2.49	0.46
58:C1:826:G:O5'	58:C1:826:G:H8	1.98	0.46
41:CS:27:THR:O	41:CS:28:VAL:CG2	2.50	0.46
42:CT:54:LYS:HE3	58:C1:1039:C:H3'	1.98	0.46
43:CU:15:GLU:O	43:CU:16:PRO:C	2.54	0.46
47:CZ:149:SER:HB2	47:CZ:173:ALA:HA	1.98	0.46
58:D1:1220:G:O2'	58:D1:1221:A:H5'	2.16	0.46
58:D1:1548:U:C4	58:D1:1549:C:N4	2.84	0.46
58:D1:1772:C:H2'	58:D1:1773:C:H5'	1.96	0.46
25:D3:34:G:C2	25:D3:35:A:N3	2.84	0.46
56:D9:29:LYS:HD3	56:D9:44:LYS:HD3	1.97	0.46
30:DD:128:ALA:O	30:DD:142:TRP:NE1	2.48	0.46
49:DH:67:ILE:N	49:DH:68:PRO:HD2	2.30	0.46
33:DI:1:MET:O	33:DI:20:ASP:HA	2.16	0.46
43:DU:49:THR:HG22	43:DU:50:PRO:HD3	1.98	0.46
46:DY:7:VAL:HB	46:DY:8:LYS:HD2	1.97	0.46
5:AE:48:ALA:HB1	5:AE:49:PRO:HD2	1.98	0.46
9:AI:95:LYS:HD3	9:AI:96:LEU:N	2.31	0.46
58:C1:2139:U:H5	58:C1:2169:G:HO2'	1.63	0.46
58:C1:2443:A:H2'	58:C1:2444:A:C8	2.51	0.46
58:C1:274:C:O2'	58:C1:275:C:P	2.73	0.46
54:C7:36:LEU:HD13	54:C7:50:ARG:NH2	2.30	0.46
56:C9:52:LYS:N	56:C9:53:PRO:CD	2.79	0.46
31:CE:171:ALA:O	31:CE:175:LEU:HG	2.15	0.46
39:CQ:84:ALA:N	39:CQ:85:PRO:CD	2.79	0.46
58:D1:1254:A:C8	58:D1:1254:A:H5'	2.46	0.46
58:D1:1276:G:H2'	58:D1:1277:G:H8	1.81	0.46
58:D1:2523:C:H2'	58:D1:2524:G:O4'	2.16	0.46
58:D1:2813:C:H2'	58:D1:2814:C:C6	2.51	0.46
58:D1:2890:C:C4	58:D1:2891:A:N7	2.84	0.46
58:D1:906:U:O4'	58:D1:906:U:O2	2.33	0.46
28:DB:34:VAL:HG23	28:DB:35:LYS:N	2.30	0.46
29:DC:105:THR:OG1	29:DC:199:ARG:NH2	2.45	0.46
29:DC:24:THR:HG23	29:DC:184:VAL:HG23	1.98	0.46
32:DF:158:HIS:HE2	32:DF:170:ARG:C	2.19	0.46
35:DM:133:GLN:O	35:DM:134:ARG:CB	2.64	0.46
35:DM:133:GLN:O	35:DM:134:ARG:HB3	2.16	0.46
40:DR:41:ASP:OD2	40:DR:44:LYS:HB2	2.15	0.46
42:DT:66:ASN:HD21	42:DT:70:ARG:NE	2.13	0.46
45:DX:14:SER:O	45:DX:15:GLU:C	2.54	0.46
10:AJ:57:LYS:O	10:AJ:57:LYS:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:AL:47:LYS:HB3	12:AL:48:PRO:HD3	1.98	0.46
32:CF:110:SER:HB2	58:C1:2664:U:O2'	2.16	0.46
58:C1:2697:G:C2	58:C1:2736:C:O2	2.69	0.46
58:C1:2612:C:P	66:C1:3001:3V6:H19	2.55	0.46
25:C3:61:C:H2'	25:C3:62:C:C6	2.50	0.46
27:CA:50:ASP:N	27:CA:51:PRO:HD3	2.30	0.46
37:CO:23:PRO:HD2	37:CO:33:ARG:NH2	2.31	0.46
58:D1:2249:G:H2'	58:D1:2249:G:N3	2.31	0.46
56:D9:12:LYS:NZ	58:D1:237:C:O2	2.37	0.46
58:D1:820:A:O2'	58:D1:821:G:P	2.74	0.46
58:D1:977:A:H2'	58:D1:978:G:O5'	2.16	0.46
56:D9:2:PRO:O	56:D9:3:LYS:CB	2.64	0.46
32:DF:138:LYS:O	32:DF:139:GLN:C	2.54	0.46
38:DP:27:VAL:O	38:DP:28:ALA:HB3	2.15	0.46
46:DY:44:ILE:HG22	46:DY:45:VAL:H	1.81	0.46
14:BN:13:THR:N	14:BN:14:PRO:CD	2.79	0.46
17:BR:63:ARG:HG2	17:BR:64:PRO:HD2	1.98	0.46
58:C1:144:G:O2'	58:C1:145:G:H5'	2.15	0.46
58:C1:2083:A:C5'	58:C1:2083:A:C4	2.98	0.46
58:C1:2124:C:O2	58:C1:2208:G:C2	2.69	0.46
58:C1:298:G:O4'	58:C1:298:G:OP1	2.34	0.46
53:C6:35:GLU:O	53:C6:36:CYS:HB2	2.15	0.46
28:CB:76:PRO:HA	28:CB:118:VAL:HG23	1.97	0.46
28:CB:242:ARG:NH2	58:C1:1856:G:O2'	2.49	0.46
28:CB:270:ILE:HD12	28:CB:270:ILE:O	2.15	0.46
33:CI:6:LEU:O	33:CI:7:GLU:C	2.54	0.46
42:CT:17:ILE:O	42:CT:20:LEU:HB2	2.16	0.46
46:CY:18:GLY:HA2	58:C1:333:A:P	2.55	0.46
58:D1:162:C:H5'	58:D1:163:G:OP2	2.15	0.46
54:D7:24:GLU:OE2	58:D1:2357:A:C8	2.69	0.46
58:D1:99:G:H5"	58:D1:99:G:C8	2.51	0.46
37:DO:108:LYS:O	37:DO:110:TYR:N	2.49	0.46
36:DN:77:ILE:HD12	41:DS:74:ARG:HG2	1.97	0.46
46:DY:31:LEU:HD23	46:DY:36:ALA:HB3	1.98	0.46
9:AI:48:GLU:N	9:AI:49:PRO:CD	2.79	0.46
13:BM:78:ILE:HA	13:BM:81:LEU:HD12	1.97	0.46
19:BT:19:VAL:O	19:BT:23:ASN:N	2.49	0.46
19:BT:58:VAL:CG2	19:BT:58:VAL:O	2.63	0.46
42:CT:55:ARG:HD2	58:C1:1200:A:OP1	2.16	0.46
58:C1:139:A:H8	58:C1:1640:G:H21	1.60	0.46
58:C1:1799:G:O2'	58:C1:1979:C:OP1	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:C7:24:GLU:OE2	58:C1:2357:A:O2'	2.27	0.46
35:CM:3:THR:O	35:CM:5:VAL:N	2.48	0.46
37:CO:126:VAL:HG12	37:CO:148:LEU:HD11	1.98	0.46
40:CR:14:VAL:HG12	40:CR:15:ARG:N	2.30	0.46
45:CX:12:VAL:HB	45:CX:17:ALA:HB1	1.98	0.46
58:D1:2139:U:P	58:D1:2168:G:HO2'	2.39	0.46
54:D7:37:ARG:NH1	58:D1:2355:U:C5	2.83	0.46
29:DC:151:TYR:O	58:D1:2630:C:H4'	2.15	0.46
58:D1:821:G:C4	58:D1:840:G:C8	3.03	0.46
28:DB:35:LYS:HE2	28:DB:36:PRO:HB3	1.98	0.46
29:DC:111:ARG:HD2	29:DC:160:TYR:CE1	2.51	0.46
35:DM:131:GLN:HA	35:DM:131:GLN:OE1	2.16	0.46
36:DN:17:ARG:HB2	36:DN:45:GLU:HG3	1.98	0.46
9:AI:43:ALA:C	9:AI:45:ALA:H	2.19	0.45
19:AT:11:VAL:HG23	19:AT:38:SER:HB2	1.97	0.45
19:AT:41:VAL:HG13	19:AT:42:PRO:HD2	1.97	0.45
58:C1:1319:A:N3	58:C1:1342:C:H1'	2.31	0.45
28:CB:211:ARG:NH1	58:C1:1612:A:OP1	2.49	0.45
58:C1:1636:G:H5''	58:C1:1636:G:C8	2.47	0.45
58:C1:25:G:C6	58:C1:26:G:N1	2.83	0.45
25:C2:64:A:H2'	25:C2:65:G:C8	2.48	0.45
25:C2:74:C:H2'	25:C2:75:C:O5'	2.15	0.45
47:CZ:24:LEU:HB2	47:CZ:41:LEU:HG	1.98	0.45
58:D1:1004:A:H5''	58:D1:1005:C:OP2	2.16	0.45
58:D1:668:A:O2'	58:D1:669:C:H5'	2.15	0.45
25:D3:30:G:C2	25:D3:41:C:N3	2.84	0.45
52:D5:61:VAL:HG13	52:D5:65:CYS:SG	2.56	0.45
28:DB:28:GLU:HB2	28:DB:29:PRO:HD3	1.99	0.45
29:DC:181:LEU:HD21	41:DS:7:ILE:CG2	2.46	0.45
29:DC:1:MET:HG2	29:DC:83:ASP:O	2.16	0.45
33:DI:129:THR:HG22	33:DI:130:TYR:H	1.80	0.45
46:DY:29:GLU:N	46:DY:29:GLU:OE1	2.49	0.45
47:DZ:68:PRO:O	47:DZ:91:LEU:HD12	2.16	0.45
10:AJ:38:ILE:HG13	10:AJ:71:LEU:HB3	1.97	0.45
19:AT:43:GLU:C	19:AT:45:VAL:H	2.20	0.45
4:BD:13:ARG:O	4:BD:15:GLU:N	2.48	0.45
17:BR:33:GLY:O	17:BR:34:LYS:C	2.55	0.45
58:C1:1698:A:O3'	58:C1:1699:G:H8	1.99	0.45
28:CB:270:ILE:C	28:CB:270:ILE:HD12	2.36	0.45
28:CB:43:ARG:HB2	28:CB:54:ARG:HB2	1.99	0.45
31:CE:152:LEU:H	31:CE:152:LEU:HD23	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:CF:17:VAL:O	32:CF:45:VAL:HG22	2.15	0.45
33:CI:60:GLU:C	33:CI:62:LYS:H	2.20	0.45
50:CK:16:LEU:O	50:CK:17:SER:HB3	2.16	0.45
37:CO:107:LYS:C	37:CO:109:GLY:H	2.18	0.45
44:CW:84:ARG:NE	58:C1:1368:U:OP1	2.50	0.45
58:D1:1729:C:H2'	58:D1:1730:C:C6	2.52	0.45
58:D1:1865:G:H2'	58:D1:1865:G:N3	2.31	0.45
58:D1:2433:A:H4'	58:D1:2434:U:OP1	2.17	0.45
58:D1:534:C:OP1	58:D1:535:U:OP2	2.34	0.45
61:D4:31:G:N2	61:D4:42:C:C2	2.83	0.45
28:DB:240:ALA:HB1	28:DB:241:PRO:HD3	1.98	0.45
46:DY:49:VAL:O	46:DY:50:ARG:HB2	2.17	0.45
13:BM:28:ALA:O	13:BM:30:ALA:N	2.49	0.45
58:C1:1326:G:H5''	58:C1:1326:G:H8	1.81	0.45
58:C1:1777:G:C2'	58:C1:1778:G:H5'	2.47	0.45
58:C1:1984:U:C2'	58:C1:1984:U:O2	2.62	0.45
58:C1:2200:C:N4	58:C1:2203:G:O6	2.49	0.45
42:CT:2:PRO:HA	58:C1:470:C:OP1	2.16	0.45
26:C4:12:G:H4'	58:C1:1929:C:O2	2.16	0.45
36:CN:47:ILE:HG12	36:CN:48:PRO:HD2	1.98	0.45
39:CQ:84:ALA:HB3	39:CQ:85:PRO:HD3	1.98	0.45
41:CS:89:VAL:HG12	41:CS:91:ARG:HG3	1.97	0.45
42:CT:49:HIS:CD2	58:C1:558:U:O2'	2.66	0.45
58:D1:1766:A:N6	58:D1:1769:A:C2	2.85	0.45
58:D1:1883:A:H2'	58:D1:1884:A:C8	2.51	0.45
58:D1:1937:A:H5'	58:D1:1938:U:OP2	2.17	0.45
58:D1:1813:A:C2	58:D1:2598:A:C5	3.04	0.45
58:D1:552:A:O2'	58:D1:553:A:H5'	2.16	0.45
61:D4:14:A:C6	61:D4:23:G:C5	3.05	0.45
40:DR:83:LYS:HE3	40:DR:105:ALA:CB	2.47	0.45
42:DT:112:ARG:HH11	42:DT:112:ARG:CG	2.29	0.45
46:DY:2:ARG:O	46:DY:4:LYS:N	2.49	0.45
1:A2:19:U:H2'	1:A2:20:U:O5'	2.16	0.45
4:AD:22:LYS:HG3	4:AD:26:CYS:SG	2.56	0.45
5:AE:16:THR:O	5:AE:17:ALA:HB2	2.17	0.45
17:AR:66:SER:OG	17:AR:69:LYS:HB2	2.16	0.45
18:AS:43:PHE:C	18:AS:51:LEU:HD12	2.37	0.45
10:BJ:82:ILE:O	10:BJ:86:MET:HB2	2.17	0.45
15:BO:56:LEU:O	15:BO:60:VAL:HG23	2.16	0.45
20:BU:97:ALA:O	20:BU:99:LEU:N	2.49	0.45
58:C1:2124:C:O2	58:C1:2208:G:N2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:C1:264:U:H2'	58:C1:265:C:C6	2.51	0.45
58:C1:393:C:H2'	58:C1:393:C:O2	2.16	0.45
29:CC:120:TRP:CE3	29:CC:155:LYS:HE3	2.51	0.45
30:CD:181:LEU:CG	30:CD:186:ILE:HD11	2.47	0.45
31:CE:46:ALA:O	31:CE:82:LEU:HD11	2.16	0.45
36:CN:68:GLU:HB3	36:CN:78:ARG:HB2	1.98	0.45
41:CS:28:VAL:HG12	41:CS:29:ARG:HD3	1.97	0.45
42:CT:109:LEU:HD21	43:CU:46:VAL:HG23	1.98	0.45
43:CU:49:THR:HB	43:CU:50:PRO:HD2	1.97	0.45
58:D1:1156:A:O2'	58:D1:1157:G:C4'	2.64	0.45
58:D1:139:A:C8	58:D1:1453:C:H1'	2.52	0.45
58:D1:2323:U:H2'	58:D1:2324:C:H5'	1.99	0.45
58:D1:2845:U:H2'	58:D1:2846:G:C8	2.51	0.45
58:D1:516:A:H2'	58:D1:517:G:O4'	2.17	0.45
50:DK:55:ARG:NH1	58:D1:73:G:H4'	2.32	0.45
54:D7:42:TRP:CH2	58:D1:667:A:N7	2.84	0.45
56:D9:47:LYS:HD2	56:D9:48:PHE:O	2.17	0.45
39:DQ:103:ARG:HD3	63:DW:40:ASN:ND2	2.31	0.45
46:DY:17:SER:HB2	46:DY:71:LYS:HE2	1.99	0.45
11:AK:84:VAL:HG23	11:AK:110:ASP:OD1	2.16	0.45
13:AM:89:GLY:C	13:AM:90:LEU:O	2.52	0.45
5:BE:126:ARG:O	5:BE:127:ASN:C	2.54	0.45
5:BE:76:ILE:HG22	5:BE:93:PRO:HB3	1.98	0.45
19:BT:31:ILE:O	19:BT:31:ILE:HG23	2.17	0.45
58:C1:1685:U:H2'	58:C1:1686:C:H5''	1.98	0.45
58:C1:1766:A:H2	58:C1:1768:G:H2'	1.82	0.45
28:CB:52:ARG:NH1	58:C1:1854:G:OP1	2.45	0.45
58:C1:2723:U:H1'	58:C1:2724:A:C8	2.52	0.45
58:C1:646:G:O2'	58:C1:647:G:H5'	2.16	0.45
25:C3:61:C:H2'	25:C3:62:C:C5	2.51	0.45
13:AM:7:VAL:HG23	31:CE:115:ARG:HG3	1.97	0.45
38:CP:137:TYR:CE2	47:CZ:81:ARG:NH1	2.85	0.45
38:CP:98:LYS:HB3	38:CP:99:PRO:CD	2.47	0.45
29:CC:14:ILE:HB	41:CS:14:TYR:CZ	2.51	0.45
57:D0:18:ARG:O	58:D1:2769:A:OP1	2.33	0.45
58:D1:154:C:O3'	58:D1:157:U:P	2.75	0.45
58:D1:2057:C:C5'	58:D1:2057:C:H6	2.29	0.45
58:D1:2562:C:H2'	58:D1:2563:U:C6	2.50	0.45
58:D1:566:C:O2'	58:D1:567:C:OP1	2.21	0.45
52:D5:36:VAL:O	52:D5:52:SER:O	2.35	0.45
30:DD:169:ASN:ND2	58:D1:345:A:H3'	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:DE:85:GLY:C	31:DE:87:PRO:HD2	2.37	0.45
33:DI:74:ASN:OD1	33:DI:75:LEU:N	2.50	0.45
43:DU:49:THR:CB	43:DU:50:PRO:CD	2.95	0.45
5:AE:76:ILE:HD11	5:AE:142:LEU:HD21	1.98	0.45
7:AG:16:LEU:HD12	9:AI:42:ARG:HA	1.98	0.45
7:AG:54:THR:OG1	7:AG:56:GLN:HG2	2.17	0.45
13:AM:86:CYS:O	13:AM:89:GLY:N	2.45	0.45
18:AS:56:THR:CB	18:AS:58:LEU:HD13	2.47	0.45
58:C1:149:C:H2'	58:C1:150:C:C6	2.51	0.45
58:C1:904:U:O2	58:C1:2279:A:H2'	2.17	0.45
36:CN:101:PRO:HG3	41:CS:67:SER:CB	2.47	0.45
46:CY:74:PRO:O	46:CY:80:GLY:HA2	2.16	0.45
46:CY:7:VAL:HB	46:CY:8:LYS:CD	2.47	0.45
58:D1:2352:G:H2'	58:D1:2353:C:C6	2.52	0.45
58:D1:2859:A:OP2	58:D1:2875:U:H5	1.98	0.45
25:D3:34:G:N1	25:D3:35:A:N3	2.64	0.45
30:DD:132:VAL:HG13	30:DD:133:ASN:CG	2.37	0.45
30:DD:188:ARG:HA	37:DO:7:ARG:CD	2.47	0.45
41:DS:28:VAL:O	41:DS:29:ARG:CD	2.62	0.45
11:AK:99:GLN:HG2	11:AK:105:VAL:HG21	1.97	0.45
16:AP:3:LYS:O	16:AP:21:VAL:HA	2.17	0.45
20:AU:14:LYS:O	20:AU:18:GLN:HB2	2.16	0.45
24:BC:11:ARG:O	24:BC:14:ILE:N	2.47	0.45
6:BF:41:GLU:HB3	6:BF:43:LEU:HD12	1.99	0.45
19:BT:40:ILE:HG21	19:BT:62:ILE:CD1	2.44	0.45
57:C0:19:ARG:O	57:C0:20:HIS:HB2	2.17	0.45
58:C1:1540:A:O4'	58:C1:1540:A:P	2.75	0.45
58:C1:552:A:C2	58:C1:2064:C:C5'	3.00	0.45
28:CB:245:PRO:O	28:CB:246:PRO:C	2.55	0.45
30:CD:103:LYS:HA	30:CD:106:ARG:HG3	1.98	0.45
41:CS:129:ARG:NH1	41:CS:131:ALA:HB2	2.32	0.45
41:CS:28:VAL:HG22	41:CS:46:GLU:CG	2.47	0.45
58:D1:1092:G:H4'	58:D1:1092:G:OP1	2.11	0.45
58:D1:1451:U:H2'	58:D1:1452:C:C6	2.52	0.45
29:DC:109:LYS:HE2	58:D1:2829:A:C8	2.51	0.45
58:D1:554:G:O4'	58:D1:554:G:N3	2.49	0.45
25:D3:61:C:H2'	25:D3:62:C:H6	1.82	0.45
56:D9:8:LYS:HB3	56:D9:12:LYS:HE3	1.99	0.45
28:DB:143:HIS:HD2	28:DB:144:ALA:HB2	1.82	0.45
28:DB:172:TYR:CD1	28:DB:186:HIS:HA	2.52	0.45
50:DK:29:LYS:HD3	50:DK:57:ILE:HD13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:DL:10:LYS:HB3	51:DL:53:LEU:HD23	1.98	0.45
41:DS:3:ARG:CZ	58:D1:2885:G:O3'	2.65	0.45
43:DU:5:VAL:HG22	43:DU:6:LYS:N	2.32	0.45
46:DY:2:ARG:C	46:DY:4:LYS:N	2.69	0.45
47:DZ:105:VAL:O	47:DZ:141:VAL:CG1	2.64	0.45
47:DZ:113:ALA:HB3	47:DZ:146:ILE:HG21	1.99	0.45
4:AD:61:LYS:HE2	4:AD:62:GLN:HE21	1.82	0.45
3:AC:60:ALA:HB2	10:AJ:91:PRO:O	2.17	0.45
23:B2:19:U:O4'	23:B2:19:U:P	2.74	0.45
2:BA:19:HIS:O	2:BA:39:ILE:HG23	2.17	0.45
19:BT:29:ARG:O	19:BT:31:ILE:N	2.49	0.45
58:C1:1625:A:H8	58:C1:1625:A:H5'	1.82	0.45
58:C1:2100:U:H2'	58:C1:2101:G:O4'	2.17	0.45
58:C1:2121:G:C6	58:C1:2122:G:C6	3.04	0.45
58:C1:323:A:H2'	58:C1:357:C:H1'	1.99	0.45
58:C1:347:A:N6	58:C1:361:G:O2'	2.45	0.45
26:C4:75:C:O5'	26:C4:75:C:H6	1.99	0.45
53:C6:57:VAL:HB	53:C6:58:LEU:HD12	1.99	0.45
54:C7:9:LEU:HD22	54:C7:10:LEU:N	2.32	0.45
28:CB:226:MET:HB3	28:CB:230:ASP:HB2	1.99	0.45
29:CC:144:ARG:HB3	29:CC:145:LYS:H	1.59	0.45
30:CD:80:ALA:O	30:CD:83:PHE:HB2	2.17	0.45
58:D1:1357:U:C2	58:D1:1648:A:C2	3.04	0.45
58:D1:2052:A:C6	58:D1:2509:C:H1'	2.51	0.45
58:D1:2845:U:C4	58:D1:2892:A:N6	2.85	0.45
58:D1:715:G:H8	58:D1:715:G:H5'	1.81	0.45
28:DB:266:SER:C	28:DB:267:SER:O	2.55	0.45
32:DF:30:LYS:HE3	32:DF:81:GLU:HG3	1.98	0.45
46:DY:39:VAL:HG12	46:DY:40:GLU:H	1.81	0.45
10:AJ:50:ILE:HA	10:AJ:60:ARG:HB2	1.99	0.45
2:BA:185:ILE:CG2	2:BA:199:TYR:HB2	2.46	0.45
13:BM:117:VAL:O	13:BM:118:ALA:HB2	2.16	0.45
13:BM:16:ASP:HA	13:BM:34:LEU:HD11	1.99	0.45
19:BT:23:ASN:O	19:BT:25:LYS:N	2.50	0.45
58:C1:1041:A:N6	58:C1:1205:G:C6	2.84	0.45
58:C1:1701:A:C8	58:C1:1702:C:C5	3.04	0.45
58:C1:271:U:H6	58:C1:271:U:H3'	1.82	0.45
53:C6:16:ARG:NH2	58:C1:541:C:OP1	2.50	0.45
53:C6:51:TYR:HB3	53:C6:52:TYR:H	1.62	0.45
46:CY:31:LEU:CB	46:CY:32:PRO:HA	2.46	0.45
58:D1:154:C:O3'	58:D1:157:U:OP1	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:D1:2714:C:C2	58:D1:2715:C:C5	3.05	0.45
58:D1:495:A:H2'	58:D1:496:A:O4'	2.17	0.45
62:DA:47:LEU:N	62:DA:47:LEU:HD23	2.31	0.45
29:DC:116:VAL:CG2	29:DC:122:PHE:CG	3.00	0.45
38:DP:82:ARG:HG2	58:D1:2507:C:OP2	2.17	0.45
1:A2:14:A:H2'	1:A2:15:A:O5'	2.17	0.45
1:A2:17:U:C2'	1:A2:18:G:C5'	2.89	0.45
3:AC:47:LEU:HD11	3:AC:76:VAL:HG12	1.98	0.45
13:AM:63:THR:HG22	13:AM:64:TRP:N	2.32	0.45
5:BE:33:VAL:HG12	5:BE:34:VAL:N	2.32	0.45
8:BH:112:LEU:N	8:BH:112:LEU:HD23	2.32	0.45
9:BI:21:PRO:HA	9:BI:58:ARG:O	2.16	0.45
10:BJ:23:ILE:O	10:BJ:23:ILE:HG22	2.17	0.45
10:BJ:8:LEU:HD23	10:BJ:96:ILE:CG2	2.46	0.45
58:C1:1036:C:H6	58:C1:1036:C:H5'	1.81	0.45
58:C1:1069:G:H3'	58:C1:1070:G:H5''	1.98	0.45
58:C1:2121:G:C2	58:C1:2122:G:C4	3.04	0.45
30:CD:51:THR:HG23	30:CD:92:PRO:HG2	1.99	0.45
42:CT:83:LEU:CD1	42:CT:88:ILE:HD11	2.44	0.45
47:CZ:54:HIS:CG	47:CZ:101:PRO:HG3	2.52	0.45
58:D1:1538:C:C5	58:D1:2226:G:O2'	2.62	0.45
58:D1:1636:G:C8	58:D1:1636:G:H5''	2.49	0.45
58:D1:25:G:C6	58:D1:26:G:N1	2.84	0.45
58:D1:275:C:O2'	58:D1:276:G:H5'	2.17	0.45
58:D1:609:C:C5	58:D1:717:C:H1'	2.52	0.45
37:DO:38:GLN:OE1	58:D1:987:U:OP2	2.35	0.45
52:D5:40:ILE:HA	52:D5:57:ILE:HB	1.99	0.45
29:DC:132:HIS:CD2	29:DC:135:HIS:CE1	3.05	0.45
31:DE:113:ARG:NH1	52:D5:60:GLU:O	2.49	0.45
37:DO:16:ARG:HD3	37:DO:16:ARG:C	2.37	0.45
38:DP:108:GLY:O	38:DP:109:VAL:HG23	2.17	0.45
39:DQ:47:PHE:O	39:DQ:51:LEU:HD13	2.17	0.45
40:DR:34:HIS:HB3	40:DR:53:SER:HB3	1.98	0.45
43:DU:47:VAL:HB	43:DU:49:THR:O	2.16	0.45
4:AD:108:LEU:HB3	4:AD:110:PHE:CE1	2.52	0.44
6:AF:9:VAL:HB	6:AF:87:ARG:HB2	1.99	0.44
12:AL:84:LEU:HB2	12:AL:104:VAL:HG11	1.99	0.44
17:BR:67:LYS:HA	17:BR:70:ARG:HH12	1.82	0.44
58:C1:353:A:H2	58:C1:1254:A:H2'	1.82	0.44
28:CB:166:GLN:NE2	28:CB:166:GLN:HA	2.31	0.44
29:CC:102:VAL:HG12	29:CC:199:ARG:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:CK:25:VAL:O	50:CK:26:ARG:C	2.55	0.44
39:CQ:24:GLN:HE22	39:CQ:36:THR:HG21	1.82	0.44
41:CS:29:ARG:CB	41:CS:85:LYS:HA	2.47	0.44
47:CZ:145:GLU:HG3	47:CZ:146:ILE:HD12	1.98	0.44
58:D1:2723:U:H5'	58:D1:2723:U:O2	2.17	0.44
58:D1:745:A:H2'	58:D1:746:G:O4'	2.18	0.44
33:DI:88:ILE:HG22	33:DI:89:TYR:N	2.32	0.44
35:DM:134:ARG:O	35:DM:136:GLU:N	2.50	0.44
63:DW:89:ALA:O	63:DW:90:ARG:HB2	2.17	0.44
46:DY:31:LEU:HD13	46:DY:31:LEU:HA	1.78	0.44
13:AM:19:LEU:O	13:AM:22:ILE:HD12	2.17	0.44
2:BA:233:SER:CB	2:BA:234:PRO:HD2	2.47	0.44
57:C0:22:ARG:HB2	57:C0:24:TYR:HE1	1.81	0.44
58:C1:1450:U:H2'	58:C1:1451:U:C6	2.53	0.44
58:C1:1648:A:H5'	58:C1:1648:A:H8	1.82	0.44
58:C1:1703:C:H2'	58:C1:1704:C:C6	2.52	0.44
36:CN:6:THR:HA	58:C1:1713:G:OP1	2.18	0.44
28:CB:88:ARG:NH2	58:C1:1847:G:OP1	2.50	0.44
58:C1:2155:A:H2'	58:C1:2155:A:N3	2.31	0.44
58:C1:2722:A:OP1	58:C1:2724:A:P	2.75	0.44
58:C1:635:G:H5''	58:C1:635:G:H8	1.81	0.44
29:CC:77:ILE:HG22	29:CC:78:LEU:N	2.32	0.44
39:CQ:75:LEU:O	39:CQ:75:LEU:HD13	2.18	0.44
43:CU:23:GLU:O	43:CU:24:LYS:C	2.55	0.44
58:D1:2535:G:C8	58:D1:2535:G:C5'	3.00	0.44
32:DF:43:VAL:CG1	32:DF:52:VAL:HA	2.47	0.44
37:DO:62:LEU:HD23	37:DO:62:LEU:N	2.31	0.44
38:DP:109:VAL:HG13	38:DP:113:GLN:OE1	2.17	0.44
39:DQ:117:VAL:O	39:DQ:118:GLU:CB	2.62	0.44
42:DT:91:ASP:O	42:DT:95:LEU:HB2	2.16	0.44
64:DV:5:G:H2'	64:DV:6:G:C8	2.52	0.44
2:AA:54:THR:HG21	2:AA:201:ILE:HD11	1.99	0.44
8:AH:51:VAL:HG11	8:AH:60:ARG:HD2	1.99	0.44
5:BE:72:GLN:O	5:BE:73:ASN:HB2	2.17	0.44
58:C1:1653:A:O2'	58:C1:1655:A:OP2	2.31	0.44
58:C1:1875:G:C2'	58:C1:1876:G:C5'	2.93	0.44
58:C1:88:U:O2	58:C1:88:U:H2'	2.17	0.44
29:CC:30:PRO:O	29:CC:32:PRO:HD3	2.18	0.44
32:CF:160:LYS:HE2	58:C1:2668:A:O2'	2.17	0.44
38:CP:58:PHE:CD1	38:CP:58:PHE:O	2.69	0.44
58:D1:1991:A:H5''	58:D1:1992:A:OP1	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:D1:2045:G:H2'	58:D1:2046:C:H6	1.82	0.44
58:D1:2344:A:O4'	58:D1:2346:A:C5	2.71	0.44
61:D4:24:C:H2'	61:D4:25:U:C6	2.52	0.44
29:DC:144:ARG:O	58:D1:2074:G:H5'	2.16	0.44
29:DC:58:ARG:HH22	58:D1:2840:G:P	2.40	0.44
30:DD:115:ALA:O	30:DD:116:ASP:C	2.56	0.44
39:DQ:38:VAL:O	39:DQ:41:ALA:HB3	2.18	0.44
41:DS:18:ASP:OD1	41:DS:18:ASP:N	2.49	0.44
41:DS:29:ARG:CG	41:DS:85:LYS:HA	2.47	0.44
41:DS:56:GLY:O	41:DS:59:THR:CG2	2.64	0.44
64:DV:46:U:H2'	64:DV:47:C:C6	2.52	0.44
63:DW:15:ARG:NH2	58:D1:1311:G:O4'	2.47	0.44
4:AD:64:LEU:HD12	4:AD:64:LEU:O	2.18	0.44
13:BM:82:MET:O	13:BM:82:MET:CG	2.65	0.44
58:C1:2209:C:C2'	58:C1:2210:U:O4'	2.65	0.44
58:C1:2710:C:H2'	58:C1:2711:C:O4'	2.17	0.44
58:C1:2732:U:C2'	58:C1:2732:U:O2	2.64	0.44
66:C1:3001:3V6:O	66:C1:3001:3V6:CLI	2.72	0.44
58:C1:65:U:H2'	58:C1:66:G:C8	2.53	0.44
28:CB:108:PRO:HA	28:CB:196:VAL:O	2.17	0.44
29:CC:176:ILE:HB	29:CC:181:LEU:HB2	1.99	0.44
41:CS:25:GLY:HA2	41:CS:92:GLY:CA	2.48	0.44
45:CX:3:THR:O	45:CX:4:ALA:HB3	2.18	0.44
58:D1:1337:U:O2'	58:D1:1338:C:H5'	2.17	0.44
58:D1:1811:C:O2	58:D1:1811:C:O4'	2.31	0.44
58:D1:1922:A:H2'	58:D1:1922:A:N3	2.32	0.44
28:DB:210:GLY:O	28:DB:211:ARG:HB3	2.17	0.44
28:DB:240:ALA:HA	58:D1:1992:A:N3	2.33	0.44
32:DF:158:HIS:CE1	32:DF:169:VAL:O	2.71	0.44
32:DF:43:VAL:HG11	32:DF:52:VAL:HA	1.99	0.44
35:DM:3:THR:O	35:DM:5:VAL:HG12	2.18	0.44
4:AD:61:LYS:HD3	4:AD:206:PHE:CE2	2.53	0.44
5:AE:143:ARG:NH1	8:AH:77:GLU:CD	2.70	0.44
19:AT:43:GLU:O	19:AT:45:VAL:N	2.46	0.44
24:BC:150:LYS:HG3	24:BC:169:ALA:HB2	2.00	0.44
19:BT:6:LYS:CG	19:BT:7:LYS:HE3	2.45	0.44
58:C1:1090:A:H3'	58:C1:1090:A:N3	2.33	0.44
58:C1:69:A:OP2	58:C1:69:A:H3'	2.18	0.44
27:CA:42:GLU:O	27:CA:213:UNK:N	2.50	0.44
28:CB:47:GLY:HA2	58:C1:819:U:H5'	1.98	0.44
31:CE:145:THR:CG2	31:CE:148:MET:HB2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:CS:88:ILE:HG22	41:CS:89:VAL:N	2.31	0.44
42:CT:66:ASN:HD21	42:CT:70:ARG:CZ	2.31	0.44
46:CY:76:CYS:SG	46:CY:77:PRO:HD3	2.57	0.44
47:CZ:53:ILE:CG2	47:CZ:71:VAL:HB	2.46	0.44
47:CZ:54:HIS:HB3	47:CZ:101:PRO:CD	2.46	0.44
42:DT:76:TYR:CE2	58:D1:1198:C:H5'	2.51	0.44
58:D1:1766:A:N6	58:D1:1769:A:N1	2.66	0.44
58:D1:2113:U:H4'	58:D1:2114:G:O5'	2.17	0.44
58:D1:2555:G:C2'	58:D1:2556:G:O5'	2.66	0.44
41:DS:5:ALA:HB2	58:D1:2884:C:H4'	1.99	0.44
58:D1:566:C:C2'	58:D1:567:C:OP1	2.65	0.44
58:D1:909:A:O2'	58:D1:910:G:H5'	2.18	0.44
53:D6:57:VAL:C	53:D6:58:LEU:HD12	2.38	0.44
35:DM:68:GLU:O	35:DM:69:GLN:HG2	2.17	0.44
39:DQ:57:ARG:O	39:DQ:59:ASP:N	2.48	0.44
40:DR:16:ASN:OD1	40:DR:17:ARG:N	2.50	0.44
40:DR:36:TYR:CD1	40:DR:36:TYR:N	2.86	0.44
46:DY:42:VAL:HG23	46:DY:67:LEU:CD1	2.48	0.44
46:DY:12:THR:HG22	46:DY:75:ILE:HG23	1.99	0.44
11:AK:80:VAL:HG23	11:AK:80:VAL:O	2.17	0.44
19:AT:51:VAL:O	19:AT:58:VAL:HG22	2.18	0.44
4:BD:120:LEU:HB3	4:BD:126:ILE:CD1	2.48	0.44
6:BF:45:LEU:HD23	6:BF:46:ARG:N	2.33	0.44
14:BN:12:ARG:HB3	14:BN:14:PRO:HD3	2.00	0.44
6:BF:98:LEU:HA	18:BS:30:ASP:HA	2.00	0.44
20:BU:50:GLU:CG	20:BU:100:ILE:HB	2.48	0.44
58:C1:1066:A:C8	58:C1:1066:A:C3'	3.01	0.44
58:C1:2595:U:O4'	58:C1:2595:U:O2	2.36	0.44
41:CS:2:ASN:O	58:C1:2885:G:P	2.76	0.44
58:C1:624:G:N2	58:C1:702:G:C5	2.86	0.44
28:CB:35:LYS:HD2	28:CB:36:PRO:CA	2.47	0.44
42:CT:66:ASN:HD21	42:CT:70:ARG:NH2	2.15	0.44
58:D1:1187:A:C5	58:D1:1189:G:C5	3.05	0.44
58:D1:1336:C:C2	58:D1:1337:U:C5	3.06	0.44
58:D1:1431:C:H2'	58:D1:1432:C:C6	2.52	0.44
58:D1:1816:A:C2	58:D1:2617:C:H1'	2.53	0.44
58:D1:2097:U:H2'	58:D1:2097:U:O2	2.17	0.44
54:D7:28:ARG:HA	54:D7:32:ASN:HD22	1.82	0.44
29:DC:65:GLY:HA2	29:DC:70:ALA:CB	2.48	0.44
33:DI:31:LEU:HB2	33:DI:32:PRO:HD3	1.99	0.44
64:DV:25:C:H2'	64:DV:26:A:H8	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:110:ASN:O	3:AC:141:VAL:HG22	2.17	0.44
23:B2:19:U:N3	64:DV:37:A:C2	2.86	0.44
5:BE:36:ASP:O	5:BE:38:GLN:HG2	2.18	0.44
18:BS:44:LEU:O	18:BS:45:SER:C	2.56	0.44
58:C1:2088:G:O2'	58:C1:2090:G:H5''	2.16	0.44
58:C1:2120:U:O2	58:C1:2120:U:C2'	2.66	0.44
58:C1:2709:U:H2'	58:C1:2710:C:C6	2.53	0.44
42:CT:53:ARG:NH1	58:C1:559:C:O3'	2.50	0.44
58:C1:875:A:N7	58:C1:2258:A:O2'	2.49	0.44
25:C2:72:C:O2	25:C2:72:C:C2'	2.65	0.44
26:C4:67:C:H2'	26:C4:68:C:C6	2.53	0.44
30:CD:36:VAL:O	30:CD:40:GLN:HG3	2.16	0.44
35:CM:43:THR:O	35:CM:46:VAL:HG12	2.18	0.44
36:CN:49:ARG:HA	36:CN:53:LYS:NZ	2.32	0.44
42:CT:112:ARG:NH2	43:CU:46:VAL:HG11	2.32	0.44
58:D1:107:G:C6	58:D1:108:A:N7	2.86	0.44
58:D1:353:A:H2	58:D1:1254:A:H2'	1.80	0.44
58:D1:1766:A:O2'	58:D1:1767:U:C5'	2.66	0.44
31:DE:40:ASN:ND2	58:D1:2324:C:C4'	2.80	0.44
58:D1:303:C:C2	58:D1:384:G:N2	2.85	0.44
28:DB:24:ILE:HD13	28:DB:25:THR:N	2.32	0.44
31:DE:87:PRO:C	31:DE:88:ILE:HD12	2.37	0.44
31:DE:96:ARG:O	31:DE:99:MET:N	2.48	0.44
41:DS:28:VAL:O	41:DS:28:VAL:HG12	2.17	0.44
42:DT:91:ASP:O	42:DT:92:ARG:HB3	2.18	0.44
19:AT:36:ARG:HA	19:AT:71:LEU:HB2	2.00	0.44
16:BP:28:ARG:CG	16:BP:29:ASP:OD2	2.62	0.44
49:CH:3:LYS:HE2	58:C1:1409:G:N7	2.33	0.44
58:C1:2741:G:H2'	58:C1:2742:C:C6	2.53	0.44
58:C1:2763:G:N3	58:C1:2763:G:H2'	2.31	0.44
58:C1:2801:C:N3	58:C1:2902:G:O6	2.51	0.44
58:C1:296:C:C2'	58:C1:297:G:OP1	2.66	0.44
58:C1:619:U:H2'	58:C1:620:G:C8	2.53	0.44
26:C4:16:C:O2'	26:C4:62:C:OP1	2.35	0.44
26:C4:51:U:N3	26:C4:52:C:C4	2.86	0.44
26:C4:53:G:O2'	26:C4:54:G:P	2.76	0.44
30:CD:113:ALA:HB1	30:CD:186:ILE:HG21	1.99	0.44
30:CD:2:LYS:O	30:CD:3:GLU:HB3	2.17	0.44
32:CF:137:ASP:O	32:CF:138:LYS:HB2	2.18	0.44
50:CK:59:ARG:HD3	58:C1:75:C:OP1	2.17	0.44
35:CM:96:GLU:OE2	35:CM:96:GLU:N	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:CX:35:THR:HG21	58:C1:141:G:H4'	1.99	0.44
47:CZ:126:VAL:HA	47:CZ:163:LEU:HA	1.99	0.44
58:D1:1334:C:O2'	58:D1:1335:C:H5'	2.18	0.44
58:D1:1337:U:H2'	58:D1:1338:C:C6	2.53	0.44
58:D1:1376:A:HO2'	58:D1:1377:G:H8	1.66	0.44
61:D4:17:C:C2'	61:D4:18:U:C5	3.01	0.44
54:D7:46:HIS:CA	54:D7:47:THR:HG21	2.48	0.44
29:DC:68:ALA:O	29:DC:70:ALA:N	2.49	0.44
40:DR:97:ARG:NH2	40:DR:98:VAL:HA	2.33	0.44
2:AA:140:HIS:HA	2:AA:143:GLU:HG3	2.00	0.44
5:AE:142:LEU:O	5:AE:143:ARG:NE	2.48	0.44
12:AL:38:THR:CG2	12:AL:57:LYS:HB3	2.48	0.44
13:AM:20:THR:C	13:AM:22:ILE:H	2.22	0.44
13:AM:94:ARG:CZ	19:AT:81:ARG:HG2	2.48	0.44
11:BK:86:GLY:H	11:BK:112:THR:HG1	1.56	0.44
13:BM:13:LYS:HA	13:BM:44:ARG:HH11	1.82	0.44
58:C1:1094:C:C4	58:C1:1156:A:C2	3.06	0.44
58:C1:553:A:H62	58:C1:2062:U:H3	1.66	0.44
43:CU:78:LYS:NZ	58:C1:595:G:OP2	2.50	0.44
58:C1:906:U:C5	58:C1:962:A:N7	2.81	0.44
25:C3:48:C:C5	25:C3:59:U:H1'	2.52	0.44
33:CI:60:GLU:HG3	33:CI:61:ARG:HD3	2.00	0.44
37:CO:57:THR:HB	37:CO:59:LEU:N	2.33	0.44
41:CS:93:ARG:HD2	41:CS:93:ARG:HA	1.77	0.44
42:CT:114:LYS:HA	42:CT:117:GLN:HB2	2.00	0.44
63:DW:15:ARG:NH1	58:D1:1311:G:C5	2.86	0.44
58:D1:1527:U:H5'	58:D1:1528:G:OP2	2.18	0.44
58:D1:2228:A:H1'	58:D1:2230:G:C5	2.53	0.44
63:DW:18:ARG:NH1	58:D1:542:G:H4'	2.33	0.44
25:D3:36:A:H2'	25:D3:37:A:O5'	2.18	0.44
25:D3:2:C:O2'	25:D3:3:C:O5'	2.36	0.44
29:DC:164:ARG:NH2	58:D1:2785:C:OP1	2.49	0.44
50:DK:2:LYS:HB2	58:D1:95:C:H5''	2.00	0.44
36:DN:61:VAL:HG13	36:DN:61:VAL:O	2.18	0.44
37:DO:47:ASP:HB3	37:DO:48:PRO:CA	2.48	0.44
4:AD:155:LEU:O	4:AD:156:GLU:C	2.57	0.43
4:AD:88:VAL:O	4:AD:92:VAL:HG23	2.17	0.43
9:AI:77:ILE:O	9:AI:81:ILE:HG12	2.17	0.43
5:BE:72:GLN:O	5:BE:75:THR:HG22	2.18	0.43
19:BT:45:VAL:HA	19:BT:62:ILE:HG23	1.99	0.43
58:C1:1006:G:OP1	58:C1:1007:U:OP2	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:C1:139:A:C5'	58:C1:140:C:OP2	2.66	0.43
58:C1:2301:G:C2	58:C1:2354:C:O2	2.71	0.43
25:C2:47:U:O2	25:C2:47:U:O4'	2.35	0.43
35:CM:2:LYS:HB3	35:CM:4:TYR:CE2	2.53	0.43
37:CO:125:VAL:HG11	37:CO:138:LEU:HD21	1.99	0.43
37:CO:55:ARG:NH1	58:C1:879:U:O2	2.50	0.43
46:CY:76:CYS:HB3	46:CY:96:ILE:CD1	2.47	0.43
47:CZ:166:SER:HB2	47:CZ:167:PRO:C	2.38	0.43
58:D1:1087:G:H2'	58:D1:1087:G:N3	2.33	0.43
58:D1:1217:G:H5'	58:D1:1218:A:O5'	2.18	0.43
31:DE:71:THR:HG23	58:D1:2323:U:H4'	2.00	0.43
37:DO:35:HIS:HB3	58:D1:986:G:OP1	2.18	0.43
58:D1:99:G:C4'	58:D1:99:G:OP1	2.66	0.43
40:DR:42:ASP:O	40:DR:43:GLU:HB2	2.17	0.43
41:DS:90:GLN:NE2	41:DS:124:ASP:OD2	2.50	0.43
6:AF:97:PHE:HD2	18:AS:31:LEU:HD21	1.82	0.43
9:AI:9:ARG:CG	9:AI:14:VAL:HG13	2.48	0.43
9:AI:4:TYR:CE2	9:AI:88:TYR:CB	3.01	0.43
12:AL:48:PRO:C	12:AL:49:ASN:HD22	2.22	0.43
14:AN:27:CYS:C	14:AN:29:ARG:N	2.70	0.43
10:BJ:54:PHE:CE2	10:BJ:55:LYS:HE3	2.53	0.43
11:BK:48:ILE:HD13	11:BK:48:ILE:N	2.33	0.43
16:BP:28:ARG:NH1	16:BP:29:ASP:OD1	2.50	0.43
58:C1:68:G:C2'	58:C1:110:G:O2'	2.66	0.43
58:C1:1547:C:H5''	58:C1:1547:C:H6	1.82	0.43
58:C1:2319:G:O2'	58:C1:2320:A:OP1	2.28	0.43
58:C1:275:C:H2'	58:C1:276:G:H5'	2.01	0.43
58:C1:820:A:HO2'	58:C1:821:G:P	2.41	0.43
58:C1:875:A:N7	58:C1:2259:C:H5'	2.33	0.43
37:CO:63:PRO:HB3	56:C9:13:ARG:HB3	2.00	0.43
37:CO:10:PRO:O	37:CO:11:GLY:C	2.56	0.43
41:CS:32:TYR:HB3	41:CS:81:PRO:HB2	2.00	0.43
43:CU:2:PHE:O	43:CU:3:ALA:CB	2.66	0.43
46:CY:18:GLY:HA2	58:C1:333:A:OP1	2.19	0.43
57:D0:10:ILE:HG22	57:D0:10:ILE:O	2.18	0.43
58:D1:1346:A:H4'	58:D1:1347:A:OP1	2.18	0.43
58:D1:2326:G:H2'	58:D1:2327:C:C6	2.52	0.43
54:D7:37:ARG:HG3	58:D1:2355:U:O2'	2.17	0.43
52:D5:37:PRO:O	52:D5:55:PRO:HG3	2.18	0.43
28:DB:31:LYS:O	28:DB:32:SER:C	2.55	0.43
28:DB:35:LYS:HD2	28:DB:36:PRO:HA	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:DE:60:LEU:O	31:DE:64:THR:HG22	2.19	0.43
39:DQ:2:ARG:HD2	58:D1:2735:C:H5'	1.99	0.43
43:DU:34:GLU:O	43:DU:36:PRO:CD	2.66	0.43
46:DY:27:VAL:C	46:DY:29:GLU:OE1	2.55	0.43
2:AA:138:LEU:O	2:AA:141:GLU:HB3	2.18	0.43
14:AN:22:THR:OG1	14:AN:33:VAL:HG21	2.19	0.43
2:BA:69:LEU:HD12	2:BA:70:PHE:N	2.33	0.43
4:BD:28:SER:HB3	4:BD:29:PRO:CD	2.48	0.43
4:BD:73:ARG:HD2	4:BD:73:ARG:HA	1.92	0.43
13:BM:35:GLU:HG3	13:BM:36:LYS:HD2	1.99	0.43
55:C8:9:ARG:NH2	58:C1:1355:G:OP2	2.50	0.43
58:C1:2671:A:C5'	58:C1:2672:G:H21	2.32	0.43
58:C1:874:U:H3'	58:C1:874:U:O2	2.17	0.43
26:C4:50:G:C5	26:C4:51:U:C6	3.07	0.43
26:C4:60:A:H5'	26:C4:61:U:C5	2.53	0.43
40:CR:89:ARG:O	40:CR:92:TYR:HB3	2.18	0.43
30:DD:95:ARG:NH2	58:D1:1292:A:OP1	2.51	0.43
58:D1:1849:A:H4'	58:D1:1850:U:O5'	2.17	0.43
29:DC:137:HIS:HB3	29:DC:138:PRO:CD	2.47	0.43
29:DC:92:THR:O	29:DC:95:ILE:HG12	2.18	0.43
30:DD:53:THR:HG22	30:DD:56:GLU:CD	2.38	0.43
31:DE:111:LEU:O	31:DE:114:ILE:HB	2.18	0.43
33:DI:142:VAL:HG12	33:DI:143:SER:H	1.83	0.43
33:DI:6:LEU:O	33:DI:15:VAL:HG12	2.18	0.43
30:DD:188:ARG:HA	37:DO:7:ARG:HD3	2.01	0.43
38:DP:133:ARG:O	38:DP:134:ARG:HG2	2.19	0.43
42:DT:88:ILE:O	42:DT:88:ILE:HG13	2.16	0.43
42:DT:65:ILE:HD11	42:DT:96:ALA:HB3	1.99	0.43
43:DU:38:LEU:O	43:DU:39:LEU:HD13	2.18	0.43
18:AS:30:ASP:C	18:AS:32:ARG:H	2.22	0.43
4:BD:26:CYS:HA	4:BD:31:CYS:CB	2.44	0.43
6:BF:72:VAL:HG13	6:BF:73:ASN:N	2.34	0.43
11:BK:98:LEU:O	11:BK:101:SER:OG	2.23	0.43
58:C1:1064:U:H3	58:C1:1187:A:H62	1.65	0.43
58:C1:1254:A:H8	58:C1:1254:A:H5'	1.84	0.43
58:C1:164:G:O2'	58:C1:165:G:H5'	2.18	0.43
58:C1:1734:U:H1'	58:C1:1747:A:C6	2.53	0.43
49:CH:35:THR:HG21	58:C1:2101:G:OP1	2.18	0.43
58:C1:2810:A:H2'	58:C1:2810:A:N3	2.34	0.43
58:C1:666:G:C8	58:C1:666:G:H3'	2.53	0.43
25:C2:16:U:H3'	25:C2:17:C:H5'	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:C7:11:LEU:HD21	54:C7:51:GLU:HB2	2.00	0.43
27:CA:74:VAL:HB	27:CA:91:ALA:CB	2.49	0.43
44:CW:36:LEU:HD12	44:CW:48:ALA:HA	2.00	0.43
46:CY:2:ARG:NH2	58:C1:103:C:H1'	2.33	0.43
58:D1:1574:A:H3'	58:D1:1575:G:H5''	1.99	0.43
58:D1:2672:G:C2'	58:D1:2673:A:C2	2.86	0.43
58:D1:2870:G:O2'	58:D1:2871:G:H5'	2.19	0.43
56:D9:2:PRO:HB3	58:D1:613:C:H1'	2.00	0.43
62:DA:36:LYS:CE	62:DA:36:LYS:HA	2.47	0.43
32:DF:54:ARG:HG2	32:DF:65:HIS:CD2	2.53	0.43
41:DS:31:SER:OG	41:DS:32:TYR:N	2.49	0.43
1:A2:16:A:C2'	1:A2:17:U:C5'	2.92	0.43
12:AL:30:ALA:HB1	12:AL:31:PRO:CD	2.49	0.43
13:AM:116:THR:O	13:AM:116:THR:HG22	2.18	0.43
13:AM:90:LEU:C	13:AM:92:HIS:N	2.72	0.43
18:AS:44:LEU:O	18:AS:45:SER:C	2.57	0.43
10:BJ:5:ARG:HG2	10:BJ:71:LEU:HD11	2.01	0.43
15:BO:78:TYR:O	15:BO:82:ILE:HG22	2.17	0.43
58:C1:2095:U:H2'	58:C1:2096:U:C6	2.53	0.43
58:C1:676:C:C5	58:C1:676:C:OP2	2.71	0.43
31:CE:129:GLY:O	31:CE:130:ASN:CB	2.66	0.43
33:CI:61:ARG:HA	33:CI:64:GLU:HB2	2.00	0.43
41:CS:1:MET:O	41:CS:3:ARG:N	2.51	0.43
42:CT:66:ASN:O	42:CT:70:ARG:HB2	2.18	0.43
58:D1:2529:A:H5'	58:D1:2529:A:H8	1.82	0.43
56:D9:30:ARG:O	56:D9:31:HIS:HB3	2.19	0.43
28:DB:271:ILE:O	28:DB:272:ALA:CB	2.66	0.43
37:DO:23:PRO:HD2	37:DO:33:ARG:HH21	1.84	0.43
37:DO:62:LEU:HB2	37:DO:63:PRO:CD	2.49	0.43
38:DP:133:ARG:HG2	38:DP:134:ARG:N	2.34	0.43
41:DS:28:VAL:HG22	41:DS:46:GLU:HG3	2.00	0.43
64:DV:55:C:H6	64:DV:55:C:O5'	2.00	0.43
38:DP:138:ASP:OD1	47:DZ:122:ARG:NH1	2.52	0.43
8:AH:17:THR:HB	8:AH:78:GLN:OE1	2.19	0.43
13:AM:81:LEU:O	13:AM:89:GLY:HA3	2.17	0.43
4:BD:166:LYS:HG3	4:BD:178:VAL:HG11	2.00	0.43
7:BG:116:ALA:O	7:BG:117:ALA:C	2.57	0.43
8:BH:4:ASP:CG	8:BH:85:ARG:HH21	2.21	0.43
46:CY:46:LYS:NZ	58:C1:505:A:OP2	2.49	0.43
58:C1:566:C:H2'	58:C1:567:C:OP1	2.18	0.43
58:C1:82:A:N1	58:C1:96:G:O2'	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:CB:186:HIS:HD2	28:CB:188:GLU:H	1.65	0.43
28:CB:28:GLU:HB2	28:CB:29:PRO:HD3	2.00	0.43
29:CC:59:VAL:HG13	29:CC:63:LEU:HG	2.01	0.43
50:CK:47:ASN:O	50:CK:48:HIS:C	2.57	0.43
43:CU:19:LYS:CG	43:CU:20:LEU:O	2.64	0.43
45:CX:84:ALA:HB1	45:CX:85:PRO:HD2	2.01	0.43
58:D1:1887:G:O2'	58:D1:1906:A:N6	2.46	0.43
55:D8:5:TRP:CH2	58:D1:732:G:N7	2.87	0.43
58:D1:849:U:O2'	58:D1:850:A:H5'	2.18	0.43
25:D3:66:U:H2'	25:D3:67:C:C5	2.53	0.43
61:D4:32:G:C5	61:D4:33:C:C5	3.07	0.43
56:D9:51:ALA:CA	56:D9:53:PRO:HD2	2.48	0.43
56:D9:6:THR:HG22	56:D9:63:PRO:HD3	2.01	0.43
29:DC:19:ARG:HA	36:DN:73:ASP:HA	2.00	0.43
31:DE:41:GLN:HB3	31:DE:43:LEU:HD13	2.01	0.43
32:DF:156:ALA:C	32:DF:158:HIS:H	2.20	0.43
32:DF:55:PRO:O	32:DF:56:SER:C	2.57	0.43
38:DP:27:VAL:HG23	38:DP:137:TYR:CD1	2.53	0.43
4:AD:148:VAL:HG11	4:AD:158:ILE:HG21	2.00	0.43
7:AG:26:PHE:O	7:AG:30:ILE:HG12	2.18	0.43
11:AK:59:TYR:O	11:AK:62:GLN:HB3	2.18	0.43
2:BA:60:ASP:HB3	2:BA:64:ARG:NH2	2.34	0.43
17:BR:59:ILE:CG2	17:BR:71:PHE:HB3	2.48	0.43
58:C1:1578:C:O2'	58:C1:1579:G:N2	2.52	0.43
31:CE:126:ASP:HB3	58:C1:2314:G:H5''	2.00	0.43
56:C9:29:LYS:O	56:C9:29:LYS:HG3	2.19	0.43
35:CM:1:MET:HG2	35:CM:2:LYS:N	2.34	0.43
37:CO:64:LYS:C	37:CO:66:GLY:N	2.72	0.43
41:CS:129:ARG:HD2	41:CS:129:ARG:C	2.38	0.43
41:CS:82:LEU:O	41:CS:83:ILE:O	2.37	0.43
36:DN:31:LYS:CE	58:D1:2017:C:OP1	2.67	0.43
58:D1:2277:A:C2	58:D1:2283:U:C5	3.06	0.43
29:DC:166:THR:OG1	58:D1:2785:C:OP1	2.35	0.43
58:D1:2842:G:H8	58:D1:2842:G:OP1	2.02	0.43
58:D1:2873:G:O2'	58:D1:2874:U:H5'	2.19	0.43
55:D8:38:GLY:O	55:D8:39:ARG:C	2.55	0.43
62:DA:55:ASP:HB2	62:DA:56:GLN:HE21	1.83	0.43
38:DP:76:LYS:HB3	38:DP:91:GLU:CG	2.49	0.43
39:DQ:101:ALA:O	39:DQ:102:GLU:HB2	2.19	0.43
41:DS:29:ARG:HG2	41:DS:85:LYS:CA	2.49	0.43
41:DS:76:PHE:HA	41:DS:77:PRO:HD3	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:DU:28:GLU:CB	43:DU:29:PRO:HD2	2.49	0.43
2:AA:118:LEU:CB	2:AA:142:LEU:HD12	2.48	0.43
2:AA:83:MET:O	2:AA:85:ALA:N	2.52	0.43
13:AM:105:THR:O	13:AM:106:ASN:O	2.37	0.43
19:AT:39:THR:HG22	19:AT:40:ILE:O	2.19	0.43
24:BC:11:ARG:O	24:BC:13:GLY:N	2.51	0.43
58:C1:1095:A:C2	58:C1:2763:G:C4	3.07	0.43
58:C1:865:A:C4	58:C1:1233:A:C2	3.06	0.43
58:C1:1703:C:H2'	58:C1:1704:C:H6	1.84	0.43
58:C1:1920:G:N2	58:C1:1923:C:N4	2.58	0.43
58:C1:2155:A:C2	58:C1:2180:G:HI'	2.53	0.43
54:C7:20:ASN:O	54:C7:21:TYR:CD1	2.72	0.43
56:C9:33:ASN:ND2	56:C9:33:ASN:N	2.65	0.43
33:CI:123:LEU:HD23	33:CI:124:GLY:H	1.83	0.43
33:CI:6:LEU:C	33:CI:15:VAL:HG12	2.39	0.43
39:CQ:9:LYS:HD3	58:C1:1698:A:OP1	2.19	0.43
41:CS:93:ARG:HH21	41:CS:95:ARG:HD3	1.83	0.43
58:D1:1393:G:H2'	58:D1:1394:A:C5'	2.48	0.43
58:D1:2302:U:H5''	58:D1:2391:C:O2'	2.19	0.43
46:DY:2:ARG:NH2	58:D1:317:A:O2'	2.52	0.43
58:D1:510:C:O2'	58:D1:511:C:H5'	2.19	0.43
61:D4:14:A:N7	61:D4:23:G:N1	2.66	0.43
62:DA:77:ILE:HG13	62:DA:100:ILE:HD11	2.01	0.43
28:DB:28:GLU:HB2	28:DB:29:PRO:CD	2.48	0.43
30:DD:65:TRP:O	30:DD:67:GLN:N	2.52	0.43
37:DO:105:LEU:O	37:DO:106:LEU:HB3	2.19	0.43
37:DO:6:LEU:CD1	37:DO:8:PRO:O	2.67	0.43
63:DW:10:VAL:O	63:DW:11:ARG:CB	2.66	0.43
46:DY:7:VAL:HB	46:DY:8:LYS:HE3	2.00	0.43
2:AA:185:ILE:HG22	2:AA:199:TYR:HD1	1.82	0.43
4:BD:129:ASN:HD22	4:BD:129:ASN:N	2.16	0.43
6:BF:67:MET:HE1	6:BF:75:LEU:HD22	2.01	0.43
19:BT:33:THR:OG1	19:BT:34:TRP:N	2.52	0.43
20:BU:75:ASN:HA	20:BU:78:ALA:HB3	2.00	0.43
58:C1:1042:G:O2'	58:C1:1043:C:H5'	2.19	0.43
58:C1:2054:A:H4'	58:C1:2055:U:OP1	2.19	0.43
58:C1:934:C:H2'	58:C1:935:C:H5'	2.00	0.43
32:CF:98:LEU:HD12	32:CF:102:ALA:O	2.19	0.43
33:CI:40:THR:OG1	33:CI:43:ASN:ND2	2.52	0.43
38:CP:1:MET:O	38:CP:2:LEU:CB	2.62	0.43
46:CY:26:LYS:O	46:CY:27:VAL:C	2.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:D1:1066:A:C3'	58:D1:1066:A:C8	3.02	0.43
32:DF:84:SER:O	32:DF:133:VAL:O	2.36	0.43
49:DH:93:GLU:O	49:DH:95:LEU:N	2.51	0.43
33:DI:27:ARG:HD3	49:DH:71:TYR:CE1	2.54	0.43
50:DK:42:GLY:O	50:DK:44:LEU:N	2.52	0.43
50:DK:28:LYS:HB3	50:DK:53:LEU:HD21	2.01	0.43
41:DS:28:VAL:O	41:DS:29:ARG:CB	2.65	0.43
41:DS:29:ARG:HG2	41:DS:85:LYS:HA	1.99	0.43
43:DU:21:ARG:O	43:DU:22:VAL:HG13	2.19	0.43
43:DU:46:VAL:CG1	43:DU:47:VAL:N	2.75	0.43
47:DZ:103:ARG:O	47:DZ:139:VAL:HG22	2.19	0.43
1:A2:20:U:O2'	1:A2:21:C:H5'	2.19	0.43
8:AH:103:VAL:HG21	8:AH:110:ALA:HB2	2.01	0.43
8:AH:11:THR:HG22	8:AH:15:ASN:ND2	2.33	0.43
9:AI:96:LEU:HD12	9:AI:101:PHE:HB2	2.00	0.43
14:AN:24:CYS:HB3	14:AN:27:CYS:O	2.19	0.43
14:AN:24:CYS:SG	14:AN:40:CYS:HB3	2.54	0.43
6:AF:62:TRP:CD1	18:AS:35:ARG:CZ	3.01	0.43
6:BF:41:GLU:HB3	6:BF:43:LEU:CD1	2.49	0.43
7:BG:111:ARG:NH1	7:BG:113:GLU:OE2	2.52	0.43
56:C9:6:THR:CG2	58:C1:231:U:OP1	2.67	0.43
58:C1:2413:C:C2'	58:C1:2414:C:H5'	2.48	0.43
56:C9:50:LEU:O	56:C9:51:ALA:HB3	2.19	0.43
27:CA:21:THR:O	27:CA:21:THR:OG1	2.34	0.43
29:CC:153:GLY:O	29:CC:154:LYS:C	2.57	0.43
35:CM:126:PRO:O	35:CM:127:ASP:HB2	2.19	0.43
36:CN:26:LYS:O	36:CN:27:GLY:O	2.37	0.43
39:CQ:28:LEU:HD22	39:CQ:116:LEU:HG	2.01	0.43
45:CX:24:GLY:O	45:CX:82:GLN:HA	2.18	0.43
46:CY:81:LYS:HD3	46:CY:97:ARG:O	2.19	0.43
58:D1:1844:G:C6	58:D1:1845:A:C6	3.07	0.43
58:D1:1912:G:C6	58:D1:1913:C:C4	3.06	0.43
58:D1:2637:C:H2'	58:D1:2638:G:O4'	2.19	0.43
60:D2:46:G:O2'	60:D2:47:U:O5'	2.33	0.43
49:DH:3:LYS:HD3	58:D1:1409:G:OP2	2.19	0.43
36:DN:105:GLU:O	36:DN:108:GLU:HG2	2.19	0.43
37:DO:48:PRO:O	37:DO:51:PHE:N	2.52	0.43
41:DS:12:SER:O	41:DS:13:ARG:NH2	2.52	0.43
46:DY:81:LYS:HE2	46:DY:97:ARG:HE	1.83	0.43
5:AE:102:ALA:HB2	5:AE:120:THR:OG1	2.18	0.42
9:AI:125:TYR:HD2	9:AI:126:SER:N	2.16	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B2:19:U:H4'	23:B2:19:U:OP2	2.18	0.42
24:BC:167:TRP:O	24:BC:168:ALA:HB3	2.19	0.42
16:BP:53:VAL:HG12	16:BP:79:VAL:CG2	2.40	0.42
58:C1:1920:G:O2'	58:C1:1921:A:P	2.77	0.42
58:C1:2578:G:H2'	58:C1:2579:C:C6	2.54	0.42
58:C1:2715:C:H2'	58:C1:2716:A:O4'	2.19	0.42
58:C1:2842:G:H3'	58:C1:2843:G:C5'	2.48	0.42
58:C1:921:G:N2	58:C1:948:C:C2	2.87	0.42
28:CB:242:ARG:CD	28:CB:242:ARG:H	2.32	0.42
37:CO:18:ARG:NH2	58:C1:1292:A:OP2	2.52	0.42
42:CT:92:ARG:CB	43:CU:11:GLN:NE2	2.82	0.42
43:CU:21:ARG:O	43:CU:22:VAL:HG13	2.19	0.42
28:DB:62:TYR:CZ	58:D1:1846:G:N7	2.87	0.42
58:D1:2313:G:C6	58:D1:2314:G:C5	3.06	0.42
58:D1:2363:A:H2'	58:D1:2364:G:O4'	2.19	0.42
30:DD:90:PHE:HB3	58:D1:610:U:H1'	2.00	0.42
58:D1:610:U:H2'	58:D1:611:C:C6	2.54	0.42
58:D1:754:C:H5'	58:D1:755:U:OP2	2.19	0.42
61:D4:12:G:C5	61:D4:13:C:C5	3.07	0.42
28:DB:147:LEU:HD12	28:DB:155:LEU:HD21	2.00	0.42
29:DC:185:LYS:O	29:DC:186:GLY:O	2.37	0.42
30:DD:74:ARG:NH2	58:D1:2456:G:OP1	2.52	0.42
37:DO:66:GLY:O	37:DO:67:MET:HB3	2.18	0.42
63:DW:84:ARG:O	63:DW:95:ILE:HA	2.18	0.42
4:AD:8:VAL:O	4:AD:10:ARG:N	2.48	0.42
11:AK:44:SER:OG	11:AK:47:VAL:HG23	2.19	0.42
12:AL:50:SER:O	12:AL:51:ALA:CB	2.67	0.42
19:AT:29:ARG:O	19:AT:31:ILE:HG22	2.18	0.42
24:BC:47:LEU:HD23	24:BC:52:LEU:HD13	2.01	0.42
4:BD:110:PHE:CE2	4:BD:148:VAL:HG23	2.54	0.42
10:BJ:7:LYS:HE3	10:BJ:99:LYS:HE3	2.01	0.42
58:C1:1539:A:C2'	58:C1:1540:A:H5''	2.44	0.42
58:C1:1877:A:H2'	58:C1:1877:A:N3	2.34	0.42
58:C1:2667:U:H3	58:C1:2676:A:H2	1.65	0.42
44:CW:60:ASN:ND2	58:C1:511:C:H4'	2.33	0.42
58:C1:932:C:C2	58:C1:935:C:N4	2.87	0.42
26:C4:10:G:H5'	26:C4:10:G:H8	1.84	0.42
35:CM:57:ALA:O	35:CM:58:ASP:C	2.57	0.42
40:CR:16:ASN:O	40:CR:19:LYS:N	2.45	0.42
43:CU:46:VAL:HG13	43:CU:47:VAL:N	2.34	0.42
45:CX:80:ILE:O	45:CX:80:ILE:HD13	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:DP:14:ARG:NH2	58:D1:1000:G:OP2	2.52	0.42
58:D1:1557:G:O2'	58:D1:1558:C:H5'	2.20	0.42
58:D1:1772:C:C2'	58:D1:1773:C:H5'	2.48	0.42
58:D1:1935:C:H2'	58:D1:1936:U:O4'	2.19	0.42
58:D1:2272:C:C2	58:D1:2291:G:C2	3.07	0.42
58:D1:2400:G:H5''	58:D1:2401:U:H5'	2.00	0.42
58:D1:69:A:H3'	58:D1:69:A:OP2	2.20	0.42
32:DF:89:ILE:HD11	32:DF:94:TYR:O	2.19	0.42
35:DM:57:ALA:C	35:DM:58:ASP:O	2.56	0.42
37:DO:33:ARG:HD3	58:D1:609:C:C4	2.54	0.42
37:DO:71:VAL:HG12	37:DO:72:PRO:HD3	2.02	0.42
38:DP:16:ARG:O	38:DP:17:LEU:HD23	2.19	0.42
39:DQ:107:ASP:C	39:DQ:107:ASP:OD2	2.58	0.42
40:DR:98:VAL:HG12	40:DR:100:ALA:HB2	2.00	0.42
43:DU:35:LEU:HB2	43:DU:57:VAL:CG1	2.49	0.42
43:DU:34:GLU:HG2	43:DU:56:SER:HB2	2.00	0.42
64:DV:43:G:H3'	64:DV:44:A:OP2	2.18	0.42
4:AD:127:THR:HG23	4:AD:147:ALA:HB3	2.00	0.42
20:AU:26:ASN:HB2	20:AU:71:THR:HG23	2.01	0.42
24:BC:70:VAL:HG12	24:BC:71:ALA:N	2.34	0.42
17:BR:58:GLU:O	17:BR:59:ILE:HD13	2.20	0.42
19:BT:27:GLU:HB3	19:BT:28:LYS:H	1.74	0.42
58:C1:1156:A:O2'	58:C1:1157:G:H4'	2.19	0.42
58:C1:1232:U:O2'	58:C1:1233:A:H5'	2.19	0.42
58:C1:1770:G:N7	58:C1:1771:C:C4	2.87	0.42
58:C1:1902:C:H5'	58:C1:1903:C:OP2	2.20	0.42
58:C1:275:C:O2'	58:C1:276:G:H5'	2.18	0.42
58:C1:2782:G:C5'	58:C1:2783:C:OP2	2.65	0.42
28:CB:213:ARG:HA	28:CB:213:ARG:HD2	1.84	0.42
28:CB:221:VAL:HG22	28:CB:226:MET:CE	2.49	0.42
41:CS:29:ARG:HG3	41:CS:30:VAL:HG13	2.01	0.42
41:CS:28:VAL:HG22	41:CS:46:GLU:HA	1.99	0.42
46:CY:19:LYS:HB3	46:CY:20:TYR:CD1	2.53	0.42
58:D1:2328:C:C2'	58:D1:2329:G:H5'	2.50	0.42
58:D1:2420:G:H2'	58:D1:2421:G:O4'	2.18	0.42
58:D1:319:C:O2'	58:D1:320:C:H5'	2.20	0.42
58:D1:623:C:O2'	58:D1:627:C:H5''	2.20	0.42
47:DZ:113:ALA:HB1	58:D1:941:A:C2	2.54	0.42
25:D3:16:U:H3'	25:D3:17:C:C5'	2.50	0.42
54:D7:46:HIS:CB	54:D7:47:THR:CG2	2.97	0.42
28:DB:270:ILE:C	28:DB:271:ILE:HG13	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:DS:106:SER:HA	41:DS:110:ILE:HG12	2.00	0.42
43:DU:18:LEU:O	43:DU:19:LYS:O	2.38	0.42
47:DZ:79:ARG:O	47:DZ:80:ARG:CB	2.65	0.42
2:AA:102:LEU:N	2:AA:102:LEU:HD12	2.35	0.42
5:AE:68:GLU:CG	5:AE:68:GLU:O	2.65	0.42
8:AH:86:ILE:HG13	8:AH:133:LEU:HD22	2.01	0.42
13:AM:20:THR:O	13:AM:22:ILE:N	2.53	0.42
13:AM:65:LYS:HA	13:AM:66:LEU:HG	2.01	0.42
19:AT:39:THR:HG22	19:AT:40:ILE:N	2.34	0.42
23:B2:19:U:C4'	23:B2:19:U:OP2	2.66	0.42
16:BP:23:ASP:OD1	16:BP:24:ALA:N	2.53	0.42
58:C1:2623:C:C4	58:C1:2624:U:H5	2.37	0.42
58:C1:267:G:C2'	58:C1:268:G:OP2	2.67	0.42
28:CB:26:LYS:O	28:CB:27:THR:HB	2.19	0.42
36:CN:105:GLU:HA	36:CN:108:GLU:OE1	2.19	0.42
39:CQ:9:LYS:HG2	39:CQ:43:GLU:OE2	2.20	0.42
41:CS:88:ILE:HG22	41:CS:89:VAL:CG2	2.43	0.42
47:CZ:145:GLU:HG3	47:CZ:146:ILE:CD1	2.49	0.42
47:CZ:8:TYR:CD1	47:CZ:8:TYR:N	2.87	0.42
58:D1:2201:U:H2'	58:D1:2201:U:O2	2.19	0.42
58:D1:2595:U:O2	58:D1:2595:U:O4'	2.36	0.42
58:D1:634:C:H2'	58:D1:635:G:H5'	1.99	0.42
29:DC:134:ILE:CD1	29:DC:134:ILE:C	2.88	0.42
29:DC:14:ILE:HG12	29:DC:21:VAL:HG22	2.02	0.42
32:DF:158:HIS:CE1	32:DF:170:ARG:HA	2.54	0.42
49:DH:3:LYS:CD	58:D1:1409:G:OP2	2.67	0.42
39:DQ:9:LYS:C	39:DQ:10:LEU:HG	2.39	0.42
41:DS:50:ILE:HA	41:DS:99:LEU:CD1	2.50	0.42
42:DT:85:LYS:HE2	42:DT:117:GLN:HE21	1.85	0.42
42:DT:97:ASP:C	42:DT:97:ASP:OD1	2.56	0.42
42:DT:98:LEU:O	42:DT:101:ARG:O	2.37	0.42
43:DU:91:TYR:CD1	43:DU:91:TYR:C	2.93	0.42
5:AE:11:ILE:HD12	5:AE:31:LEU:CD1	2.50	0.42
10:AJ:90:LEU:N	10:AJ:91:PRO:CD	2.82	0.42
12:AL:86:ARG:HB2	12:AL:101:VAL:HG23	2.01	0.42
11:BK:37:GLY:O	11:BK:39:PRO:HD3	2.18	0.42
13:BM:108:ARG:HD2	13:BM:108:ARG:N	2.34	0.42
58:C1:209:A:H4'	58:C1:210:A:O5'	2.20	0.42
58:C1:26:G:C4	58:C1:536:G:N2	2.87	0.42
58:C1:646:G:C2'	58:C1:647:G:H5'	2.50	0.42
58:C1:919:G:N2	58:C1:950:U:C2	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:CE:143:GLU:OE2	52:C5:52:SER:HB2	2.19	0.42
54:C7:15:GLU:O	54:C7:16:CYS:C	2.58	0.42
55:C8:10:ARG:NH2	58:C1:1423:A:OP1	2.52	0.42
55:C8:40:TRP:N	55:C8:40:TRP:CD1	2.87	0.42
28:CB:220:HIS:C	28:CB:220:HIS:CD2	2.92	0.42
28:CB:224:ALA:O	28:CB:225:ALA:CB	2.67	0.42
28:CB:43:ARG:HD2	28:CB:44:ASN:OD1	2.19	0.42
30:CD:34:TRP:HB2	37:CO:10:PRO:O	2.19	0.42
30:CD:83:PHE:CE2	58:C1:1302:C:H4'	2.54	0.42
36:CN:2:ILE:HD11	36:CN:82:ASN:ND2	2.35	0.42
37:CO:47:ASP:HB2	37:CO:51:PHE:HD2	1.84	0.42
39:CQ:49:ASP:O	39:CQ:52:ILE:HB	2.19	0.42
40:CR:61:ASN:OD1	40:CR:62:LYS:N	2.52	0.42
42:CT:66:ASN:C	42:CT:66:ASN:HD22	2.22	0.42
42:CT:112:ARG:CZ	43:CU:46:VAL:HG11	2.50	0.42
46:CY:8:LYS:HB2	46:CY:28:LYS:HZ3	1.84	0.42
45:DX:35:THR:CG2	58:D1:1643:C:O3'	2.66	0.42
29:DC:120:TRP:O	29:DC:121:ASN:HB2	2.19	0.42
32:DF:149:ARG:HA	32:DF:162:ILE:CG1	2.49	0.42
35:DM:55:VAL:HG13	35:DM:56:ASN:HB2	2.00	0.42
40:DR:24:LEU:HB3	40:DR:85:VAL:HG12	2.02	0.42
43:DU:15:GLU:CB	43:DU:16:PRO:HD2	2.49	0.42
43:DU:68:LYS:HD2	43:DU:68:LYS:HA	1.82	0.42
46:DY:7:VAL:HG21	46:DY:8:LYS:NZ	2.34	0.42
1:A2:20:U:H2'	1:A2:21:C:O5'	2.20	0.42
2:BA:178:ARG:HA	2:BA:178:ARG:HD3	1.87	0.42
7:BG:140:ASP:HA	7:BG:143:ARG:NH1	2.35	0.42
12:BL:58:VAL:N	12:BL:66:VAL:O	2.47	0.42
20:BU:89:ARG:NH2	20:BU:104:LEU:HD21	2.34	0.42
21:BW:5:ASP:C	21:BW:7:ARG:H	2.23	0.42
58:C1:1311:G:O2'	58:C1:2033:G:O6	2.30	0.42
25:C3:30:G:C2	25:C3:31:A:C5	3.08	0.42
26:C4:20:G:C2	26:C4:58:A:N3	2.87	0.42
33:CI:90:GLY:O	33:CI:121:LYS:HD2	2.19	0.42
41:CS:31:SER:OG	41:CS:32:TYR:N	2.52	0.42
43:CU:25:LEU:H	43:CU:92:THR:HG21	1.84	0.42
46:CY:28:LYS:O	46:CY:29:GLU:C	2.58	0.42
58:D1:2192:A:O2'	58:D1:2193:U:C6	2.72	0.42
58:D1:2517:U:C2'	58:D1:2517:U:O2	2.66	0.42
25:D3:9:A:C2	25:D3:45:U:C4	3.07	0.42
61:D4:50:G:N2	61:D4:67:C:C2	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:DE:2:PRO:HD2	52:D5:51:TYR:CE2	2.54	0.42
62:DA:169:UNK:O	62:DA:171:UNK:N	2.53	0.42
28:DB:228:PRO:HD3	28:DB:235:GLY:CA	2.50	0.42
31:DE:166:ASP:OD1	31:DE:166:ASP:N	2.52	0.42
32:DF:88:LEU:N	32:DF:88:LEU:HD22	2.35	0.42
20:AU:10:LEU:O	20:AU:13:LEU:HD12	2.19	0.42
24:BC:189:ALA:HB3	24:BC:196:LEU:HB2	2.02	0.42
5:BE:51:VAL:O	5:BE:55:VAL:HG23	2.20	0.42
58:C1:1359:C:C2	58:C1:1384:G:N2	2.88	0.42
58:C1:1684:C:H4'	58:C1:2721:C:O2	2.19	0.42
58:C1:1684:C:H2'	58:C1:1685:U:O4'	2.20	0.42
58:C1:2048:G:H2'	58:C1:2049:U:O4'	2.19	0.42
58:C1:2125:G:O4'	58:C1:2125:G:N3	2.53	0.42
58:C1:2479:G:H22	58:C1:2492:G:C2'	2.31	0.42
58:C1:894:G:H2'	58:C1:895:A:C8	2.54	0.42
56:C9:28:GLY:O	56:C9:32:LEU:HG	2.20	0.42
27:CA:56:GLN:NE2	27:CA:168:UNK:CB	2.83	0.42
30:CD:126:VAL:HG23	30:CD:127:GLU:N	2.34	0.42
30:CD:51:THR:HB	30:CD:88:VAL:HG11	2.02	0.42
33:CI:1:MET:HG3	33:CI:23:PRO:HA	2.01	0.42
37:CO:40:SER:O	37:CO:41:ARG:NE	2.52	0.42
38:CP:52:VAL:O	38:CP:56:ARG:HG2	2.20	0.42
42:CT:112:ARG:NH2	43:CU:46:VAL:CG1	2.83	0.42
58:D1:2155:A:N6	58:D1:2178:G:O2'	2.43	0.42
58:D1:2306:C:C2'	58:D1:2307:U:H5'	2.50	0.42
58:D1:2475:C:O2'	58:D1:2476:C:O4'	2.37	0.42
58:D1:86:G:N3	58:D1:86:G:H2'	2.34	0.42
58:D1:906:U:H5	58:D1:962:A:N7	2.18	0.42
54:D7:15:GLU:OE2	54:D7:41:PRO:HG3	2.19	0.42
50:DK:61:LEU:HA	50:DK:61:LEU:HD12	1.89	0.42
40:DR:74:ALA:HB1	40:DR:103:GLU:CB	2.45	0.42
43:DU:46:VAL:HG13	43:DU:47:VAL:H	1.84	0.42
5:AE:7:GLU:HG2	5:AE:112:LEU:HD22	2.01	0.42
8:AH:51:VAL:HG11	8:AH:60:ARG:CD	2.49	0.42
11:AK:108:ILE:O	18:AS:87:ARG:N	2.49	0.42
11:AK:22:HIS:HB3	11:AK:29:ILE:HG23	2.02	0.42
17:AR:4:LYS:HG3	17:AR:5:VAL:N	2.34	0.42
19:AT:15:LEU:O	19:AT:19:VAL:HG23	2.19	0.42
8:BH:120:THR:H	8:BH:123:GLU:HB2	1.85	0.42
21:BW:12:LYS:HB3	21:BW:22:ARG:HD2	2.01	0.42
58:C1:2666:G:O2'	58:C1:2675:G:N1	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:CW:49:LYS:NZ	58:C1:514:G:N7	2.66	0.42
26:C4:17:C:C4	26:C4:18:U:C4	3.07	0.42
28:CB:266:SER:C	28:CB:267:SER:O	2.55	0.42
29:CC:104:VAL:HG11	29:CC:188:VAL:CG2	2.50	0.42
37:CO:58:THR:CG2	37:CO:58:THR:O	2.66	0.42
40:CR:91:PRO:O	40:CR:92:TYR:C	2.58	0.42
47:CZ:8:TYR:HB2	47:CZ:38:TYR:CE1	2.55	0.42
58:D1:1477:C:H2'	58:D1:1478:U:O5'	2.20	0.42
58:D1:1524:G:HO2'	58:D1:1604:A:H2	1.66	0.42
58:D1:195:A:H2'	58:D1:196:C:O4'	2.19	0.42
58:D1:978:G:H2'	58:D1:978:G:N3	2.33	0.42
54:D7:46:HIS:HB2	54:D7:47:THR:HG21	2.01	0.42
31:DE:116:ASP:O	31:DE:117:PHE:HB2	2.20	0.42
31:DE:26:GLN:HE21	31:DE:26:GLN:H	1.67	0.42
34:DJ:107:UNK:O	34:DJ:108:UNK:CB	2.68	0.42
37:DO:98:GLU:HA	37:DO:101:VAL:HG22	2.00	0.42
2:AA:162:ILE:HD11	2:AA:184:VAL:HG22	2.00	0.42
11:AK:120:ARG:HA	11:AK:121:PRO:HD3	1.81	0.42
19:AT:6:LYS:C	19:AT:7:LYS:HE3	2.40	0.42
5:BE:139:LEU:HA	5:BE:142:LEU:CD1	2.50	0.42
5:BE:76:ILE:CG1	5:BE:77:PRO:HD2	2.49	0.42
8:BH:4:ASP:HA	8:BH:5:PRO:HD2	1.92	0.42
10:BJ:38:ILE:HG13	10:BJ:71:LEU:HB3	2.01	0.42
11:BK:108:ILE:O	18:BS:87:ARG:HA	2.20	0.42
58:C1:1801:C:H1'	58:C1:1816:A:C8	2.55	0.42
58:C1:2424:G:N2	58:C1:2425:G:H1'	2.35	0.42
58:C1:576:U:C4	58:C1:577:U:C4	3.08	0.42
26:C4:53:G:O2'	26:C4:54:G:H8	2.02	0.42
31:CE:91:ARG:C	31:CE:91:ARG:HD2	2.40	0.42
37:CO:124:LYS:HA	37:CO:124:LYS:HD3	1.95	0.42
39:CQ:101:ALA:HB2	53:C6:44:THR:HG21	2.01	0.42
41:CS:98:LYS:N	41:CS:98:LYS:HD2	2.35	0.42
58:D1:1098:C:O3'	58:D1:1151:A:P	2.77	0.42
58:D1:1151:A:O4'	58:D1:1151:A:P	2.78	0.42
41:DS:96:ARG:NH1	58:D1:1784:C:P	2.93	0.42
58:D1:1923:C:H2'	58:D1:1924:G:O5'	2.19	0.42
58:D1:2555:G:H2'	58:D1:2556:G:O5'	2.20	0.42
58:D1:552:A:N1	58:D1:2063:A:H2'	2.34	0.42
58:D1:88:U:H2'	58:D1:88:U:O2	2.18	0.42
60:D2:43:C:OP1	60:D2:43:C:H4'	2.20	0.42
49:DH:86:SER:HB2	49:DH:89:GLU:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:DM:15:LEU:HD13	35:DM:16:ILE:H	1.82	0.42
35:DM:67:LEU:HB3	35:DM:88:GLU:HG2	2.01	0.42
36:DN:68:GLU:CD	36:DN:68:GLU:H	2.23	0.42
36:DN:9:GLU:OE1	36:DN:9:GLU:HA	2.20	0.42
40:DR:90:GLY:C	40:DR:92:TYR:H	2.23	0.42
42:DT:107:ALA:O	42:DT:110:VAL:HB	2.19	0.42
46:DY:77:PRO:O	46:DY:78:ALA:HB2	2.20	0.42
14:AN:24:CYS:HB3	14:AN:29:ARG:CB	2.50	0.42
18:AS:73:ALA:HB3	18:AS:79:LEU:HD12	2.02	0.42
19:AT:44:MET:HA	19:AT:44:MET:CE	2.50	0.42
18:BS:67:ALA:HA	18:BS:70:ILE:HG13	2.01	0.42
58:C1:1337:U:H2'	58:C1:1338:C:C6	2.55	0.42
58:C1:1362:A:H2'	58:C1:1363:C:C6	2.54	0.42
58:C1:1315:C:O2'	58:C1:1694:C:OP2	2.30	0.42
58:C1:1792:A:O5'	58:C1:1792:A:H8	2.02	0.42
41:CS:5:ALA:HB3	58:C1:2884:C:O2'	2.20	0.42
29:CC:111:ARG:HG3	39:CQ:2:ARG:CG	2.50	0.42
29:CC:93:VAL:O	29:CC:95:ILE:N	2.53	0.42
32:CF:136:ILE:N	32:CF:136:ILE:HD12	2.35	0.42
33:CI:91:SER:HB2	33:CI:119:PRO:O	2.19	0.42
30:CD:34:TRP:CD2	37:CO:12:ALA:HB2	2.54	0.42
38:CP:110:THR:HG23	38:CP:113:GLN:HB2	2.02	0.42
41:CS:28:VAL:HG21	41:CS:88:ILE:CG1	2.50	0.42
41:CS:34:VAL:O	41:CS:35:LYS:HB3	2.20	0.42
58:D1:1151:A:HO2'	58:D1:1152:G:C1'	2.31	0.42
42:DT:25:TRP:CZ3	58:D1:16:G:H4'	2.55	0.42
58:D1:1792:A:O5'	58:D1:1792:A:C8	2.73	0.42
58:D1:1874:C:O2'	58:D1:1875:G:H5'	2.20	0.42
58:D1:2328:C:H2'	58:D1:2329:G:C5'	2.49	0.42
58:D1:2338:A:H2'	58:D1:2339:A:H8	1.78	0.42
58:D1:2563:U:H2'	58:D1:2565:U:OP2	2.20	0.42
58:D1:2675:G:O5'	58:D1:2675:G:H8	2.03	0.42
58:D1:420:A:C6	58:D1:421:U:C4	3.07	0.42
25:D3:7:A:N6	25:D3:49:C:N4	2.67	0.42
56:D9:14:VAL:HG21	56:D9:22:VAL:HG13	2.01	0.42
29:DC:81:ILE:O	29:DC:82:ARG:C	2.58	0.42
50:DK:64:LEU:O	50:DK:64:LEU:HD23	2.19	0.42
41:DS:24:PRO:CA	41:DS:49:VAL:HG13	2.49	0.42
42:DT:66:ASN:HD21	42:DT:70:ARG:HE	1.67	0.42
43:DU:19:LYS:HG2	43:DU:94:LEU:HB2	2.01	0.42
2:AA:32:ILE:CD1	2:AA:40:HIS:CD2	3.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:AI:118:LYS:O	9:AI:119:ALA:CB	2.64	0.41
2:BA:221:LEU:HD13	2:BA:221:LEU:O	2.19	0.41
13:BM:74:VAL:O	13:BM:77:ASN:HB2	2.20	0.41
19:BT:9:VAL:HG12	19:BT:9:VAL:O	2.20	0.41
58:C1:1575:G:N3	58:C1:1575:G:H2'	2.35	0.41
58:C1:2212:G:N3	58:C1:2212:G:H2'	2.35	0.41
58:C1:2298:A:N6	58:C1:2355:U:H3	2.17	0.41
56:C9:30:ARG:CZ	58:C1:2430:U:O4	2.68	0.41
58:C1:2527:G:C6	58:C1:2528:C:N4	2.87	0.41
58:C1:271:U:H2'	58:C1:272:G:OP2	2.20	0.41
58:C1:754:C:H5''	58:C1:754:C:C6	2.55	0.41
29:CC:107:THR:HG22	29:CC:107:THR:O	2.20	0.41
29:CC:101:ARG:HD2	29:CC:169:ASN:ND2	2.34	0.41
32:CF:149:ARG:HA	32:CF:162:ILE:HG13	2.02	0.41
45:CX:36:LYS:HB2	58:C1:1643:C:H5'	2.02	0.41
58:D1:1180:G:H2'	58:D1:1180:G:N3	2.34	0.41
58:D1:1246:C:H2'	58:D1:1247:G:H5'	2.01	0.41
58:D1:157:U:C6	58:D1:157:U:OP2	2.73	0.41
58:D1:1729:C:H2'	58:D1:1730:C:H6	1.85	0.41
58:D1:193:G:O2'	58:D1:194:U:P	2.78	0.41
58:D1:2328:C:O2'	58:D1:2329:G:H5'	2.20	0.41
58:D1:2817:U:H5'	58:D1:2899:G:O6	2.19	0.41
37:DO:146:VAL:HG13	37:DO:147:LEU:HB2	2.02	0.41
1:A2:14:A:C2'	1:A2:15:A:O5'	2.68	0.41
1:A2:14:A:C5	25:C3:34:G:C6	3.08	0.41
20:AU:84:LEU:C	20:AU:84:LEU:CD1	2.89	0.41
58:C1:1488:G:H5''	58:C1:1488:G:C8	2.55	0.41
58:C1:2331:A:H2'	58:C1:2331:A:N3	2.35	0.41
58:C1:552:A:H2	58:C1:2064:C:H5'	1.84	0.41
56:C9:22:VAL:HB	56:C9:53:PRO:HB3	2.02	0.41
32:CF:150:ALA:O	32:CF:151:ILE:C	2.58	0.41
49:CH:44:PRO:O	49:CH:46:LEU:N	2.54	0.41
33:CI:81:VAL:HG22	33:CI:82:ARG:N	2.35	0.41
51:CL:40:THR:OG1	51:CL:43:ILE:HG12	2.20	0.41
35:CM:3:THR:HG22	35:CM:5:VAL:HB	2.02	0.41
47:CZ:151:HIS:HB2	47:CZ:170:THR:HA	2.02	0.41
58:D1:1177:A:C2	58:D1:1178:U:C2	3.08	0.41
58:D1:1488:G:N2	58:D1:1595:C:C2	2.88	0.41
38:DP:123:HIS:CD2	58:D1:2478:C:H4'	2.54	0.41
58:D1:949:C:H2'	58:D1:950:U:C6	2.55	0.41
58:D1:906:U:C5	58:D1:962:A:N7	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:D3:34:G:N1	25:D3:35:A:C6	2.88	0.41
28:DB:24:ILE:O	28:DB:25:THR:C	2.48	0.41
32:DF:41:MET:HE2	32:DF:42:ARG:C	2.40	0.41
32:DF:55:PRO:HG2	32:DF:61:HIS:CE1	2.55	0.41
36:DN:22:ILE:CD1	58:D1:1973:A:C5	3.02	0.41
39:DQ:21:TYR:HB3	39:DQ:47:PHE:CD2	2.55	0.41
3:AC:53:ALA:HB2	3:AC:115:LEU:CD2	2.50	0.41
18:AS:33:ASP:O	18:AS:40:LEU:HD11	2.20	0.41
4:BD:61:LYS:HD3	4:BD:206:PHE:CE2	2.55	0.41
9:BI:55:ALA:HB1	9:BI:58:ARG:HB2	2.03	0.41
20:BU:63:ILE:HG22	20:BU:77:ALA:HB1	2.03	0.41
20:BU:63:ILE:CG2	20:BU:77:ALA:HB1	2.50	0.41
58:C1:2450:A:H5''	58:C1:2450:A:C8	2.55	0.41
44:CW:80:PRO:HB3	58:C1:25:G:OP1	2.20	0.41
58:C1:997:A:C2	58:C1:998:G:C8	3.08	0.41
58:C1:998:G:C5	58:C1:999:C:C5	3.08	0.41
25:C3:64:A:H2'	25:C3:65:G:C8	2.55	0.41
30:CD:117:ARG:HD3	30:CD:117:ARG:HA	1.85	0.41
36:CN:3:GLN:HB2	36:CN:4:PRO:HD2	2.02	0.41
41:CS:3:ARG:HB3	41:CS:6:LEU:H	1.85	0.41
42:CT:81:HIS:CE1	42:CT:85:LYS:HD2	2.55	0.41
45:CX:12:VAL:HG12	45:CX:27:THR:OG1	2.21	0.41
46:CY:32:PRO:HD2	58:C1:84:C:OP1	2.20	0.41
37:DO:46:LYS:HE2	58:D1:184:A:O4'	2.21	0.41
58:D1:2045:G:H2'	58:D1:2046:C:C6	2.56	0.41
31:DE:40:ASN:CG	58:D1:2324:C:O4'	2.59	0.41
58:D1:821:G:C5	58:D1:840:G:C8	3.08	0.41
29:DC:13:ARG:HD2	29:DC:20:ALA:HB1	2.02	0.41
33:DI:81:VAL:HG21	33:DI:88:ILE:HG23	2.02	0.41
35:DM:126:PRO:O	35:DM:127:ASP:HB2	2.20	0.41
46:DY:17:SER:CA	46:DY:71:LYS:HE2	2.49	0.41
2:AA:185:ILE:HG22	2:AA:199:TYR:CB	2.50	0.41
16:AP:19:ILE:HG22	16:AP:36:ILE:CG1	2.50	0.41
4:BD:11:LEU:O	4:BD:12:CYS:C	2.57	0.41
7:BG:16:LEU:HD12	9:BI:42:ARG:HA	2.03	0.41
11:BK:23:ALA:O	11:BK:86:GLY:O	2.38	0.41
58:C1:1313:A:H2'	58:C1:1314:A:O5'	2.20	0.41
58:C1:1411:A:H2'	58:C1:1412:A:O4'	2.21	0.41
26:C4:17:C:N3	26:C4:18:U:N3	2.68	0.41
28:CB:36:PRO:HA	28:CB:62:TYR:O	2.20	0.41
33:CI:74:ASN:OD1	33:CI:75:LEU:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:CO:110:TYR:O	37:CO:111:ARG:C	2.59	0.41
40:CR:89:ARG:HG3	40:CR:92:TYR:N	2.36	0.41
44:CW:50:VAL:HG13	44:CW:105:VAL:HG21	2.03	0.41
58:D1:2272:C:O2'	58:D1:2273:U:H5'	2.21	0.41
58:D1:2597:C:O5'	58:D1:2597:C:H6	2.04	0.41
58:D1:670:A:H2'	58:D1:671:G:O4'	2.20	0.41
58:D1:799:C:H6	58:D1:799:C:O5'	2.02	0.41
58:D1:928:G:H2'	58:D1:929:G:C8	2.56	0.41
38:DP:12:GLN:HE21	38:DP:73:PRO:HD2	1.85	0.41
41:DS:3:ARG:O	41:DS:5:ALA:N	2.53	0.41
43:DU:38:LEU:O	43:DU:51:VAL:HG13	2.21	0.41
46:DY:28:LYS:HB2	46:DY:28:LYS:HE3	1.87	0.41
2:AA:55:PHE:CD1	2:AA:58:ILE:HD12	2.55	0.41
9:AI:8:GLY:HA2	9:AI:79:LEU:HD12	2.02	0.41
9:AI:97:LYS:HB3	9:AI:98:PRO:HD3	2.02	0.41
11:AK:59:TYR:CE1	11:AK:63:LEU:HD21	2.55	0.41
8:BH:6:ILE:O	8:BH:9:MET:HB3	2.20	0.41
58:C1:1679:G:H8	58:C1:1679:G:O5'	2.03	0.41
58:C1:2752:A:C6	58:C1:2753:A:C6	3.08	0.41
58:C1:497:A:H3'	58:C1:497:A:C8	2.56	0.41
25:C3:10:G:N2	25:C3:26:A:H1'	2.34	0.41
26:C4:53:G:HO2'	26:C4:54:G:P	2.43	0.41
56:C9:4:MET:HB2	56:C9:61:LEU:HD13	2.01	0.41
28:CB:77:ALA:HB2	28:CB:97:TYR:CD1	2.56	0.41
35:CM:28:THR:HG21	58:C1:1057:U:O4	2.20	0.41
41:CS:7:ILE:O	41:CS:10:VAL:HB	2.20	0.41
43:CU:19:LYS:HG2	43:CU:94:LEU:H	1.85	0.41
47:CZ:30:ASN:HB3	47:CZ:90:VAL:HB	2.02	0.41
58:D1:1090:A:N3	58:D1:1090:A:H3'	2.35	0.41
58:D1:1213:G:C2	58:D1:1226:A:C2	3.08	0.41
58:D1:1676:C:H2'	58:D1:1677:A:OP1	2.21	0.41
58:D1:2306:C:H2'	58:D1:2307:U:H5'	2.02	0.41
58:D1:594:A:H2'	58:D1:595:G:O4'	2.20	0.41
58:D1:672:G:O2'	58:D1:673:G:H5'	2.21	0.41
32:DF:20:ALA:CB	32:DF:21:PRO:CD	2.94	0.41
49:DH:84:GLY:O	49:DH:85:LEU:C	2.58	0.41
41:DS:38:ASN:ND2	41:DS:40:THR:H	2.15	0.41
42:DT:76:TYR:O	42:DT:77:SER:C	2.59	0.41
64:DV:15:G:H4'	64:DV:16:U:OP1	2.21	0.41
46:DY:52:SER:C	46:DY:54:LYS:N	2.68	0.41
9:AI:59:PHE:N	9:AI:59:PHE:CD1	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:AL:60:LEU:N	12:AL:60:LEU:HD22	2.35	0.41
24:BC:149:ALA:HA	24:BC:201:TYR:O	2.20	0.41
11:BK:57:THR:HG23	11:BK:60:ALA:H	1.86	0.41
58:C1:1092:G:H4'	58:C1:1092:G:OP1	2.19	0.41
58:C1:1218:A:OP1	58:C1:1219:U:H5''	2.20	0.41
58:C1:2077:G:C2	58:C1:2078:A:C8	3.08	0.41
58:C1:2189:G:N2	58:C1:2192:A:C8	2.89	0.41
58:C1:2640:A:H2'	58:C1:2640:A:N3	2.36	0.41
58:C1:966:G:C6	58:C1:967:U:C4	3.09	0.41
58:C1:710:C:H4'	58:C1:985:A:OP1	2.19	0.41
54:C7:13:CYS:HB2	54:C7:22:ALA:HB3	2.03	0.41
28:CB:25:THR:O	28:CB:26:LYS:CB	2.67	0.41
29:CC:23:VAL:HA	29:CC:184:VAL:O	2.20	0.41
30:CD:3:GLU:O	30:CD:19:GLU:CB	2.68	0.41
31:CE:18:GLU:O	31:CE:22:ARG:HB2	2.20	0.41
33:CI:98:ALA:HA	33:CI:109:ILE:HD13	2.02	0.41
33:CI:5:LEU:HD22	33:CI:9:LEU:HD13	2.01	0.41
47:CZ:63:ASP:C	47:CZ:65:GLN:H	2.23	0.41
58:D1:1540:A:O4'	58:D1:1540:A:OP1	2.39	0.41
58:D1:2103:A:H2'	58:D1:2104:G:O4'	2.21	0.41
58:D1:2454:C:O2'	58:D1:2455:G:H5'	2.20	0.41
58:D1:2518:C:H2'	58:D1:2518:C:O2	2.20	0.41
58:D1:2801:C:N3	58:D1:2902:G:O6	2.53	0.41
62:DA:77:ILE:O	62:DA:77:ILE:HG23	2.20	0.41
28:DB:149:PRO:O	28:DB:150:LYS:HB2	2.21	0.41
29:DC:141:ILE:HD11	58:D1:2073:G:C8	2.55	0.41
30:DD:157:VAL:HG11	30:DD:181:LEU:HD13	2.01	0.41
30:DD:3:GLU:HA	30:DD:24:LEU:HB3	2.03	0.41
33:DI:92:VAL:HG12	33:DI:120:ILE:HB	2.00	0.41
37:DO:97:PRO:O	37:DO:98:GLU:CB	2.68	0.41
63:DW:6:ILE:HG12	63:DW:104:THR:HG23	2.02	0.41
47:DZ:139:VAL:HG23	47:DZ:140:ASP:N	2.35	0.41
3:AC:64:VAL:HG12	3:AC:66:VAL:HG23	2.03	0.41
4:AD:4:TYR:O	4:AD:5:ILE:HB	2.21	0.41
13:AM:90:LEU:O	13:AM:92:HIS:N	2.46	0.41
20:AU:69:GLY:O	20:AU:73:HIS:CD2	2.74	0.41
2:BA:29:ALA:O	2:BA:32:ILE:HG22	2.21	0.41
12:BL:91:LYS:HG3	12:BL:91:LYS:O	2.20	0.41
20:BU:75:ASN:O	20:BU:79:ARG:N	2.51	0.41
58:C1:2182:C:H2'	58:C1:2183:G:C8	2.55	0.41
58:C1:2528:C:H2'	58:C1:2553:A:H2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:C1:2740:U:O2'	58:C1:2741:G:H5'	2.20	0.41
58:C1:88:U:C2'	58:C1:89:A:OP2	2.69	0.41
25:C2:10:G:H2'	25:C2:11:C:C6	2.56	0.41
28:CB:209:ALA:O	28:CB:210:GLY:O	2.39	0.41
32:CF:167:GLU:CB	32:CF:168:PRO:HD2	2.50	0.41
32:CF:54:ARG:HD2	32:CF:55:PRO:O	2.20	0.41
37:CO:124:LYS:HD3	37:CO:143:GLY:HA3	2.02	0.41
39:CQ:4:LEU:CD1	39:CQ:6:SER:O	2.69	0.41
41:CS:27:THR:HA	41:CS:87:ASP:HB2	2.01	0.41
44:CW:6:ILE:HA	44:CW:103:ILE:O	2.20	0.41
58:D1:2723:U:O2'	58:D1:2724:A:P	2.79	0.41
58:D1:329:U:H2'	58:D1:330:G:O4'	2.21	0.41
58:D1:578:G:C6	58:D1:579:U:C4	3.08	0.41
58:D1:923:U:O2'	58:D1:924:A:H5"	2.21	0.41
32:DF:62:LYS:HE2	32:DF:62:LYS:HB3	1.94	0.41
38:DP:26:TYR:CD1	38:DP:26:TYR:C	2.94	0.41
40:DR:85:VAL:H	40:DR:106:ARG:HB2	1.85	0.41
41:DS:80:SER:CB	41:DS:81:PRO:HD3	2.48	0.41
46:DY:8:LYS:HB2	46:DY:28:LYS:HE2	2.03	0.41
4:AD:24:GLU:O	4:AD:27:TYR:HB2	2.20	0.41
5:BE:27:ARG:HE	5:BE:27:ARG:HB2	1.78	0.41
58:C1:2351:G:O2'	58:C1:2352:G:H5'	2.20	0.41
58:C1:2532:C:O2'	58:C1:2575:A:N3	2.44	0.41
54:C7:28:ARG:HA	54:C7:32:ASN:HB3	2.02	0.41
29:CC:132:HIS:CD2	29:CC:135:HIS:NE2	2.89	0.41
29:CC:4:ILE:HG12	29:CC:5:LEU:O	2.21	0.41
30:CD:115:ALA:O	30:CD:116:ASP:C	2.59	0.41
37:CO:35:HIS:C	37:CO:36:LYS:HG3	2.41	0.41
43:CU:84:LYS:HD3	58:C1:1270:G:O3'	2.20	0.41
44:CW:50:VAL:HG13	44:CW:105:VAL:CG2	2.51	0.41
45:CX:3:THR:N	45:CX:6:ASP:OD2	2.53	0.41
47:CZ:45:ASP:O	47:CZ:49:ARG:HB2	2.21	0.41
58:D1:1574:A:N7	58:D1:1575:G:H8	2.19	0.41
58:D1:1846:G:C3'	58:D1:1846:G:C8	3.03	0.41
58:D1:2331:A:N3	58:D1:2331:A:C2'	2.83	0.41
58:D1:2733:A:H2'	58:D1:2734:G:O4'	2.20	0.41
58:D1:448:A:C6	58:D1:449:A:C6	3.09	0.41
58:D1:251:C:O2'	58:D1:455:A:N3	2.46	0.41
28:DB:224:ALA:O	28:DB:225:ALA:CB	2.69	0.41
28:DB:267:SER:O	28:DB:268:ARG:CB	2.69	0.41
29:DC:59:VAL:O	29:DC:62:PRO:HD2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:DD:3:GLU:O	30:DD:19:GLU:CB	2.69	0.41
51:DL:31:LEU:O	51:DL:32:GLN:HB2	2.21	0.41
43:DU:21:ARG:HG2	43:DU:91:TYR:CG	2.55	0.41
43:DU:40:LEU:CD2	43:DU:40:LEU:N	2.83	0.41
43:DU:2:PHE:HB2	43:DU:42:GLY:CA	2.51	0.41
3:AC:15:THR:HG21	3:AC:181:ASN:HA	2.02	0.41
4:AD:25:ARG:C	4:AD:27:TYR:H	2.24	0.41
8:AH:34:GLU:HA	8:AH:34:GLU:OE2	2.21	0.41
9:BI:8:GLY:HA2	9:BI:79:LEU:HD12	2.03	0.41
13:BM:113:PRO:O	13:BM:115:LYS:HD3	2.21	0.41
13:BM:8:GLU:OE1	13:BM:22:ILE:HG23	2.21	0.41
17:BR:9:VAL:O	17:BR:21:VAL:HA	2.21	0.41
58:C1:1068:U:OP2	58:C1:1069:G:N7	2.54	0.41
58:C1:158:U:H4'	58:C1:159:G:C8	2.55	0.41
58:C1:1770:G:N7	58:C1:1771:C:N3	2.68	0.41
58:C1:1966:G:C6	58:C1:1967:U:C4	3.08	0.41
58:C1:2139:U:P	58:C1:2168:G:HO2'	2.44	0.41
29:CC:61:ARG:HD3	58:C1:2799:C:H1'	2.02	0.41
58:C1:2861:G:C2	58:C1:2862:C:C2	3.09	0.41
58:C1:88:U:O2'	58:C1:89:A:OP2	2.33	0.41
26:C4:50:G:C2	26:C4:51:U:H1'	2.55	0.41
56:C9:62:LEU:N	56:C9:63:PRO:HD2	2.36	0.41
28:CB:232:PRO:HD2	28:CB:249:PRO:HA	2.03	0.41
28:CB:35:LYS:CG	28:CB:63:ARG:HG3	2.42	0.41
29:CC:9:VAL:HG22	29:CC:25:VAL:HB	2.03	0.41
31:CE:130:ASN:HB3	31:CE:160:VAL:HA	2.03	0.41
31:CE:77:ILE:HD13	31:CE:77:ILE:HG21	1.82	0.41
32:CF:25:LYS:HB3	32:CF:32:GLU:OE2	2.20	0.41
43:CU:45:THR:O	43:CU:46:VAL:HG12	2.21	0.41
58:D1:1093:A:H4'	58:D1:1094:C:OP1	2.19	0.41
58:D1:1184:C:HO2'	58:D1:1188:A:HO2'	1.69	0.41
58:D1:1313:A:OP1	58:D1:2027:C:OP1	2.39	0.41
28:DB:58:HIS:CD2	58:D1:1613:A:H5'	2.56	0.41
45:DX:36:LYS:HB2	58:D1:1643:C:H5'	2.02	0.41
58:D1:1765:G:H5'	58:D1:1766:A:OP2	2.21	0.41
58:D1:1906:A:H3'	58:D1:1907:C:H6	1.86	0.41
58:D1:1863:U:O2'	58:D1:1990:A:N1	2.50	0.41
31:DE:38:VAL:HG11	58:D1:2325:C:H5'	2.02	0.41
58:D1:2861:G:C2	58:D1:2862:C:C2	3.09	0.41
58:D1:880:C:C2	58:D1:881:A:C8	3.09	0.41
58:D1:902:C:H2'	58:D1:902:C:O2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:D2:57:G:N7	64:DV:18:G:N1	2.66	0.41
52:D5:60:GLU:O	52:D5:61:VAL:HB	2.20	0.41
29:DC:98:PRO:HD3	29:DC:175:VAL:CG1	2.51	0.41
41:DS:10:VAL:O	41:DS:13:ARG:HG2	2.20	0.41
45:DX:24:GLY:O	45:DX:82:GLN:HA	2.21	0.41
47:DZ:165:VAL:CG1	47:DZ:166:SER:N	2.84	0.41
10:AJ:90:LEU:N	10:AJ:91:PRO:HD3	2.36	0.41
12:AL:58:VAL:O	12:AL:65:GLU:HA	2.21	0.41
19:AT:44:MET:SD	19:AT:44:MET:N	2.94	0.41
20:AU:42:GLN:HE21	20:AU:42:GLN:HA	1.85	0.41
24:BC:8:ILE:O	24:BC:11:ARG:N	2.48	0.41
8:BH:112:LEU:HA	8:BH:134:ILE:HG12	2.02	0.41
11:BK:34:ASP:HB3	11:BK:40:ILE:HD11	2.02	0.41
11:BK:17:GLY:HA3	11:BK:77:MET:SD	2.61	0.41
19:BT:6:LYS:H	19:BT:6:LYS:HD2	1.85	0.41
58:C1:1670:C:H2'	58:C1:1671:G:O4'	2.21	0.41
58:C1:2220:A:H3'	58:C1:2221:C:H6	1.86	0.41
58:C1:718:C:H2'	58:C1:719:C:H5'	2.02	0.41
58:C1:754:C:H5'	58:C1:755:U:OP2	2.21	0.41
50:CK:47:ASN:ND2	58:C1:92:G:N3	2.69	0.41
26:C4:51:U:O2	26:C4:51:U:H2'	2.20	0.41
26:C4:7:G:C5'	26:C4:7:G:H8	2.34	0.41
55:C8:8:ASN:ND2	55:C8:8:ASN:C	2.75	0.41
28:CB:25:THR:C	28:CB:27:THR:H	2.24	0.41
28:CB:30:GLU:HB2	28:CB:35:LYS:CE	2.49	0.41
30:CD:177:ALA:HB1	30:CD:178:PRO:CD	2.51	0.41
31:CE:9:ARG:C	31:CE:11:TYR:H	2.25	0.41
32:CF:41:MET:HE3	32:CF:43:VAL:HG13	2.03	0.41
32:CF:67:LEU:O	32:CF:71:LEU:HD12	2.21	0.41
32:CF:84:SER:O	32:CF:85:LYS:HB3	2.20	0.41
35:CM:2:LYS:O	35:CM:4:TYR:CE2	2.73	0.41
37:CO:112:LEU:H	37:CO:128:HIS:CD2	2.39	0.41
37:CO:121:LYS:HA	37:CO:122:PRO:HD3	1.95	0.41
40:CR:36:TYR:N	40:CR:36:TYR:CD1	2.88	0.41
42:CT:9:VAL:O	42:CT:13:LYS:HE3	2.21	0.41
58:D1:1529:G:H2'	58:D1:1530:G:O5'	2.21	0.41
58:D1:2509:C:OP2	58:D1:2510:C:OP2	2.38	0.41
37:DO:25:SER:HA	58:D1:857:U:H3'	2.03	0.41
29:DC:101:ARG:NH1	29:DC:169:ASN:O	2.54	0.41
29:DC:87:GLU:O	29:DC:87:GLU:HG3	2.20	0.41
30:DD:65:TRP:HA	30:DD:66:PRO:HD2	1.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:DF:86:GLU:OE1	32:DF:86:GLU:N	2.53	0.41
37:DO:17:LYS:C	37:DO:19:VAL:N	2.74	0.41
37:DO:23:PRO:HD2	37:DO:33:ARG:CZ	2.51	0.41
40:DR:53:SER:OG	40:DR:54:LEU:N	2.53	0.41
41:DS:83:ILE:HG13	41:DS:84:GLN:H	1.86	0.41
64:DV:28:G:H2'	64:DV:29:G:H8	1.86	0.41
4:AD:13:ARG:HD2	4:AD:38:TYR:O	2.20	0.41
4:AD:61:LYS:CE	4:AD:62:GLN:HE21	2.34	0.41
7:AG:148:ASN:N	7:AG:148:ASN:HD22	2.19	0.41
9:AI:28:VAL:HA	9:AI:63:ILE:O	2.21	0.41
10:AJ:5:ARG:HB3	10:AJ:99:LYS:HB2	2.03	0.41
13:AM:23:TYR:HB3	13:AM:67:GLU:HB2	2.02	0.41
2:BA:239:VAL:O	2:BA:240:GLN:CB	2.68	0.41
2:BA:24:TRP:CH2	2:BA:26:PRO:HA	2.56	0.41
8:BH:53:VAL:HG12	8:BH:54:ASP:OD2	2.21	0.41
58:C1:139:A:H8	58:C1:1453:C:H1'	1.83	0.41
58:C1:1475:C:H2'	58:C1:1476:U:H6	1.84	0.41
58:C1:1741:G:N2	58:C1:1742:G:C8	2.88	0.41
58:C1:2801:C:H4'	58:C1:2801:C:OP1	2.21	0.41
56:C9:8:LYS:O	56:C9:12:LYS:HG3	2.21	0.41
29:CC:24:THR:HG23	29:CC:184:VAL:HG23	2.03	0.41
31:CE:170:ARG:HH22	31:CE:182:LYS:HG2	1.86	0.41
33:CI:31:LEU:HB2	33:CI:32:PRO:HD3	2.03	0.41
38:CP:51:ARG:O	38:CP:52:VAL:C	2.59	0.41
41:CS:58:ASN:HD22	41:CS:58:ASN:C	2.25	0.41
42:CT:34:LYS:HA	42:CT:34:LYS:HE3	2.03	0.41
43:CU:49:THR:HB	43:CU:50:PRO:CD	2.51	0.41
46:CY:47:LYS:CG	46:CY:60:PHE:HE2	2.34	0.41
46:CY:7:VAL:HB	46:CY:8:LYS:CE	2.51	0.41
58:D1:1042:G:O2'	58:D1:1043:C:H5'	2.21	0.41
58:D1:151:G:H2'	58:D1:152:C:C6	2.56	0.41
58:D1:1533:G:C6	58:D1:1534:U:C2	3.09	0.41
58:D1:1766:A:C6	58:D1:1769:A:C6	3.09	0.41
61:D4:12:G:H1'	58:D1:1944:U:O2'	2.21	0.41
58:D1:209:A:H4'	58:D1:210:A:O5'	2.20	0.41
28:DB:264:LYS:HA	28:DB:265:PRO:HD2	1.89	0.41
29:DC:14:ILE:HG12	29:DC:21:VAL:CG2	2.51	0.41
30:DD:199:TRP:CZ3	30:DD:203:GLN:NE2	2.89	0.41
31:DE:115:ARG:CG	31:DE:116:ASP:H	2.34	0.41
31:DE:89:GLY:HA3	58:D1:2323:U:O2'	2.21	0.41
37:DO:125:VAL:CG1	37:DO:138:LEU:HD21	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:DO:51:PHE:O	37:DO:52:GLU:HB2	2.21	0.41
38:DP:39:PRO:O	38:DP:40:ALA:HB2	2.20	0.41
64:DV:52:C:H3'	64:DV:53:A:OP2	2.21	0.41
2:AA:21:ARG:HG3	2:AA:21:ARG:O	2.21	0.40
3:AC:47:LEU:CD1	3:AC:76:VAL:HG12	2.51	0.40
5:AE:91:LEU:HD13	5:AE:120:THR:HG22	2.03	0.40
7:AG:26:PHE:CE2	7:AG:30:ILE:HD11	2.57	0.40
11:AK:114:VAL:HA	11:AK:115:PRO:HD2	1.90	0.40
2:BA:198:ASP:N	2:BA:198:ASP:OD2	2.53	0.40
2:BA:212:GLN:HE22	2:BA:216:SER:HB2	1.86	0.40
24:BC:167:TRP:O	24:BC:168:ALA:CB	2.69	0.40
24:BC:58:GLU:HB2	24:BC:65:ALA:HB3	2.03	0.40
8:BH:11:THR:HG23	8:BH:14:ARG:NH1	2.36	0.40
9:BI:9:ARG:HA	9:BI:13:ALA:O	2.21	0.40
9:BI:97:LYS:HD2	9:BI:102:LEU:HD13	2.03	0.40
14:BN:23:ARG:HD2	14:BN:28:GLY:O	2.20	0.40
42:CT:33:ARG:NH1	58:C1:1297:G:O4'	2.55	0.40
58:C1:1967:U:H2'	58:C1:1968:C:H6	1.86	0.40
58:C1:338:G:H2'	58:C1:339:C:O4'	2.22	0.40
58:C1:635:G:C5'	58:C1:635:G:H8	2.33	0.40
28:CB:130:ALA:C	28:CB:131:LEU:HD12	2.42	0.40
32:CF:148:ILE:O	32:CF:151:ILE:HG12	2.21	0.40
32:CF:155:SER:O	32:CF:157:TYR:N	2.55	0.40
51:CL:13:ILE:HD11	58:C1:1034:G:C8	2.57	0.40
36:CN:1:MET:HE2	36:CN:32:TYR:CD2	2.55	0.40
41:CS:65:LYS:HE3	41:CS:66:VAL:H	1.86	0.40
47:CZ:130:PRO:O	47:CZ:133:ILE:HG12	2.22	0.40
58:D1:1574:A:N7	58:D1:1575:G:C8	2.89	0.40
58:D1:1589:C:C6	58:D1:1589:C:H3'	2.56	0.40
41:DS:3:ARG:HD3	58:D1:2885:G:H4'	1.99	0.40
58:D1:666:G:OP2	58:D1:2413:C:N4	2.54	0.40
61:D4:10:G:O5'	61:D4:10:G:H8	2.05	0.40
40:DR:36:TYR:HD1	40:DR:36:TYR:N	2.19	0.40
41:DS:23:ARG:NH1	58:D1:2876:G:N7	2.69	0.40
45:DX:12:VAL:HG22	45:DX:27:THR:O	2.21	0.40
3:AC:27:LYS:HB2	3:AC:27:LYS:HE3	1.93	0.40
9:AI:12:GLU:O	9:AI:68:GLY:CA	2.69	0.40
23:B2:20:U:H2'	23:B2:21:C:H6	1.81	0.40
2:BA:168:THR:HG23	2:BA:192:SER:CB	2.52	0.40
2:BA:18:GLY:HA2	2:BA:42:ILE:HG22	2.03	0.40
11:BK:21:ILE:HG13	11:BK:30:VAL:HG12	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:BP:56:ALA:O	16:BP:60:LEU:HD12	2.21	0.40
58:C1:1088:C:H6	58:C1:1088:C:H3'	1.86	0.40
58:C1:1812:C:C4	58:C1:2598:A:C2	3.09	0.40
58:C1:2001:G:O2'	58:C1:2003:C:OP2	2.35	0.40
58:C1:2270:G:C6	58:C1:2271:C:C4	3.09	0.40
58:C1:1813:A:C2	58:C1:2598:A:C5	3.10	0.40
58:C1:353:A:HO2'	58:C1:354:A:H8	1.65	0.40
58:C1:928:G:H2'	58:C1:929:G:H8	1.86	0.40
28:CB:9:TYR:C	28:CB:10:THR:HG22	2.41	0.40
28:CB:28:GLU:HB2	28:CB:29:PRO:CD	2.51	0.40
30:CD:78:ILE:HA	30:CD:83:PHE:CD1	2.57	0.40
31:CE:20:ILE:O	31:CE:24:GLY:HA2	2.22	0.40
35:CM:58:ASP:C	35:CM:60:ILE:H	2.24	0.40
58:D1:1812:C:H1'	58:D1:2620:U:H5''	2.01	0.40
58:D1:1902:C:C6	58:D1:1902:C:H5''	2.55	0.40
58:D1:2131:G:O2'	58:D1:2141:G:H5'	2.21	0.40
58:D1:2163:C:O2	58:D1:2170:G:N2	2.36	0.40
58:D1:551:C:H4'	58:D1:552:A:O5'	2.21	0.40
58:D1:928:G:H2'	58:D1:929:G:H8	1.86	0.40
25:D3:2:C:H2'	25:D3:3:C:H6	1.87	0.40
61:D4:67:C:H2'	61:D4:68:C:C6	2.54	0.40
54:D7:51:GLU:O	54:D7:52:VAL:HB	2.22	0.40
56:D9:50:LEU:O	56:D9:51:ALA:HB3	2.21	0.40
29:DC:9:VAL:HG13	29:DC:25:VAL:O	2.21	0.40
30:DD:134:GLY:HA2	30:DD:166:ALA:HB2	2.04	0.40
32:DF:43:VAL:HG11	32:DF:52:VAL:CG2	2.49	0.40
50:DK:16:LEU:O	50:DK:17:SER:CB	2.69	0.40
37:DO:49:ARG:HD2	56:D9:58:ILE:HG22	2.03	0.40
40:DR:61:ASN:OD1	40:DR:64:GLU:OE2	2.39	0.40
41:DS:40:THR:O	41:DS:41:ARG:CB	2.70	0.40
41:DS:58:ASN:C	41:DS:58:ASN:HD22	2.25	0.40
43:DU:2:PHE:O	43:DU:3:ALA:HB3	2.21	0.40
46:DY:27:VAL:O	46:DY:29:GLU:OE1	2.40	0.40
1:A2:19:U:O2'	1:A2:20:U:H5'	2.20	0.40
4:AD:107:ARG:HD2	4:AD:173:TRP:HZ2	1.86	0.40
12:AL:17:LYS:HD3	12:AL:18:VAL:HG22	2.03	0.40
13:AM:84:ILE:HG13	19:AT:66:MET:SD	2.61	0.40
13:AM:83:ASP:C	13:AM:85:GLY:N	2.74	0.40
20:AU:13:LEU:O	20:AU:16:HIS:N	2.52	0.40
2:BA:19:HIS:CD2	2:BA:189:ASP:OD2	2.73	0.40
4:BD:61:LYS:NZ	4:BD:72:GLU:OE2	2.49	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:BH:100:ILE:HG23	8:BH:101:PRO:HD2	2.02	0.40
9:BI:4:TYR:N	9:BI:4:TYR:CD1	2.89	0.40
12:BL:49:ASN:HD22	12:BL:49:ASN:N	2.19	0.40
16:BP:28:ARG:HG2	16:BP:28:ARG:NH1	2.37	0.40
18:BS:56:THR:CB	18:BS:58:LEU:HD13	2.51	0.40
58:C1:1186:U:O2	58:C1:1186:U:H2'	2.20	0.40
58:C1:1549:C:O2'	58:C1:1550:C:P	2.79	0.40
58:C1:1902:C:H5''	58:C1:1902:C:C6	2.56	0.40
58:C1:1910:A:O2'	58:C1:2108:G:H5'	2.22	0.40
58:C1:2194:A:N3	58:C1:2194:A:H2'	2.36	0.40
58:C1:2746:A:H5''	58:C1:2747:G:OP2	2.21	0.40
58:C1:66:G:H2'	58:C1:67:C:C6	2.57	0.40
25:C3:67:C:H2'	25:C3:68:C:C6	2.55	0.40
26:C4:3:C:C4	26:C4:4:G:N7	2.89	0.40
31:CE:64:THR:OG1	31:CE:94:LEU:HD21	2.21	0.40
37:CO:80:TYR:CE1	37:CO:111:ARG:HD3	2.56	0.40
37:CO:116:GLY:H	37:CO:134:ALA:HB2	1.86	0.40
46:CY:42:VAL:CB	46:CY:65:ALA:HB3	2.50	0.40
37:DO:51:PHE:CE1	58:D1:184:A:OP2	2.75	0.40
58:D1:2667:U:H3	58:D1:2676:A:H2	1.68	0.40
58:D1:538:A:H1'	58:D1:603:C:O2'	2.22	0.40
60:D2:56:C:H5'	58:D1:942:C:H4'	2.02	0.40
60:D2:53:G:H2'	60:D2:53:G:N3	2.36	0.40
28:DB:145:VAL:HG12	28:DB:146:GLU:O	2.21	0.40
28:DB:65:ILE:HD11	28:DB:67:PHE:CD2	2.56	0.40
29:DC:69:LYS:C	29:DC:71:GLY:N	2.75	0.40
32:DF:19:VAL:HG21	32:DF:44:VAL:HA	2.03	0.40
33:DI:113:ARG:O	33:DI:130:TYR:CD1	2.74	0.40
50:DK:71:ASN:C	50:DK:71:ASN:OD1	2.59	0.40
51:DL:31:LEU:O	58:D1:1203:C:H4'	2.21	0.40
37:DO:16:ARG:NH1	37:DO:16:ARG:HB2	2.36	0.40
4:AD:9:CYS:SG	4:AD:31:CYS:C	2.84	0.40
16:AP:48:TRP:O	16:AP:49:LEU:HB2	2.21	0.40
15:BO:81:LEU:CD1	15:BO:85:LEU:HD13	2.49	0.40
58:C1:1333:U:C4'	58:C1:1334:C:OP2	2.68	0.40
58:C1:2708:G:C2	58:C1:2722:A:C2	3.08	0.40
58:C1:282:G:H5''	58:C1:283:G:OP2	2.22	0.40
41:CS:3:ARG:HE	58:C1:2885:G:H4'	1.83	0.40
58:C1:38:C:H2'	58:C1:39:C:C6	2.56	0.40
37:CO:64:LYS:HE2	58:C1:655:A:OP1	2.21	0.40
58:C1:781:A:C8	58:C1:782:C:C5	3.10	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:C1:894:G:C4	58:C1:977:A:H8	2.40	0.40
29:CC:70:ALA:O	29:CC:71:GLY:C	2.59	0.40
49:CH:66:HIS:O	49:CH:67:ILE:C	2.59	0.40
35:CM:46:VAL:HG13	35:CM:47:ALA:N	2.36	0.40
37:CO:108:LYS:C	37:CO:110:TYR:N	2.75	0.40
58:D1:108:A:C2	58:D1:109:U:C2	3.10	0.40
58:D1:2183:G:H2'	58:D1:2184:C:O4'	2.21	0.40
58:D1:2449:U:C3'	58:D1:2449:U:C6	3.04	0.40
29:DC:61:ARG:HD3	58:D1:2799:C:H1'	2.01	0.40
61:D4:6:G:O6	61:D4:68:C:N4	2.49	0.40
28:DB:70:TRP:C	28:DB:70:TRP:CD1	2.95	0.40
32:DF:68:THR:O	32:DF:69:ARG:C	2.60	0.40
33:DI:123:LEU:HD23	33:DI:142:VAL:HB	2.03	0.40
41:DS:92:GLY:C	41:DS:94:ALA:N	2.75	0.40
63:DW:17:VAL:O	63:DW:18:ARG:C	2.58	0.40
46:DY:101:LYS:HG2	46:DY:101:LYS:OXT	2.21	0.40
11:AK:17:GLY:HA3	11:AK:77:MET:SD	2.61	0.40
12:AL:38:THR:HG23	12:AL:39:VAL:HG23	2.04	0.40
20:AU:26:ASN:HB3	20:AU:71:THR:OG1	2.22	0.40
2:BA:118:LEU:HB3	2:BA:142:LEU:HD12	2.03	0.40
4:BD:110:PHE:H	4:BD:110:PHE:HD1	1.69	0.40
17:BR:50:LYS:HE3	17:BR:51:TYR:CZ	2.56	0.40
58:C1:1332:A:C5	58:C1:1333:U:C4	3.09	0.40
58:C1:1740:C:O2	58:C1:1740:C:C2'	2.68	0.40
58:C1:1865:G:N3	58:C1:1865:G:H2'	2.37	0.40
58:C1:1967:U:H2'	58:C1:1968:C:C6	2.56	0.40
58:C1:554:G:C5	58:C1:2043:U:H5''	2.57	0.40
58:C1:874:U:C3'	58:C1:874:U:O2	2.70	0.40
26:C4:52:C:H2'	26:C4:53:G:H5'	2.04	0.40
56:C9:6:THR:HG22	56:C9:63:PRO:HD3	2.03	0.40
28:CB:136:ILE:HG22	28:CB:140:THR:OG1	2.22	0.40
28:CB:166:GLN:NE2	28:CB:166:GLN:CA	2.84	0.40
28:CB:241:PRO:O	28:CB:242:ARG:C	2.59	0.40
30:CD:124:LEU:O	30:CD:193:VAL:HA	2.22	0.40
30:CD:22:ALA:CB	30:CD:26:ALA:HB2	2.41	0.40
30:CD:65:TRP:HB3	30:CD:66:PRO:HD2	2.03	0.40
37:CO:98:GLU:O	37:CO:101:VAL:HG22	2.21	0.40
37:CO:144:GLU:N	37:CO:145:PRO:HD3	2.36	0.40
37:CO:15:ARG:HD2	58:C1:620:G:H5'	2.04	0.40
46:CY:13:VAL:HG21	46:CY:72:VAL:HB	2.03	0.40
58:D1:1862:C:H2'	58:D1:1863:U:O5'	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:D1:2186:G:H2'	58:D1:2187:G:O4'	2.21	0.40
58:D1:2239:G:C5	58:D1:2240:C:C5	3.10	0.40
58:D1:2484:U:C5	58:D1:2485:C:C5	3.10	0.40
58:D1:2793:A:H5''	58:D1:2794:G:H5'	2.04	0.40
58:D1:406:U:O2'	58:D1:407:G:H5'	2.22	0.40
58:D1:876:G:H4'	58:D1:877:G:OP2	2.22	0.40
28:DB:182:LEU:HB2	28:DB:271:ILE:O	2.20	0.40
29:DC:70:ALA:O	29:DC:71:GLY:C	2.59	0.40
29:DC:74:PRO:O	29:DC:75:VAL:C	2.59	0.40
31:DE:151:ALA:O	31:DE:153:ARG:HD3	2.21	0.40
33:DI:1:MET:HG3	33:DI:23:PRO:HG3	2.03	0.40
40:DR:89:ARG:HB3	40:DR:92:TYR:HB3	2.03	0.40
41:DS:102:ILE:HB	41:DS:110:ILE:HD11	2.00	0.40
63:DW:26:GLY:HA2	63:DW:71:VAL:O	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:Bb:364:U:OP1	33:CI:91:SER:OG[4_455]	2.14	0.06

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AA	232/234 (99%)	174 (75%)	47 (20%)	11 (5%)	2	15
2	BA	232/234 (99%)	180 (78%)	41 (18%)	11 (5%)	2	15
3	AC	204/238 (86%)	145 (71%)	42 (21%)	17 (8%)	1	5
4	AD	206/208 (99%)	161 (78%)	33 (16%)	12 (6%)	1	11
4	BD	206/208 (99%)	168 (82%)	27 (13%)	11 (5%)	2	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	AE	148/150 (99%)	130 (88%)	15 (10%)	3 (2%)	7	30
5	BE	148/150 (99%)	130 (88%)	14 (10%)	4 (3%)	5	26
6	AF	99/101 (98%)	92 (93%)	5 (5%)	2 (2%)	7	30
6	BF	99/101 (98%)	89 (90%)	9 (9%)	1 (1%)	15	46
7	AG	153/155 (99%)	124 (81%)	26 (17%)	3 (2%)	7	30
7	BG	153/155 (99%)	135 (88%)	17 (11%)	1 (1%)	22	55
8	AH	136/138 (99%)	110 (81%)	24 (18%)	2 (2%)	10	36
8	BH	136/138 (99%)	116 (85%)	19 (14%)	1 (1%)	22	55
9	AI	125/127 (98%)	97 (78%)	23 (18%)	5 (4%)	3	18
9	BI	125/127 (98%)	98 (78%)	22 (18%)	5 (4%)	3	18
10	AJ	96/98 (98%)	79 (82%)	13 (14%)	4 (4%)	3	18
10	BJ	96/98 (98%)	76 (79%)	15 (16%)	5 (5%)	2	13
11	AK	117/119 (98%)	102 (87%)	14 (12%)	1 (1%)	17	49
11	BK	117/119 (98%)	93 (80%)	20 (17%)	4 (3%)	3	21
12	AL	122/124 (98%)	92 (75%)	20 (16%)	10 (8%)	1	5
12	BL	122/124 (98%)	94 (77%)	16 (13%)	12 (10%)	0	4
13	AM	122/124 (98%)	83 (68%)	26 (21%)	13 (11%)	0	3
13	BM	122/124 (98%)	83 (68%)	26 (21%)	13 (11%)	0	3
14	AN	58/60 (97%)	43 (74%)	12 (21%)	3 (5%)	2	13
14	BN	58/60 (97%)	41 (71%)	14 (24%)	3 (5%)	2	13
15	AO	86/88 (98%)	73 (85%)	9 (10%)	4 (5%)	2	15
15	BO	86/88 (98%)	72 (84%)	13 (15%)	1 (1%)	13	41
16	AP	81/83 (98%)	63 (78%)	15 (18%)	3 (4%)	3	20
16	BP	81/83 (98%)	67 (83%)	14 (17%)	0	100	100
17	AR	97/99 (98%)	89 (92%)	5 (5%)	3 (3%)	4	23
17	BR	97/99 (98%)	84 (87%)	10 (10%)	3 (3%)	4	23
18	AS	68/70 (97%)	57 (84%)	5 (7%)	6 (9%)	1	5
18	BS	68/70 (97%)	54 (79%)	10 (15%)	4 (6%)	1	11
19	AT	76/78 (97%)	61 (80%)	7 (9%)	8 (10%)	0	3
19	BT	76/78 (97%)	55 (72%)	13 (17%)	8 (10%)	0	3
20	AU	97/99 (98%)	77 (79%)	14 (14%)	6 (6%)	1	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	BU	97/99 (98%)	75 (77%)	19 (20%)	3 (3%)	4	23
21	AW	22/24 (92%)	19 (86%)	2 (9%)	1 (4%)	2	16
21	BW	22/24 (92%)	17 (77%)	3 (14%)	2 (9%)	1	4
24	BC	204/206 (99%)	153 (75%)	41 (20%)	10 (5%)	2	14
27	CA	83/206 (40%)	56 (68%)	22 (26%)	5 (6%)	1	10
28	CB	269/271 (99%)	210 (78%)	39 (14%)	20 (7%)	1	7
28	DB	269/271 (99%)	209 (78%)	38 (14%)	22 (8%)	1	5
29	CC	202/204 (99%)	143 (71%)	43 (21%)	16 (8%)	1	6
29	DC	202/204 (99%)	145 (72%)	32 (16%)	25 (12%)	0	2
30	CD	205/207 (99%)	162 (79%)	30 (15%)	13 (6%)	1	9
30	DD	205/207 (99%)	166 (81%)	24 (12%)	15 (7%)	1	7
31	CE	179/181 (99%)	132 (74%)	32 (18%)	15 (8%)	1	5
31	DE	179/181 (99%)	139 (78%)	28 (16%)	12 (7%)	1	8
32	CF	157/159 (99%)	112 (71%)	25 (16%)	20 (13%)	0	2
32	DF	157/159 (99%)	113 (72%)	26 (17%)	18 (12%)	0	3
33	CI	143/145 (99%)	112 (78%)	22 (15%)	9 (6%)	1	9
33	DI	143/145 (99%)	104 (73%)	29 (20%)	10 (7%)	1	7
35	CM	136/138 (99%)	103 (76%)	24 (18%)	9 (7%)	1	8
35	DM	136/138 (99%)	96 (71%)	30 (22%)	10 (7%)	1	7
36	CN	120/122 (98%)	106 (88%)	10 (8%)	4 (3%)	4	22
36	DN	120/122 (98%)	110 (92%)	8 (7%)	2 (2%)	9	34
37	CO	144/146 (99%)	84 (58%)	29 (20%)	31 (22%)	0	0
37	DO	144/146 (99%)	86 (60%)	26 (18%)	32 (22%)	0	0
38	CP	139/141 (99%)	118 (85%)	17 (12%)	4 (3%)	4	24
38	DP	139/141 (99%)	117 (84%)	17 (12%)	5 (4%)	3	21
39	CQ	115/117 (98%)	93 (81%)	14 (12%)	8 (7%)	1	7
39	DQ	115/117 (98%)	98 (85%)	11 (10%)	6 (5%)	2	13
40	CR	96/98 (98%)	62 (65%)	23 (24%)	11 (12%)	0	3
40	DR	96/98 (98%)	66 (69%)	15 (16%)	15 (16%)	0	0
41	CS	135/137 (98%)	92 (68%)	24 (18%)	19 (14%)	0	1
41	DS	135/137 (98%)	89 (66%)	28 (21%)	18 (13%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	CT	115/117 (98%)	103 (90%)	10 (9%)	2 (2%)	9	34
42	DT	115/117 (98%)	93 (81%)	15 (13%)	7 (6%)	1	10
43	CU	99/101 (98%)	75 (76%)	11 (11%)	13 (13%)	0	1
43	DU	99/101 (98%)	72 (73%)	13 (13%)	14 (14%)	0	1
44	CW	111/113 (98%)	92 (83%)	12 (11%)	7 (6%)	1	9
45	CX	90/92 (98%)	77 (86%)	7 (8%)	6 (7%)	1	8
45	DX	90/92 (98%)	79 (88%)	9 (10%)	2 (2%)	6	29
46	CY	98/100 (98%)	60 (61%)	17 (17%)	21 (21%)	0	0
46	DY	98/100 (98%)	60 (61%)	18 (18%)	20 (20%)	0	0
47	CZ	174/176 (99%)	121 (70%)	42 (24%)	11 (6%)	1	9
47	DZ	174/176 (99%)	136 (78%)	28 (16%)	10 (6%)	1	12
48	Ca	82/84 (98%)	72 (88%)	9 (11%)	1 (1%)	13	41
48	Da	82/84 (98%)	74 (90%)	7 (8%)	1 (1%)	13	41
49	CH	91/93 (98%)	73 (80%)	10 (11%)	8 (9%)	1	5
49	DH	91/93 (98%)	73 (80%)	12 (13%)	6 (7%)	1	8
50	CK	69/71 (97%)	50 (72%)	12 (17%)	7 (10%)	0	4
50	DK	69/71 (97%)	54 (78%)	11 (16%)	4 (6%)	1	11
51	CL	57/59 (97%)	51 (90%)	5 (9%)	1 (2%)	8	32
51	DL	57/59 (97%)	52 (91%)	3 (5%)	2 (4%)	3	21
52	C5	28/30 (93%)	20 (71%)	5 (18%)	3 (11%)	0	3
52	D5	28/30 (93%)	18 (64%)	7 (25%)	3 (11%)	0	3
53	C6	57/59 (97%)	48 (84%)	5 (9%)	4 (7%)	1	7
53	D6	57/59 (97%)	46 (81%)	7 (12%)	4 (7%)	1	7
54	C7	40/44 (91%)	22 (55%)	9 (22%)	9 (22%)	0	0
54	D7	40/44 (91%)	21 (52%)	8 (20%)	11 (28%)	0	0
55	C8	46/48 (96%)	42 (91%)	4 (9%)	0	100	100
55	D8	46/48 (96%)	45 (98%)	1 (2%)	0	100	100
56	C9	61/63 (97%)	47 (77%)	11 (18%)	3 (5%)	2	14
56	D9	61/63 (97%)	41 (67%)	15 (25%)	5 (8%)	1	5
57	C0	34/36 (94%)	32 (94%)	2 (6%)	0	100	100
57	D0	34/36 (94%)	32 (94%)	2 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
62	DA	83/206 (40%)	52 (63%)	28 (34%)	3 (4%)	3	21
63	DW	111/113 (98%)	94 (85%)	11 (10%)	6 (5%)	2	13
All	All	11440/11918 (96%)	8901 (78%)	1752 (15%)	787 (7%)	1	8

All (787) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AA	83	MET
2	AA	165	VAL
3	AC	4	LYS
3	AC	12	LEU
3	AC	47	LEU
3	AC	156	ARG
4	AD	3	ARG
4	AD	4	TYR
4	AD	18	LYS
4	AD	30	LYS
4	AD	129	ASN
7	AG	117	ALA
9	AI	42	ARG
12	AL	18	VAL
12	AL	51	ALA
12	AL	91	LYS
12	AL	92	ASP
12	AL	115	LYS
13	AM	113	PRO
13	AM	117	VAL
19	AT	10	PHE
19	AT	24	ALA
19	AT	80	TYR
20	AU	97	ALA
2	BA	165	VAL
24	BC	12	LEU
24	BC	47	LEU
4	BD	9	CYS
4	BD	26	CYS
4	BD	30	LYS
7	BG	7	ALA
8	BH	2	LEU
9	BI	54	ASP
9	BI	89	ASN

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Mol	Chain	Res	Type
10	BJ	59	SER
11	BK	122	LYS
12	BL	18	VAL
12	BL	27	LEU
12	BL	64	TYR
12	BL	92	ASP
13	BM	63	THR
13	BM	67	GLU
13	BM	83	ASP
13	BM	113	PRO
13	BM	116	THR
13	BM	117	VAL
14	BN	15	LYS
14	BN	16	PHE
17	BR	34	LYS
18	BS	45	SER
18	BS	54	ARG
18	BS	87	ARG
19	BT	10	PHE
19	BT	24	ALA
19	BT	80	TYR
27	CA	55	ASP
28	CB	23	GLU
28	CB	25	THR
28	CB	33	LEU
28	CB	234	GLY
28	CB	271	ILE
29	CC	66	HIS
29	CC	71	GLY
29	CC	94	GLU
30	CD	3	GLU
30	CD	21	ALA
30	CD	26	ALA
30	CD	89	VAL
30	CD	167	ALA
31	CE	82	LEU
31	CE	87	PRO
31	CE	96	ARG
31	CE	97	ASP
31	CE	115	ARG
32	CF	83	TYR
32	CF	154	PRO

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Mol	Chain	Res	Type
32	CF	156	ALA
32	CF	159	GLU
32	CF	168	PRO
33	CI	14	ASP
33	CI	115	ALA
33	CI	133	HIS
35	CM	4	TYR
35	CM	5	VAL
35	CM	134	ARG
35	CM	135	PRO
36	CN	27	GLY
36	CN	48	PRO
37	CO	9	ASN
37	CO	14	LYS
37	CO	19	VAL
37	CO	31	ALA
37	CO	35	HIS
37	CO	42	SER
37	CO	47	ASP
37	CO	49	ARG
37	CO	52	GLU
37	CO	57	THR
37	CO	58	THR
37	CO	107	LYS
38	CP	2	LEU
38	CP	135	ASP
40	CR	59	LYS
40	CR	89	ARG
40	CR	97	ARG
41	CS	2	ASN
41	CS	18	ASP
41	CS	24	PRO
41	CS	28	VAL
41	CS	33	LYS
41	CS	80	SER
41	CS	83	ILE
41	CS	107	ASP
41	CS	129	ARG
42	CT	91	ASP
43	CU	3	ALA
43	CU	19	LYS
43	CU	46	VAL

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Mol	Chain	Res	Type
44	CW	11	ARG
45	CX	12	VAL
46	CY	3	VAL
46	CY	7	VAL
46	CY	17	SER
46	CY	27	VAL
46	CY	38	ILE
46	CY	56	PRO
46	CY	77	PRO
46	CY	78	ALA
46	CY	99	CYS
49	CH	58	ILE
49	CH	85	LEU
50	CK	45	SER
50	CK	70	GLN
53	C6	4	HIS
53	C6	36	CYS
53	C6	57	VAL
54	C7	31	PRO
54	C7	49	HIS
56	C9	31	HIS
28	DB	23	GLU
28	DB	25	THR
28	DB	33	LEU
28	DB	225	ALA
28	DB	241	PRO
29	DC	2	LYS
29	DC	18	ASP
29	DC	60	ASN
29	DC	66	HIS
29	DC	72	VAL
29	DC	82	ARG
29	DC	87	GLU
29	DC	88	GLY
29	DC	116	VAL
29	DC	131	ALA
30	DD	21	ALA
30	DD	25	PRO
30	DD	66	PRO
30	DD	89	VAL
31	DE	82	LEU
31	DE	87	PRO

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Mol	Chain	Res	Type
31	DE	117	PHE
32	DF	45	VAL
32	DF	83	TYR
32	DF	92	ILE
32	DF	137	ASP
32	DF	138	LYS
32	DF	154	PRO
32	DF	157	TYR
32	DF	159	GLU
32	DF	160	LYS
33	DI	15	VAL
33	DI	85	GLU
33	DI	133	HIS
35	DM	4	TYR
35	DM	5	VAL
35	DM	134	ARG
36	DN	48	PRO
37	DO	11	GLY
37	DO	18	ARG
37	DO	19	VAL
37	DO	31	ALA
37	DO	35	HIS
37	DO	39	LYS
37	DO	49	ARG
37	DO	52	GLU
37	DO	65	ARG
37	DO	107	LYS
38	DP	2	LEU
38	DP	135	ASP
39	DQ	8	ARG
39	DQ	45	ARG
39	DQ	58	GLY
39	DQ	117	VAL
40	DR	59	LYS
40	DR	97	ARG
40	DR	102	ALA
41	DS	24	PRO
41	DS	26	ASP
41	DS	28	VAL
41	DS	30	VAL
41	DS	33	LYS
41	DS	58	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
41	DS	80	SER
41	DS	107	ASP
41	DS	129	ARG
42	DT	32	ALA
42	DT	91	ASP
43	DU	16	PRO
43	DU	19	LYS
43	DU	23	GLU
43	DU	46	VAL
43	DU	49	THR
63	DW	11	ARG
45	DX	12	VAL
45	DX	19	ALA
46	DY	3	VAL
46	DY	27	VAL
46	DY	56	PRO
46	DY	77	PRO
46	DY	78	ALA
46	DY	99	CYS
47	DZ	119	GLU
47	DZ	166	SER
49	DH	83	GLU
50	DK	43	GLN
50	DK	71	ASN
52	D5	46	ASN
53	D6	4	HIS
53	D6	36	CYS
53	D6	57	VAL
54	D7	17	LYS
54	D7	19	ARG
54	D7	20	ASN
54	D7	28	ARG
54	D7	49	HIS
2	AA	233	SER
3	AC	52	LEU
3	AC	145	GLY
4	AD	5	ILE
4	AD	42	GLN
4	AD	44	GLY
9	AI	44	VAL
10	AJ	27	ALA
11	AK	49	GLY

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Mol	Chain	Res	Type
12	AL	29	GLY
12	AL	46	LYS
12	AL	121	GLY
13	AM	5	ALA
13	AM	63	THR
13	AM	66	LEU
13	AM	83	ASP
13	AM	106	ASN
14	AN	15	LYS
14	AN	16	PHE
15	AO	84	LYS
16	AP	81	ARG
17	AR	34	LYS
18	AS	45	SER
18	AS	55	ARG
20	AU	103	GLY
21	AW	9	ARG
2	BA	14	GLY
2	BA	77	ALA
24	BC	145	GLY
24	BC	156	ARG
24	BC	168	ALA
4	BD	4	TYR
4	BD	5	ILE
4	BD	14	ARG
4	BD	18	LYS
4	BD	44	GLY
6	BF	40	VAL
10	BJ	27	ALA
12	BL	29	GLY
12	BL	91	LYS
13	BM	6	GLY
13	BM	12	ASN
13	BM	29	ARG
13	BM	66	LEU
13	BM	106	ASN
13	BM	124	PRO
17	BR	49	GLU
19	BT	26	GLY
19	BT	29	ARG
19	BT	30	LEU
19	BT	67	VAL

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Mol	Chain	Res	Type
20	BU	97	ALA
20	BU	99	LEU
20	BU	103	GLY
28	CB	10	THR
28	CB	27	THR
28	CB	32	SER
28	CB	225	ALA
28	CB	267	SER
29	CC	72	VAL
29	CC	77	ILE
29	CC	130	GLY
30	CD	67	GLN
31	CE	52	ILE
32	CF	45	VAL
32	CF	56	SER
32	CF	92	ILE
32	CF	137	ASP
32	CF	138	LYS
33	CI	15	VAL
33	CI	85	GLU
35	CM	58	ASP
35	CM	133	GLN
36	CN	5	GLN
37	CO	11	GLY
37	CO	18	ARG
37	CO	34	GLY
37	CO	39	LYS
37	CO	65	ARG
37	CO	106	LEU
37	CO	111	ARG
38	CP	134	ARG
39	CQ	4	LEU
39	CQ	8	ARG
39	CQ	45	ARG
39	CQ	117	VAL
40	CR	14	VAL
40	CR	92	TYR
40	CR	94	TYR
40	CR	102	ALA
41	CS	35	LYS
41	CS	92	GLY
41	CS	93	ARG

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Mol	Chain	Res	Type
42	CT	93	LYS
43	CU	16	PRO
43	CU	23	GLU
43	CU	37	VAL
43	CU	49	THR
44	CW	63	ASP
45	CX	4	ALA
45	CX	11	PRO
46	CY	29	GLU
46	CY	90	LEU
47	CZ	52	SER
47	CZ	136	PHE
47	CZ	166	SER
49	CH	26	ARG
49	CH	45	ASN
49	CH	53	VAL
50	CK	43	GLN
50	CK	47	ASN
52	C5	61	VAL
53	C6	49	CYS
54	C7	16	CYS
54	C7	28	ARG
56	C9	34	TRP
62	DA	55	ASP
28	DB	26	LYS
28	DB	27	THR
28	DB	99	ASP
28	DB	246	PRO
28	DB	271	ILE
29	DC	69	LYS
29	DC	70	ALA
29	DC	71	GLY
29	DC	186	GLY
29	DC	189	PRO
30	DD	53	THR
30	DD	134	GLY
30	DD	206	ILE
31	DE	14	GLU
31	DE	126	ASP
31	DE	128	ARG
31	DE	129	GLY
32	DF	56	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	DF	81	GLU
32	DF	84	SER
33	DI	120	ILE
35	DM	58	ASP
36	DN	5	GLN
37	DO	40	SER
37	DO	42	SER
37	DO	67	MET
37	DO	98	GLU
37	DO	109	GLY
37	DO	111	ARG
38	DP	134	ARG
40	DR	15	ARG
40	DR	23	ARG
40	DR	85	VAL
40	DR	89	ARG
41	DS	35	LYS
41	DS	90	GLN
41	DS	92	GLY
41	DS	93	ARG
41	DS	126	ALA
43	DU	18	LEU
43	DU	37	VAL
63	DW	59	VAL
46	DY	10	GLY
46	DY	22	GLY
46	DY	80	GLY
46	DY	90	LEU
47	DZ	81	ARG
47	DZ	142	SER
47	DZ	152	ALA
47	DZ	163	LEU
48	Da	55	ARG
49	DH	53	VAL
49	DH	84	GLY
49	DH	85	LEU
49	DH	94	LEU
52	D5	54	LYS
52	D5	61	VAL
54	D7	16	CYS
54	D7	31	PRO
54	D7	33	LYS

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Mol	Chain	Res	Type
56	D9	34	TRP
2	AA	153	ARG
2	AA	183	PRO
3	AC	30	ARG
3	AC	154	SER
3	AC	165	THR
3	AC	179	ARG
3	AC	206	GLU
4	AD	14	ARG
4	AD	26	CYS
5	AE	153	LYS
6	AF	38	GLU
6	AF	40	VAL
8	AH	2	LEU
9	AI	41	VAL
10	AJ	58	ASP
10	AJ	59	SER
12	AL	27	LEU
13	AM	21	TYR
13	AM	90	LEU
14	AN	28	GLY
15	AO	21	ASP
16	AP	72	ARG
17	AR	49	GLU
2	BA	130	ARG
24	BC	4	LYS
24	BC	15	THR
24	BC	61	ALA
24	BC	81	GLY
5	BE	153	LYS
9	BI	105	ASP
11	BK	49	GLY
12	BL	115	LYS
17	BR	31	LEU
19	BT	28	LYS
21	BW	6	ARG
21	BW	9	ARG
27	CA	52	ARG
28	CB	3	VAL
28	CB	35	LYS
28	CB	210	GLY
28	CB	238	GLY

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Mol	Chain	Res	Type
29	CC	17	ASP
29	CC	54	GLN
29	CC	88	GLY
29	CC	89	ASP
29	CC	118	LYS
30	CD	7	TYR
30	CD	168	ARG
31	CE	50	ALA
32	CF	110	SER
32	CF	157	TYR
35	CM	47	ALA
35	CM	57	ALA
35	CM	59	LYS
37	CO	56	SER
37	CO	90	ARG
37	CO	103	ALA
37	CO	109	GLY
39	CQ	86	ARG
43	CU	22	VAL
43	CU	53	GLU
43	CU	79	VAL
44	CW	65	LEU
44	CW	112	GLY
46	CY	39	VAL
46	CY	62	GLU
46	CY	98	VAL
47	CZ	146	ILE
50	CK	69	ARG
51	CL	13	ILE
54	C7	18	ARG
54	C7	19	ARG
62	DA	52	ARG
28	DB	267	SER
29	DC	53	PRO
29	DC	77	ILE
29	DC	178	GLU
30	DD	3	GLU
30	DD	14	PRO
30	DD	26	ALA
30	DD	128	ALA
30	DD	167	ALA
30	DD	168	ARG

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Mol	Chain	Res	Type
31	DE	97	ASP
33	DI	115	ALA
35	DM	17	ASP
35	DM	57	ALA
35	DM	60	ILE
35	DM	135	PRO
37	DO	14	LYS
37	DO	17	LYS
37	DO	43	GLY
37	DO	47	ASP
37	DO	57	THR
37	DO	102	ARG
37	DO	108	LYS
37	DO	140	ALA
39	DQ	102	GLU
39	DQ	106	GLY
40	DR	24	LEU
40	DR	53	SER
40	DR	94	TYR
43	DU	22	VAL
43	DU	29	PRO
63	DW	63	ASP
63	DW	65	LEU
46	DY	39	VAL
46	DY	41	GLY
46	DY	53	PRO
46	DY	81	LYS
50	DK	44	LEU
50	DK	47	ASN
54	D7	18	ARG
56	D9	3	LYS
56	D9	31	HIS
3	AC	15	THR
5	AE	49	PRO
7	AG	131	LYS
9	AI	105	ASP
10	AJ	23	ILE
15	AO	24	SER
17	AR	33	GLY
18	AS	87	ARG
19	AT	44	MET
19	AT	47	HIS

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Mol	Chain	Res	Type
20	AU	48	LYS
20	AU	71	THR
20	AU	99	LEU
2	BA	83	MET
2	BA	84	GLU
2	BA	87	ARG
4	BD	12	CYS
10	BJ	23	ILE
12	BL	46	LYS
12	BL	47	LYS
12	BL	62	SER
13	BM	107	ALA
18	BS	41	LYS
28	CB	11	PRO
28	CB	58	HIS
28	CB	244	ARG
29	CC	69	LYS
29	CC	144	ARG
30	CD	14	PRO
30	CD	25	PRO
31	CE	43	LEU
31	CE	81	LYS
31	CE	104	GLU
31	CE	126	ASP
32	CF	81	GLU
32	CF	158	HIS
33	CI	120	ILE
37	CO	48	PRO
37	CO	108	LYS
37	CO	132	LYS
37	CO	141	ALA
39	CQ	67	LEU
40	CR	53	SER
40	CR	107	GLU
41	CS	27	THR
41	CS	88	ILE
43	CU	29	PRO
43	CU	31	ALA
44	CW	93	ALA
45	CX	10	ALA
45	CX	13	LEU
46	CY	24	VAL

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Mol	Chain	Res	Type
46	CY	81	LYS
47	CZ	92	SER
47	CZ	142	SER
47	CZ	165	VAL
47	CZ	168	GLU
48	Ca	13	GLY
49	CH	52	ARG
49	CH	84	GLY
50	CK	18	PRO
52	C5	46	ASN
52	C5	54	LYS
54	C7	17	LYS
54	C7	33	LYS
54	C7	41	PRO
28	DB	28	GLU
28	DB	242	ARG
28	DB	245	PRO
29	DC	45	THR
29	DC	64	LYS
31	DE	96	ARG
33	DI	12	LEU
33	DI	70	GLU
35	DM	133	GLN
37	DO	37	GLY
37	DO	48	PRO
37	DO	61	ARG
37	DO	147	LEU
38	DP	27	VAL
40	DR	19	LYS
40	DR	82	ILE
41	DS	31	SER
42	DT	86	ALA
63	DW	9	TYR
46	DY	7	VAL
46	DY	24	VAL
46	DY	29	GLU
47	DZ	168	GLU
47	DZ	177	PRO
54	D7	44	ARG
2	AA	14	GLY
2	AA	84	GLU
2	AA	130	ARG

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Mol	Chain	Res	Type
2	AA	152	PHE
3	AC	81	GLY
5	AE	17	ALA
7	AG	153	HIS
9	AI	89	ASN
18	AS	31	LEU
18	AS	36	ASN
19	AT	67	VAL
2	BA	19	HIS
2	BA	153	ARG
4	BD	13	ARG
5	BE	8	GLU
5	BE	146	ALA
9	BI	42	ARG
10	BJ	58	ASP
11	BK	62	GLN
11	BK	67	ASP
12	BL	51	ALA
15	BO	24	SER
28	CB	239	ARG
29	CC	60	ASN
29	CC	90	THR
31	CE	10	LYS
31	CE	84	LYS
31	CE	129	GLY
32	CF	49	VAL
37	CO	38	GLN
37	CO	140	ALA
37	CO	147	LEU
38	CP	27	VAL
39	CQ	14	SER
41	CS	12	SER
41	CS	31	SER
41	CS	41	ARG
41	CS	68	TYR
43	CU	18	LEU
44	CW	6	ILE
45	CX	22	ALA
46	CY	53	PRO
46	CY	67	LEU
50	CK	44	LEU
28	DB	3	VAL

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Mol	Chain	Res	Type
28	DB	127	VAL
28	DB	239	ARG
28	DB	257	LEU
29	DC	89	ASP
29	DC	129	HIS
31	DE	53	LEU
31	DE	115	ARG
32	DF	85	LYS
32	DF	127	GLU
32	DF	158	HIS
37	DO	12	ALA
37	DO	38	GLN
38	DP	136	ALA
41	DS	85	LYS
42	DT	92	ARG
42	DT	97	ASP
43	DU	3	ALA
43	DU	48	GLY
63	DW	6	ILE
46	DY	38	ILE
47	DZ	80	ARG
56	D9	52	LYS
2	AA	19	HIS
3	AC	20	SER
3	AC	168	ALA
15	AO	85	LEU
16	AP	16	HIS
19	AT	30	LEU
19	AT	73	GLU
2	BA	48	MET
2	BA	233	SER
24	BC	8	ILE
4	BD	172	PRO
5	BE	21	ALA
12	BL	19	ARG
27	CA	68	LEU
29	CC	64	LYS
30	CD	84	VAL
32	CF	85	LYS
33	CI	78	THR
39	CQ	106	GLY
40	CR	103	GLU

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Mol	Chain	Res	Type
44	CW	91	GLY
46	CY	37	VAL
47	CZ	177	PRO
56	C9	3	LYS
62	DA	64	LEU
28	DB	211	ARG
28	DB	244	ARG
29	DC	138	PRO
30	DD	9	ILE
30	DD	58	ALA
31	DE	45	GLU
33	DI	78	THR
33	DI	144	VAL
37	DO	34	GLY
40	DR	57	LYS
41	DS	41	ARG
42	DT	99	ALA
43	DU	35	LEU
43	DU	52	VAL
53	D6	56	LYS
54	D7	45	LYS
3	AC	66	VAL
4	AD	28	SER
13	AM	6	GLY
10	BJ	90	LEU
27	CA	60	GLY
28	CB	245	PRO
30	CD	206	ILE
32	CF	126	PRO
36	CN	4	PRO
29	DC	75	VAL
32	DF	24	VAL
32	DF	93	GLY
35	DM	36	GLY
56	D9	53	PRO
4	AD	171	GLY
13	AM	100	GLY
9	BI	44	VAL
27	CA	90	GLY
28	CB	28	GLU
33	CI	7	GLU
41	CS	30	VAL

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Mol	Chain	Res	Type
47	CZ	128	VAL
47	CZ	147	GLY
49	CH	28	GLY
28	DB	35	LYS
28	DB	236	GLY
43	DU	79	VAL
46	DY	98	VAL
49	DH	28	GLY
51	DL	2	PRO
51	DL	13	ILE
8	AH	73	ASP
12	AL	90	VAL
13	AM	10	PRO
18	AS	65	ILE
20	AU	96	GLY
32	CF	20	ALA
33	CI	111	PRO
37	CO	23	PRO
40	CR	85	VAL
46	CY	80	GLY
40	DR	90	GLY
41	DS	81	PRO
3	AC	195	VAL
13	AM	7	VAL
14	BN	13	THR
30	CD	24	LEU
31	CE	142	PRO
32	CF	21	PRO
32	CF	39	PRO
29	DC	29	GLY
32	DF	49	VAL
37	DO	63	PRO
40	DR	14	VAL
42	DT	90	VAL
46	DY	37	VAL
47	DZ	139	VAL
2	AA	72	GLY
46	CY	31	LEU
33	DI	92	VAL



### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AA	202/202 (100%)	180 (89%)	22 (11%)	6	23
2	BA	202/202 (100%)	181 (90%)	21 (10%)	7	25
3	AC	160/187 (86%)	142 (89%)	18 (11%)	6	21
4	AD	180/180 (100%)	162 (90%)	18 (10%)	7	27
4	BD	180/180 (100%)	160 (89%)	20 (11%)	6	22
5	AE	115/115 (100%)	101 (88%)	14 (12%)	5	18
5	BE	115/115 (100%)	102 (89%)	13 (11%)	6	21
6	AF	90/90 (100%)	85 (94%)	5 (6%)	21	51
6	BF	90/90 (100%)	86 (96%)	4 (4%)	28	58
7	AG	126/126 (100%)	113 (90%)	13 (10%)	7	26
7	BG	126/126 (100%)	114 (90%)	12 (10%)	8	29
8	AH	119/119 (100%)	104 (87%)	15 (13%)	4	17
8	BH	119/119 (100%)	104 (87%)	15 (13%)	4	17
9	AI	98/98 (100%)	82 (84%)	16 (16%)	2	9
9	BI	98/98 (100%)	88 (90%)	10 (10%)	7	26
10	AJ	88/88 (100%)	77 (88%)	11 (12%)	4	17
10	BJ	88/88 (100%)	77 (88%)	11 (12%)	4	17
11	AK	90/90 (100%)	82 (91%)	8 (9%)	9	33
11	BK	90/90 (100%)	82 (91%)	8 (9%)	9	33
12	AL	104/104 (100%)	87 (84%)	17 (16%)	2	9
12	BL	104/104 (100%)	88 (85%)	16 (15%)	2	11
13	AM	99/99 (100%)	87 (88%)	12 (12%)	5	18
13	BM	99/99 (100%)	82 (83%)	17 (17%)	2	8
14	AN	49/49 (100%)	45 (92%)	4 (8%)	11	37
14	BN	49/49 (100%)	43 (88%)	6 (12%)	5	18
15	AO	79/79 (100%)	75 (95%)	4 (5%)	24	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	BO	79/79 (100%)	72 (91%)	7 (9%)	9	33
16	AP	72/72 (100%)	65 (90%)	7 (10%)	8	28
16	BP	72/72 (100%)	62 (86%)	10 (14%)	3	13
17	AR	94/94 (100%)	90 (96%)	4 (4%)	29	59
17	BR	94/94 (100%)	87 (93%)	7 (7%)	13	42
18	AS	61/61 (100%)	56 (92%)	5 (8%)	11	37
18	BS	61/61 (100%)	53 (87%)	8 (13%)	4	15
19	AT	69/69 (100%)	55 (80%)	14 (20%)	1	3
19	BT	69/69 (100%)	54 (78%)	15 (22%)	1	3
20	AU	76/76 (100%)	68 (90%)	8 (10%)	7	25
20	BU	76/76 (100%)	63 (83%)	13 (17%)	2	8
21	AW	19/19 (100%)	17 (90%)	2 (10%)	7	25
21	BW	19/19 (100%)	17 (90%)	2 (10%)	7	25
24	BC	160/160 (100%)	141 (88%)	19 (12%)	5	19
27	CA	61/74 (82%)	53 (87%)	8 (13%)	4	15
28	CB	213/213 (100%)	179 (84%)	34 (16%)	2	10
28	DB	213/213 (100%)	179 (84%)	34 (16%)	2	10
29	CC	165/165 (100%)	137 (83%)	28 (17%)	2	8
29	DC	165/165 (100%)	142 (86%)	23 (14%)	3	13
30	CD	165/165 (100%)	139 (84%)	26 (16%)	2	10
30	DD	165/165 (100%)	139 (84%)	26 (16%)	2	10
31	CE	155/155 (100%)	140 (90%)	15 (10%)	8	28
31	DE	155/155 (100%)	123 (79%)	32 (21%)	1	3
32	CF	132/132 (100%)	113 (86%)	19 (14%)	3	13
32	DF	132/132 (100%)	110 (83%)	22 (17%)	2	8
33	CI	122/122 (100%)	109 (89%)	13 (11%)	6	24
33	DI	122/122 (100%)	110 (90%)	12 (10%)	8	28
35	CM	117/117 (100%)	96 (82%)	21 (18%)	2	6
35	DM	117/117 (100%)	95 (81%)	22 (19%)	1	4
36	CN	100/100 (100%)	84 (84%)	16 (16%)	2	10
36	DN	100/100 (100%)	88 (88%)	12 (12%)	5	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	CO	112/112 (100%)	82 (73%)	30 (27%)	0	1
37	DO	112/112 (100%)	83 (74%)	29 (26%)	0	2
38	CP	111/111 (100%)	99 (89%)	12 (11%)	6	24
38	DP	111/111 (100%)	97 (87%)	14 (13%)	4	17
39	CQ	100/100 (100%)	81 (81%)	19 (19%)	1	4
39	DQ	100/100 (100%)	83 (83%)	17 (17%)	2	8
40	CR	77/77 (100%)	60 (78%)	17 (22%)	1	2
40	DR	77/77 (100%)	58 (75%)	19 (25%)	0	2
41	CS	120/120 (100%)	92 (77%)	28 (23%)	1	2
41	DS	120/120 (100%)	100 (83%)	20 (17%)	2	8
42	CT	92/92 (100%)	79 (86%)	13 (14%)	3	13
42	DT	92/92 (100%)	81 (88%)	11 (12%)	5	19
43	CU	82/82 (100%)	69 (84%)	13 (16%)	2	10
43	DU	82/82 (100%)	61 (74%)	21 (26%)	0	2
44	CW	91/92 (99%)	82 (90%)	9 (10%)	8	27
45	CX	74/74 (100%)	63 (85%)	11 (15%)	3	12
45	DX	74/74 (100%)	60 (81%)	14 (19%)	1	4
46	CY	84/84 (100%)	67 (80%)	17 (20%)	1	3
46	DY	84/84 (100%)	68 (81%)	16 (19%)	1	4
47	CZ	155/155 (100%)	142 (92%)	13 (8%)	11	36
47	DZ	155/155 (100%)	136 (88%)	19 (12%)	4	17
48	Ca	66/66 (100%)	57 (86%)	9 (14%)	3	14
48	Da	66/66 (100%)	56 (85%)	10 (15%)	3	11
49	CH	78/78 (100%)	56 (72%)	22 (28%)	0	1
49	DH	78/78 (100%)	62 (80%)	16 (20%)	1	3
50	CK	66/66 (100%)	55 (83%)	11 (17%)	2	8
50	DK	66/66 (100%)	53 (80%)	13 (20%)	1	4
51	CL	51/51 (100%)	49 (96%)	2 (4%)	32	61
51	DL	51/51 (100%)	48 (94%)	3 (6%)	19	49
52	C5	27/27 (100%)	24 (89%)	3 (11%)	6	22
52	D5	27/27 (100%)	21 (78%)	6 (22%)	1	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
53	C6	51/51 (100%)	43 (84%)	8 (16%)	2	10
53	D6	51/51 (100%)	42 (82%)	9 (18%)	2	6
54	C7	43/43 (100%)	36 (84%)	7 (16%)	2	9
54	D7	43/43 (100%)	35 (81%)	8 (19%)	1	5
55	C8	41/41 (100%)	37 (90%)	4 (10%)	8	28
55	D8	41/41 (100%)	32 (78%)	9 (22%)	1	3
56	C9	53/53 (100%)	40 (76%)	13 (24%)	0	2
56	D9	53/53 (100%)	43 (81%)	10 (19%)	1	4
57	C0	33/33 (100%)	30 (91%)	3 (9%)	9	32
57	D0	33/33 (100%)	27 (82%)	6 (18%)	1	6
62	DA	61/74 (82%)	53 (87%)	8 (13%)	4	15
63	DW	91/91 (100%)	86 (94%)	5 (6%)	21	51
All	All	9654/9708 (99%)	8293 (86%)	1361 (14%)	3	13

All (1361) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	AA	11	LEU
2	AA	20	GLU
2	AA	36	ARG
2	AA	42	ILE
2	AA	46	LYS
2	AA	63	MET
2	AA	98	LEU
2	AA	101	MET
2	AA	107	THR
2	AA	119	GLU
2	AA	130	ARG
2	AA	137	ARG
2	AA	145	LEU
2	AA	172	ILE
2	AA	178	ARG
2	AA	187	LEU
2	AA	195	ASP
2	AA	196	LEU
2	AA	206	ASP
2	AA	221	LEU
2	AA	236	TYR

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Mol	Chain	Res	Type
2	AA	238	LEU
3	AC	5	ILE
3	AC	16	ARG
3	AC	17	ASP
3	AC	20	SER
3	AC	22	TRP
3	AC	23	TYR
3	AC	27	LYS
3	AC	34	LEU
3	AC	37	GLN
3	AC	42	LEU
3	AC	44	GLU
3	AC	89	GLU
3	AC	104	GLN
3	AC	107	GLN
3	AC	127	ARG
3	AC	170	GLN
3	AC	192	THR
3	AC	202	ILE
4	AD	3	ARG
4	AD	8	VAL
4	AD	10	ARG
4	AD	11	LEU
4	AD	15	GLU
4	AD	31	CYS
4	AD	36	ARG
4	AD	47	ARG
4	AD	50	ARG
4	AD	58	LEU
4	AD	86	LYS
4	AD	110	PHE
4	AD	132	ARG
4	AD	135	LEU
4	AD	168	ARG
4	AD	170	VAL
4	AD	187	ARG
4	AD	200	GLU
5	AE	10	MET
5	AE	12	LEU
5	AE	20	GLN
5	AE	24	ARG
5	AE	27	ARG

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Mol	Chain	Res	Type
5	AE	31	LEU
5	AE	41	VAL
5	AE	53	LEU
5	AE	72	GLN
5	AE	79	GLU
5	AE	91	LEU
5	AE	101	ILE
5	AE	116	THR
5	AE	147	ASP
6	AF	15	ASP
6	AF	40	VAL
6	AF	77	ARG
6	AF	81	ILE
6	AF	98	LEU
7	AG	4	ARG
7	AG	6	ARG
7	AG	13	GLN
7	AG	32	ARG
7	AG	41	ARG
7	AG	54	THR
7	AG	60	LYS
7	AG	63	LYS
7	AG	86	GLN
7	AG	104	LEU
7	AG	114	ARG
7	AG	137	LYS
7	AG	146	GLU
8	AH	1	MET
8	AH	2	LEU
8	AH	23	SER
8	AH	25	ASP
8	AH	30	ARG
8	AH	52	ASP
8	AH	60	ARG
8	AH	83	ILE
8	AH	85	ARG
8	AH	91	ARG
8	AH	98	LYS
8	AH	102	ARG
8	AH	112	LEU
8	AH	116	LYS
8	AH	119	LEU

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Mol	Chain	Res	Type
9	AI	4	TYR
9	AI	10	ARG
9	AI	40	LEU
9	AI	42	ARG
9	AI	78	LYS
9	AI	79	LEU
9	AI	89	ASN
9	AI	95	LYS
9	AI	102	LEU
9	AI	103	THR
9	AI	112	LYS
9	AI	114	TYR
9	AI	121	ARG
9	AI	125	TYR
9	AI	126	SER
9	AI	128	ARG
10	AJ	19	SER
10	AJ	22	LYS
10	AJ	49	VAL
10	AJ	50	ILE
10	AJ	55	LYS
10	AJ	59	SER
10	AJ	62	HIS
10	AJ	69	ASN
10	AJ	79	ARG
10	AJ	96	ILE
10	AJ	98	ILE
11	AK	28	THR
11	AK	30	VAL
11	AK	51	LYS
11	AK	87	THR
11	AK	119	CYS
11	AK	124	LYS
11	AK	125	PHE
11	AK	126	ARG
12	AL	7	ILE
12	AL	17	LYS
12	AL	20	LYS
12	AL	41	ARG
12	AL	42	THR
12	AL	43	VAL
12	AL	47	LYS

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Mol	Chain	Res	Type
12	AL	49	ASN
12	AL	53	ARG
12	AL	55	VAL
12	AL	57	LYS
12	AL	62	SER
12	AL	85	ILE
12	AL	89	ARG
12	AL	102	ARG
12	AL	115	LYS
12	AL	126	LYS
13	AM	32	GLU
13	AM	35	GLU
13	AM	47	ASP
13	AM	56	LEU
13	AM	64	TRP
13	AM	70	LEU
13	AM	79	LYS
13	AM	82	MET
13	AM	93	ARG
13	AM	108	ARG
13	AM	115	LYS
13	AM	120	LYS
14	AN	33	VAL
14	AN	40	CYS
14	AN	41	ARG
14	AN	44	LEU
15	AO	51	HIS
15	AO	65	ARG
15	AO	82	ILE
15	AO	88	ARG
16	AP	1	MET
16	AP	2	VAL
16	AP	16	HIS
16	AP	21	VAL
16	AP	55	ARG
16	AP	67	THR
16	AP	69	THR
17	AR	9	VAL
17	AR	38	ARG
17	AR	52	LYS
17	AR	74	LEU
18	AS	31	LEU

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Mol	Chain	Res	Type
18	AS	32	ARG
18	AS	47	THR
18	AS	61	LYS
18	AS	82	THR
19	AT	6	LYS
19	AT	7	LYS
19	AT	13	ASP
19	AT	15	LEU
19	AT	22	LEU
19	AT	27	GLU
19	AT	29	ARG
19	AT	37	ARG
19	AT	44	MET
19	AT	56	GLN
19	AT	65	ASN
19	AT	67	VAL
19	AT	70	LYS
19	AT	80	TYR
20	AU	26	ASN
20	AU	36	LEU
20	AU	42	GLN
20	AU	45	GLN
20	AU	54	LYS
20	AU	73	HIS
20	AU	84	LEU
20	AU	93	GLU
21	AW	12	LYS
21	AW	24	ARG
2	BA	17	PHE
2	BA	30	ARG
2	BA	36	ARG
2	BA	69	LEU
2	BA	76	GLN
2	BA	87	ARG
2	BA	107	THR
2	BA	117	GLU
2	BA	133	LYS
2	BA	137	ARG
2	BA	145	LEU
2	BA	172	ILE
2	BA	178	ARG
2	BA	179	LYS

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Mol	Chain	Res	Type
2	BA	187	LEU
2	BA	195	ASP
2	BA	196	LEU
2	BA	204	ASN
2	BA	206	ASP
2	BA	221	LEU
2	BA	238	LEU
24	BC	5	ILE
24	BC	14	ILE
24	BC	16	ARG
24	BC	17	ASP
24	BC	21	ARG
24	BC	26	LYS
24	BC	27	LYS
24	BC	29	TYR
24	BC	34	LEU
24	BC	37	GLN
24	BC	44	GLU
24	BC	94	LEU
24	BC	98	ASN
24	BC	127	ARG
24	BC	132	ARG
24	BC	167	TRP
24	BC	190	ARG
24	BC	202	ILE
24	BC	207	VAL
4	BD	3	ARG
4	BD	9	CYS
4	BD	10	ARG
4	BD	11	LEU
4	BD	33	MET
4	BD	36	ARG
4	BD	53	ASP
4	BD	58	LEU
4	BD	77	ASN
4	BD	80	GLU
4	BD	86	LYS
4	BD	96	LEU
4	BD	108	LEU
4	BD	110	PHE
4	BD	131	ARG
4	BD	132	ARG

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Mol	Chain	Res	Type
4	BD	135	LEU
4	BD	168	ARG
4	BD	200	GLU
4	BD	209	ARG
5	BE	10	MET
5	BE	12	LEU
5	BE	20	GLN
5	BE	24	ARG
5	BE	25	ARG
5	BE	41	VAL
5	BE	47	LYS
5	BE	53	LEU
5	BE	64	ARG
5	BE	72	GLN
5	BE	79	GLU
5	BE	100	VAL
5	BE	101	ILE
6	BF	40	VAL
6	BF	64	GLN
6	BF	70	ASP
6	BF	98	LEU
7	BG	5	ARG
7	BG	63	LYS
7	BG	75	VAL
7	BG	94	ARG
7	BG	104	LEU
7	BG	113	GLU
7	BG	114	ARG
7	BG	118	VAL
7	BG	126	ASP
7	BG	136	LYS
7	BG	137	LYS
7	BG	148	ASN
8	BH	1	MET
8	BH	3	THR
8	BH	26	VAL
8	BH	41	ARG
8	BH	45	ILE
8	BH	50	ARG
8	BH	52	ASP
8	BH	60	ARG
8	BH	63	LEU

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Mol	Chain	Res	Type
8	BH	70	GLN
8	BH	80	ILE
8	BH	98	LYS
8	BH	102	ARG
8	BH	112	LEU
8	BH	137	VAL
9	BI	4	TYR
9	BI	10	ARG
9	BI	42	ARG
9	BI	47	LEU
9	BI	95	LYS
9	BI	105	ASP
9	BI	112	LYS
9	BI	114	TYR
9	BI	121	ARG
9	BI	128	ARG
10	BJ	16	LEU
10	BJ	22	LYS
10	BJ	43	ARG
10	BJ	46	ARG
10	BJ	49	VAL
10	BJ	50	ILE
10	BJ	62	HIS
10	BJ	74	ILE
10	BJ	86	MET
10	BJ	96	ILE
10	BJ	98	ILE
11	BK	29	ILE
11	BK	79	SER
11	BK	87	THR
11	BK	117	ASN
11	BK	119	CYS
11	BK	124	LYS
11	BK	126	ARG
11	BK	129	SER
12	BL	13	LYS
12	BL	18	VAL
12	BL	19	ARG
12	BL	20	LYS
12	BL	21	LYS
12	BL	36	VAL
12	BL	41	ARG

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Mol	Chain	Res	Type
12	BL	45	PRO
12	BL	47	LYS
12	BL	53	ARG
12	BL	62	SER
12	BL	85	ILE
12	BL	89	ARG
12	BL	92	ASP
12	BL	102	ARG
12	BL	113	ARG
13	BM	11	ARG
13	BM	32	GLU
13	BM	47	ASP
13	BM	56	LEU
13	BM	64	TRP
13	BM	79	LYS
13	BM	82	MET
13	BM	93	ARG
13	BM	94	ARG
13	BM	101	GLN
13	BM	108	ARG
13	BM	114	ARG
13	BM	115	LYS
13	BM	117	VAL
13	BM	120	LYS
13	BM	121	LYS
13	BM	122	LYS
14	BN	3	ARG
14	BN	13	THR
14	BN	27	CYS
14	BN	32	SER
14	BN	41	ARG
14	BN	44	LEU
15	BO	10	LYS
15	BO	39	LEU
15	BO	41	GLU
15	BO	48	LYS
15	BO	65	ARG
15	BO	82	ILE
15	BO	88	ARG
16	BP	2	VAL
16	BP	12	LYS
16	BP	27	LYS

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Mol	Chain	Res	Type
16	BP	28	ARG
16	BP	32	TYR
16	BP	47	ASP
16	BP	54	GLU
16	BP	55	ARG
16	BP	67	THR
16	BP	69	THR
17	BR	9	VAL
17	BR	11	VAL
17	BR	35	VAL
17	BR	49	GLU
17	BR	52	LYS
17	BR	60	ILE
17	BR	74	LEU
18	BS	31	LEU
18	BS	32	ARG
18	BS	41	LYS
18	BS	47	THR
18	BS	65	ILE
18	BS	68	LYS
18	BS	82	THR
18	BS	87	ARG
19	BT	5	LEU
19	BT	6	LYS
19	BT	7	LYS
19	BT	13	ASP
19	BT	17	GLU
19	BT	27	GLU
19	BT	29	ARG
19	BT	37	ARG
19	BT	44	MET
19	BT	60	VAL
19	BT	64	GLU
19	BT	67	VAL
19	BT	70	LYS
19	BT	77	THR
19	BT	79	THR
20	BU	10	LEU
20	BU	21	LYS
20	BU	26	ASN
20	BU	30	LYS
20	BU	38	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
20	BU	42	GLN
20	BU	54	LYS
20	BU	58	LYS
20	BU	62	LEU
20	BU	73	HIS
20	BU	75	ASN
20	BU	84	LEU
20	BU	93	GLU
21	BW	10	ARG
21	BW	12	LYS
27	CA	21	THR
27	CA	23	ASP
27	CA	36	LYS
27	CA	50	ASP
27	CA	53	ARG
27	CA	56	GLN
27	CA	58	VAL
27	CA	63	SER
28	CB	10	THR
28	CB	13	ARG
28	CB	20	ASP
28	CB	23	GLU
28	CB	24	ILE
28	CB	25	THR
28	CB	26	LYS
28	CB	33	LEU
28	CB	35	LYS
28	CB	46	GLN
28	CB	49	ILE
28	CB	61	LEU
28	CB	64	ILE
28	CB	65	ILE
28	CB	92	ILE
28	CB	94	LEU
28	CB	98	VAL
28	CB	103	ARG
28	CB	111	LEU
28	CB	116	GLN
28	CB	138	VAL
28	CB	147	LEU
28	CB	166	GLN
28	CB	168	ARG

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Mol	Chain	Res	Type
28	CB	173	VAL
28	CB	192	THR
28	CB	211	ARG
28	CB	212	SER
28	CB	218	ARG
28	CB	229	VAL
28	CB	257	LEU
28	CB	259	THR
28	CB	260	ARG
28	CB	271	ILE
29	CC	16	ARG
29	CC	17	ASP
29	CC	18	ASP
29	CC	33	VAL
29	CC	34	VAL
29	CC	52	LEU
29	CC	54	GLN
29	CC	55	ASN
29	CC	57	LYS
29	CC	58	ARG
29	CC	63	LEU
29	CC	64	LYS
29	CC	67	PHE
29	CC	76	ARG
29	CC	78	LEU
29	CC	79	ARG
29	CC	82	ARG
29	CC	107	THR
29	CC	117	MET
29	CC	119	ARG
29	CC	128	SER
29	CC	144	ARG
29	CC	152	LYS
29	CC	175	VAL
29	CC	196	VAL
29	CC	197	ILE
29	CC	202	LYS
29	CC	203	LYS
30	CD	2	LYS
30	CD	20	LEU
30	CD	23	ASP
30	CD	24	LEU

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Mol	Chain	Res	Type
30	CD	28	ILE
30	CD	33	LEU
30	CD	38	ARG
30	CD	43	LYS
30	CD	65	TRP
30	CD	66	PRO
30	CD	74	ARG
30	CD	83	PHE
30	CD	110	LEU
30	CD	125	LEU
30	CD	137	LYS
30	CD	140	LEU
30	CD	165	ARG
30	CD	169	ASN
30	CD	170	LEU
30	CD	179	GLU
30	CD	183	VAL
30	CD	191	ARG
30	CD	192	LEU
30	CD	197	ASP
30	CD	199	TRP
30	CD	206	ILE
31	CE	5	VAL
31	CE	16	ARG
31	CE	22	ARG
31	CE	34	LEU
31	CE	36	LYS
31	CE	39	ILE
31	CE	59	GLU
31	CE	80	PHE
31	CE	96	ARG
31	CE	97	ASP
31	CE	98	ARG
31	CE	116	ASP
31	CE	152	LEU
31	CE	155	MET
31	CE	159	VAL
32	CF	13	LYS
32	CF	34	GLU
32	CF	40	GLU
32	CF	53	GLU
32	CF	54	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	CF	71	LEU
32	CF	84	SER
32	CF	86	GLU
32	CF	89	ILE
32	CF	111	HIS
32	CF	119	GLU
32	CF	122	THR
32	CF	143	GLN
32	CF	149	ARG
32	CF	153	LYS
32	CF	155	SER
32	CF	157	TYR
32	CF	162	ILE
32	CF	170	ARG
33	CI	12	LEU
33	CI	20	ASP
33	CI	35	LEU
33	CI	41	GLU
33	CI	61	ARG
33	CI	77	LEU
33	CI	86	THR
33	CI	87	LYS
33	CI	99	GLU
33	CI	109	ILE
33	CI	114	LEU
33	CI	123	LEU
33	CI	129	THR
35	CM	4	TYR
35	CM	5	VAL
35	CM	19	GLU
35	CM	33	LEU
35	CM	34	LEU
35	CM	39	ARG
35	CM	43	THR
35	CM	45	ASN
35	CM	48	MET
35	CM	55	VAL
35	CM	56	ASN
35	CM	60	ILE
35	CM	63	THR
35	CM	65	LYS
35	CM	87	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
35	CM	97	ARG
35	CM	99	LEU
35	CM	109	LYS
35	CM	121	LYS
35	CM	131	GLN
35	CM	134	ARG
36	CN	7	TYR
36	CN	8	LEU
36	CN	20	MET
36	CN	24	VAL
36	CN	28	SER
36	CN	32	TYR
36	CN	49	ARG
36	CN	66	LYS
36	CN	70	LYS
36	CN	73	ASP
36	CN	85	VAL
36	CN	92	GLU
36	CN	98	VAL
36	CN	99	PHE
36	CN	108	GLU
36	CN	117	LEU
37	CO	6	LEU
37	CO	13	ASN
37	CO	16	ARG
37	CO	27	HIS
37	CO	30	THR
37	CO	32	THR
37	CO	38	GLN
37	CO	39	LYS
37	CO	41	ARG
37	CO	45	LEU
37	CO	52	GLU
37	CO	56	SER
37	CO	57	THR
37	CO	59	LEU
37	CO	61	ARG
37	CO	62	LEU
37	CO	64	LYS
37	CO	67	MET
37	CO	70	GLN
37	CO	81	GLN

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Mol	Chain	Res	Type
37	CO	84	ASN
37	CO	85	LEU
37	CO	95	VAL
37	CO	98	GLU
37	CO	105	LEU
37	CO	107	LYS
37	CO	108	LYS
37	CO	114	ILE
37	CO	125	VAL
37	CO	130	PHE
38	CP	5	ARG
38	CP	16	ARG
38	CP	18	LYS
38	CP	21	THR
38	CP	45	GLN
38	CP	58	PHE
38	CP	67	ARG
38	CP	75	THR
38	CP	76	LYS
38	CP	79	LEU
38	CP	110	THR
38	CP	131	ILE
39	CQ	2	ARG
39	CQ	8	ARG
39	CQ	18	LEU
39	CQ	28	LEU
39	CQ	29	LEU
39	CQ	33	ARG
39	CQ	35	THR
39	CQ	44	LEU
39	CQ	54	LEU
39	CQ	63	ARG
39	CQ	67	LEU
39	CQ	71	GLN
39	CQ	74	LYS
39	CQ	79	LEU
39	CQ	90	ARG
39	CQ	95	THR
39	CQ	99	LYS
39	CQ	100	LEU
39	CQ	105	ARG
40	CR	11	LYS

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Mol	Chain	Res	Type
40	CR	13	ARG
40	CR	17	ARG
40	CR	20	ARG
40	CR	21	THR
40	CR	25	ARG
40	CR	30	ARG
40	CR	33	LYS
40	CR	36	TYR
40	CR	44	LYS
40	CR	56	LEU
40	CR	73	LEU
40	CR	89	ARG
40	CR	92	TYR
40	CR	97	ARG
40	CR	106	ARG
40	CR	107	GLU
41	CS	6	LEU
41	CS	9	LEU
41	CS	13	ARG
41	CS	17	THR
41	CS	24	PRO
41	CS	29	ARG
41	CS	32	TYR
41	CS	35	LYS
41	CS	38	ASN
41	CS	41	ARG
41	CS	58	ASN
41	CS	59	THR
41	CS	63	VAL
41	CS	67	SER
41	CS	74	ARG
41	CS	78	LEU
41	CS	82	LEU
41	CS	83	ILE
41	CS	85	LYS
41	CS	89	VAL
41	CS	98	LYS
41	CS	99	LEU
41	CS	106	SER
41	CS	107	ASP
41	CS	108	ARG
41	CS	113	LYS

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Mol	Chain	Res	Type
41	CS	125	ARG
41	CS	128	GLU
42	CT	8	VAL
42	CT	17	ILE
42	CT	33	ARG
42	CT	34	LYS
42	CT	52	ARG
42	CT	60	LEU
42	CT	66	ASN
42	CT	74	LEU
42	CT	77	SER
42	CT	83	LEU
42	CT	101	ARG
42	CT	102	GLU
42	CT	108	GLU
43	CU	2	PHE
43	CU	13	ARG
43	CU	18	LEU
43	CU	19	LYS
43	CU	39	LEU
43	CU	40	LEU
43	CU	44	LYS
43	CU	45	THR
43	CU	46	VAL
43	CU	49	THR
43	CU	91	TYR
43	CU	95	LEU
43	CU	99	ILE
44	CW	11	ARG
44	CW	19	LEU
44	CW	20	VAL
44	CW	23	LEU
44	CW	52	GLU
44	CW	67	ASP
44	CW	76	VAL
44	CW	98	LYS
44	CW	107	LEU
45	CX	15	GLU
45	CX	23	GLU
45	CX	27	THR
45	CX	48	LYS
45	CX	52	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
45	CX	57	LEU
45	CX	68	ARG
45	CX	70	LEU
45	CX	73	ARG
45	CX	76	ARG
45	CX	80	ILE
46	CY	2	ARG
46	CY	7	VAL
46	CY	14	LEU
46	CY	28	LYS
46	CY	34	LYS
46	CY	46	LYS
46	CY	50	ARG
46	CY	55	TYR
46	CY	56	PRO
46	CY	61	ILE
46	CY	62	GLU
46	CY	71	LYS
46	CY	76	CYS
46	CY	83	THR
46	CY	89	PHE
46	CY	96	ILE
46	CY	97	ARG
47	CZ	3	TYR
47	CZ	5	LEU
47	CZ	6	LYS
47	CZ	8	TYR
47	CZ	11	GLU
47	CZ	36	LYS
47	CZ	41	LEU
47	CZ	46	LYS
47	CZ	80	ARG
47	CZ	81	ARG
47	CZ	89	PHE
47	CZ	155	LEU
47	CZ	166	SER
48	Ca	5	LYS
48	Ca	11	ARG
48	Ca	12	ASN
48	Ca	19	LYS
48	Ca	20	ARG
48	Ca	36	ILE

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Mol	Chain	Res	Type
48	Ca	41	ARG
48	Ca	74	ARG
48	Ca	84	LEU
49	CH	3	LYS
49	CH	17	SER
49	CH	38	SER
49	CH	39	LYS
49	CH	40	ARG
49	CH	41	ARG
49	CH	45	ASN
49	CH	46	LEU
49	CH	48	LYS
49	CH	57	GLU
49	CH	58	ILE
49	CH	59	THR
49	CH	61	ARG
49	CH	68	PRO
49	CH	69	LYS
49	CH	72	GLU
49	CH	75	GLU
49	CH	80	LEU
49	CH	82	LEU
49	CH	88	LYS
49	CH	92	LYS
49	CH	94	LEU
50	CK	2	LYS
50	CK	3	LEU
50	CK	16	LEU
50	CK	17	SER
50	CK	32	LEU
50	CK	34	GLU
50	CK	35	LEU
50	CK	53	LEU
50	CK	55	ARG
50	CK	64	LEU
50	CK	70	GLN
51	CL	8	LEU
51	CL	31	LEU
52	C5	39	ARG
52	C5	51	TYR
52	C5	53	THR
53	C6	7	PRO

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Mol	Chain	Res	Type
53	C6	29	THR
53	C6	44	THR
53	C6	46	CYS
53	C6	48	GLU
53	C6	49	CYS
53	C6	56	LYS
53	C6	57	VAL
54	C7	10	LEU
54	C7	18	ARG
54	C7	30	THR
54	C7	33	LYS
54	C7	42	TRP
54	C7	44	ARG
54	C7	46	HIS
55	C8	8	ASN
55	C8	24	THR
55	C8	43	THR
55	C8	48	LYS
56	C9	4	MET
56	C9	8	LYS
56	C9	15	LYS
56	C9	16	ILE
56	C9	30	ARG
56	C9	31	HIS
56	C9	33	ASN
56	C9	34	TRP
56	C9	44	LYS
56	C9	46	ARG
56	C9	49	VAL
56	C9	56	GLU
56	C9	61	LEU
57	C0	9	ARG
57	C0	26	ILE
57	C0	28	GLU
62	DA	23	ASP
62	DA	36	LYS
62	DA	47	LEU
62	DA	50	ASP
62	DA	53	ARG
62	DA	56	GLN
62	DA	64	LEU
62	DA	75	LEU

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Mol	Chain	Res	Type
28	DB	5	LYS
28	DB	10	THR
28	DB	20	ASP
28	DB	24	ILE
28	DB	25	THR
28	DB	26	LYS
28	DB	35	LYS
28	DB	46	GLN
28	DB	49	ILE
28	DB	61	LEU
28	DB	65	ILE
28	DB	69	ARG
28	DB	78	LYS
28	DB	92	ILE
28	DB	94	LEU
28	DB	99	ASP
28	DB	103	ARG
28	DB	141	VAL
28	DB	147	LEU
28	DB	154	LYS
28	DB	155	LEU
28	DB	157	ARG
28	DB	166	GLN
28	DB	168	ARG
28	DB	173	VAL
28	DB	192	THR
28	DB	212	SER
28	DB	221	VAL
28	DB	229	VAL
28	DB	239	ARG
28	DB	257	LEU
28	DB	259	THR
28	DB	260	ARG
28	DB	271	ILE
29	DC	1	MET
29	DC	11	MET
29	DC	17	ASP
29	DC	18	ASP
29	DC	33	VAL
29	DC	34	VAL
29	DC	55	ASN
29	DC	60	ASN

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Mol	Chain	Res	Type
29	DC	63	LEU
29	DC	64	LYS
29	DC	67	PHE
29	DC	78	LEU
29	DC	79	ARG
29	DC	82	ARG
29	DC	111	ARG
29	DC	113	PHE
29	DC	119	ARG
29	DC	145	LYS
29	DC	169	ASN
29	DC	175	VAL
29	DC	181	LEU
29	DC	202	LYS
29	DC	203	LYS
30	DD	2	LYS
30	DD	17	ARG
30	DD	20	LEU
30	DD	23	ASP
30	DD	27	GLU
30	DD	28	ILE
30	DD	38	ARG
30	DD	50	SER
30	DD	59	TYR
30	DD	65	TRP
30	DD	67	GLN
30	DD	74	ARG
30	DD	78	ILE
30	DD	83	PHE
30	DD	110	LEU
30	DD	125	LEU
30	DD	127	GLU
30	DD	149	ASP
30	DD	164	ARG
30	DD	165	ARG
30	DD	170	LEU
30	DD	175	THR
30	DD	192	LEU
30	DD	199	TRP
30	DD	200	GLU
30	DD	205	ARG
31	DE	4	ASP

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Mol	Chain	Res	Type
31	DE	5	VAL
31	DE	16	ARG
31	DE	21	ARG
31	DE	26	GLN
31	DE	34	LEU
31	DE	35	GLU
31	DE	39	ILE
31	DE	43	LEU
31	DE	45	GLU
31	DE	51	ARG
31	DE	53	LEU
31	DE	63	ILE
31	DE	67	LYS
31	DE	68	PRO
31	DE	70	VAL
31	DE	79	ASN
31	DE	80	PHE
31	DE	82	LEU
31	DE	84	LYS
31	DE	88	ILE
31	DE	96	ARG
31	DE	97	ASP
31	DE	108	ASN
31	DE	113	ARG
31	DE	115	ARG
31	DE	128	ARG
31	DE	130	ASN
31	DE	147	ASP
31	DE	153	ARG
31	DE	159	VAL
31	DE	179	PRO
32	DF	23	ARG
32	DF	24	VAL
32	DF	34	GLU
32	DF	46	GLU
32	DF	53	GLU
32	DF	54	ARG
32	DF	77	LYS
32	DF	85	LYS
32	DF	86	GLU
32	DF	88	LEU
32	DF	89	ILE

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Mol	Chain	Res	Type
32	DF	105	LEU
32	DF	119	GLU
32	DF	127	GLU
32	DF	132	ARG
32	DF	134	SER
32	DF	143	GLN
32	DF	144	VAL
32	DF	153	LYS
32	DF	157	TYR
32	DF	162	ILE
32	DF	170	ARG
33	DI	1	MET
33	DI	7	GLU
33	DI	12	LEU
33	DI	52	ARG
33	DI	61	ARG
33	DI	77	LEU
33	DI	82	ARG
33	DI	86	THR
33	DI	103	ARG
33	DI	110	ASP
33	DI	123	LEU
33	DI	140	LEU
35	DM	2	LYS
35	DM	4	TYR
35	DM	12	ARG
35	DM	22	THR
35	DM	34	LEU
35	DM	35	ARG
35	DM	39	ARG
35	DM	41	ASP
35	DM	43	THR
35	DM	48	MET
35	DM	55	VAL
35	DM	56	ASN
35	DM	60	ILE
35	DM	63	THR
35	DM	65	LYS
35	DM	73	THR
35	DM	87	LEU
35	DM	109	LYS
35	DM	119	ARG

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Mol	Chain	Res	Type
35	DM	121	LYS
35	DM	130	HIS
35	DM	131	GLN
36	DN	8	LEU
36	DN	20	MET
36	DN	23	ARG
36	DN	48	PRO
36	DN	49	ARG
36	DN	66	LYS
36	DN	73	ASP
36	DN	80	ASP
36	DN	98	VAL
36	DN	104	ARG
36	DN	108	GLU
36	DN	117	LEU
37	DO	6	LEU
37	DO	13	ASN
37	DO	16	ARG
37	DO	29	LYS
37	DO	32	THR
37	DO	36	LYS
37	DO	39	LYS
37	DO	41	ARG
37	DO	52	GLU
37	DO	57	THR
37	DO	59	LEU
37	DO	61	ARG
37	DO	62	LEU
37	DO	64	LYS
37	DO	67	MET
37	DO	68	GLN
37	DO	70	GLN
37	DO	76	LYS
37	DO	81	GLN
37	DO	85	LEU
37	DO	95	VAL
37	DO	98	GLU
37	DO	105	LEU
37	DO	108	LYS
37	DO	114	ILE
37	DO	123	LEU
37	DO	125	VAL

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Mol	Chain	Res	Type
37	DO	135	LEU
37	DO	139	LYS
38	DP	5	ARG
38	DP	18	LYS
38	DP	45	GLN
38	DP	58	PHE
38	DP	59	ARG
38	DP	63	LYS
38	DP	67	ARG
38	DP	75	THR
38	DP	79	LEU
38	DP	110	THR
38	DP	115	MET
38	DP	131	ILE
38	DP	133	ARG
38	DP	139	GLU
39	DQ	8	ARG
39	DQ	12	ARG
39	DQ	18	LEU
39	DQ	27	SER
39	DQ	28	LEU
39	DQ	29	LEU
39	DQ	57	ARG
39	DQ	67	LEU
39	DQ	71	GLN
39	DQ	74	LYS
39	DQ	76	VAL
39	DQ	79	LEU
39	DQ	103	ARG
39	DQ	104	ARG
39	DQ	111	LEU
39	DQ	113	LEU
39	DQ	118	GLU
40	DR	11	LYS
40	DR	13	ARG
40	DR	17	ARG
40	DR	18	ILE
40	DR	23	ARG
40	DR	26	LEU
40	DR	30	ARG
40	DR	32	LEU
40	DR	35	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
40	DR	36	TYR
40	DR	50	SER
40	DR	52	SER
40	DR	56	LEU
40	DR	78	LEU
40	DR	84	GLN
40	DR	89	ARG
40	DR	92	TYR
40	DR	97	ARG
40	DR	101	LEU
41	DS	11	GLU
41	DS	13	ARG
41	DS	18	ASP
41	DS	29	ARG
41	DS	32	TYR
41	DS	38	ASN
41	DS	41	ARG
41	DS	44	ASP
41	DS	51	ARG
41	DS	58	ASN
41	DS	59	THR
41	DS	65	LYS
41	DS	74	ARG
41	DS	78	LEU
41	DS	85	LYS
41	DS	87	ASP
41	DS	93	ARG
41	DS	98	LYS
41	DS	99	LEU
41	DS	108	ARG
42	DT	8	VAL
42	DT	17	ILE
42	DT	59	ARG
42	DT	60	LEU
42	DT	64	ARG
42	DT	66	ASN
42	DT	71	GLN
42	DT	74	LEU
42	DT	83	LEU
42	DT	84	LYS
42	DT	112	ARG
43	DU	13	ARG

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Mol	Chain	Res	Type
43	DU	18	LEU
43	DU	19	LYS
43	DU	20	LEU
43	DU	21	ARG
43	DU	32	THR
43	DU	35	LEU
43	DU	39	LEU
43	DU	40	LEU
43	DU	45	THR
43	DU	46	VAL
43	DU	49	THR
43	DU	53	GLU
43	DU	62	LEU
43	DU	64	HIS
43	DU	68	LYS
43	DU	82	ARG
43	DU	89	GLN
43	DU	91	TYR
43	DU	95	LEU
43	DU	99	ILE
63	DW	11	ARG
63	DW	51	LEU
63	DW	52	GLU
63	DW	70	TYR
63	DW	107	LEU
45	DX	25	LYS
45	DX	27	THR
45	DX	35	THR
45	DX	50	LYS
45	DX	53	LYS
45	DX	57	LEU
45	DX	64	LYS
45	DX	68	ARG
45	DX	72	LYS
45	DX	76	ARG
45	DX	80	ILE
45	DX	81	VAL
45	DX	88	LYS
45	DX	90	GLU
46	DY	2	ARG
46	DY	7	VAL
46	DY	8	LYS

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Mol	Chain	Res	Type
46	DY	9	LYS
46	DY	14	LEU
46	DY	33	LYS
46	DY	34	LYS
46	DY	55	TYR
46	DY	62	GLU
46	DY	66	PRO
46	DY	76	CYS
46	DY	79	CYS
46	DY	85	VAL
46	DY	89	PHE
46	DY	96	ILE
46	DY	97	ARG
47	DZ	14	LYS
47	DZ	18	LEU
47	DZ	20	ARG
47	DZ	34	ASN
47	DZ	37	VAL
47	DZ	39	VAL
47	DZ	63	ASP
47	DZ	76	LEU
47	DZ	79	ARG
47	DZ	80	ARG
47	DZ	81	ARG
47	DZ	91	LEU
47	DZ	92	SER
47	DZ	116	VAL
47	DZ	121	HIS
47	DZ	123	ASP
47	DZ	125	LEU
47	DZ	131	ARG
47	DZ	163	LEU
48	Da	10	THR
48	Da	11	ARG
48	Da	12	ASN
48	Da	14	ARG
48	Da	19	LYS
48	Da	29	GLN
48	Da	31	VAL
48	Da	41	ARG
48	Da	64	ASP
48	Da	84	LEU

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Mol	Chain	Res	Type
49	DH	3	LYS
49	DH	4	VAL
49	DH	25	LYS
49	DH	26	ARG
49	DH	40	ARG
49	DH	45	ASN
49	DH	46	LEU
49	DH	56	GLN
49	DH	58	ILE
49	DH	59	THR
49	DH	61	ARG
49	DH	75	GLU
49	DH	80	LEU
49	DH	82	LEU
49	DH	92	LYS
49	DH	94	LEU
50	DK	3	LEU
50	DK	10	LEU
50	DK	14	ARG
50	DK	15	LYS
50	DK	17	SER
50	DK	28	LYS
50	DK	32	LEU
50	DK	51	ARG
50	DK	53	LEU
50	DK	56	GLN
50	DK	61	LEU
50	DK	69	ARG
50	DK	70	GLN
51	DL	8	LEU
51	DL	18	ASP
51	DL	29	ARG
52	D5	39	ARG
52	D5	46	ASN
52	D5	49	GLU
52	D5	51	TYR
52	D5	53	THR
52	D5	58	TYR
53	D6	3	LYS
53	D6	11	THR
53	D6	29	THR
53	D6	36	CYS

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Mol	Chain	Res	Type
53	D6	44	THR
53	D6	49	CYS
53	D6	51	TYR
53	D6	56	LYS
53	D6	57	VAL
54	D7	10	LEU
54	D7	17	LYS
54	D7	30	THR
54	D7	33	LYS
54	D7	36	LEU
54	D7	37	ARG
54	D7	44	ARG
54	D7	46	HIS
55	D8	1	MET
55	D8	4	THR
55	D8	8	ASN
55	D8	24	THR
55	D8	36	GLN
55	D8	43	THR
55	D8	44	PRO
55	D8	47	ARG
55	D8	48	LYS
56	D9	8	LYS
56	D9	11	LYS
56	D9	14	VAL
56	D9	30	ARG
56	D9	31	HIS
56	D9	33	ASN
56	D9	34	TRP
56	D9	36	LYS
56	D9	44	LYS
56	D9	61	LEU
57	D0	2	LYS
57	D0	9	ARG
57	D0	12	ASP
57	D0	26	ILE
57	D0	27	CYS
57	D0	28	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (195) such sidechains are listed below:

Mol	Chain	Res	Type
2	AA	40	HIS
2	AA	78	GLN
2	AA	146	GLN
3	AC	170	GLN
4	AD	62	GLN
4	AD	123	HIS
4	AD	129	ASN
4	AD	161	ASN
5	AE	20	GLN
6	AF	18	GLN
6	AF	32	ASN
6	AF	73	ASN
6	AF	100	ASN
7	AG	37	ASN
7	AG	86	GLN
7	AG	148	ASN
10	AJ	56	HIS
10	AJ	78	ASN
11	AK	38	ASN
12	AL	8	ASN
12	AL	9	GLN
12	AL	49	ASN
12	AL	75	HIS
15	AO	37	ASN
15	AO	46	HIS
16	AP	16	HIS
18	AS	36	ASN
20	AU	26	ASN
20	AU	42	GLN
20	AU	75	ASN
2	BA	19	HIS
2	BA	78	GLN
2	BA	146	GLN
2	BA	212	GLN
24	BC	69	HIS
24	BC	118	GLN
24	BC	170	GLN
4	BD	62	GLN
4	BD	74	GLN
4	BD	77	ASN
4	BD	123	HIS
4	BD	129	ASN
5	BE	20	GLN

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Mol	Chain	Res	Type
6	BF	18	GLN
6	BF	32	ASN
6	BF	73	ASN
7	BG	28	ASN
7	BG	37	ASN
7	BG	148	ASN
9	BI	124	GLN
10	BJ	33	GLN
10	BJ	56	HIS
10	BJ	68	HIS
10	BJ	78	ASN
10	BJ	84	GLN
11	BK	13	GLN
11	BK	26	ASN
11	BK	78	GLN
11	BK	117	ASN
12	BL	9	GLN
12	BL	49	ASN
12	BL	75	HIS
13	BM	62	ASN
13	BM	92	HIS
15	BO	37	ASN
15	BO	46	HIS
16	BP	76	GLN
18	BS	36	ASN
19	BT	14	HIS
19	BT	23	ASN
20	BU	26	ASN
27	CA	56	GLN
28	CB	58	HIS
28	CB	96	HIS
28	CB	126	GLN
28	CB	166	GLN
28	CB	186	HIS
28	CB	198	ASN
28	CB	220	HIS
29	CC	48	GLN
29	CC	55	ASN
29	CC	129	HIS
29	CC	192	ASN
30	CD	75	HIS
30	CD	169	ASN

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Mol	Chain	Res	Type
32	CF	139	GLN
32	CF	147	ASN
33	CI	43	ASN
35	CM	45	ASN
35	CM	56	ASN
36	CN	5	GLN
36	CN	82	ASN
37	CO	13	ASN
37	CO	68	GLN
37	CO	128	HIS
38	CP	45	GLN
38	CP	123	HIS
39	CQ	16	HIS
39	CQ	23	ASN
39	CQ	24	GLN
39	CQ	53	HIS
39	CQ	71	GLN
40	CR	34	HIS
41	CS	38	ASN
41	CS	43	GLN
41	CS	90	GLN
42	CT	14	HIS
42	CT	49	HIS
42	CT	66	ASN
42	CT	81	HIS
43	CU	11	GLN
44	CW	34	ASN
44	CW	57	ASN
44	CW	60	ASN
44	CW	102	HIS
45	CX	41	ASN
45	CX	55	ASN
47	CZ	65	GLN
47	CZ	118	GLN
47	CZ	132	ASN
49	CH	45	ASN
51	CL	19	GLN
51	CL	46	ASN
51	CL	52	HIS
53	C6	23	HIS
53	C6	43	HIS
55	C8	8	ASN

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Mol	Chain	Res	Type
56	C9	31	HIS
56	C9	33	ASN
62	DA	56	GLN
28	DB	116	GLN
28	DB	166	GLN
28	DB	186	HIS
28	DB	198	ASN
29	DC	48	GLN
29	DC	55	ASN
29	DC	129	HIS
29	DC	192	ASN
30	DD	8	GLN
30	DD	40	GLN
30	DD	75	HIS
30	DD	169	ASN
30	DD	203	GLN
31	DE	26	GLN
31	DE	40	ASN
31	DE	121	ASN
32	DF	65	HIS
32	DF	147	ASN
33	DI	139	GLN
35	DM	69	GLN
35	DM	128	HIS
36	DN	5	GLN
37	DO	13	ASN
37	DO	35	HIS
37	DO	84	ASN
37	DO	128	HIS
38	DP	12	GLN
39	DQ	13	HIS
39	DQ	23	ASN
39	DQ	24	GLN
39	DQ	53	HIS
39	DQ	61	HIS
39	DQ	71	GLN
40	DR	84	GLN
41	DS	38	ASN
41	DS	58	ASN
41	DS	123	GLN
42	DT	14	HIS
42	DT	49	HIS

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Mol	Chain	Res	Type
42	DT	66	ASN
42	DT	117	GLN
43	DU	11	GLN
63	DW	57	ASN
63	DW	61	ASN
63	DW	102	HIS
45	DX	41	ASN
45	DX	55	ASN
46	DY	43	ASN
47	DZ	73	GLN
47	DZ	118	GLN
47	DZ	132	ASN
48	Da	12	ASN
49	DH	45	ASN
49	DH	56	GLN
50	DK	38	GLN
50	DK	70	GLN
51	DL	19	GLN
51	DL	46	ASN
51	DL	52	HIS
53	D6	23	HIS
53	D6	43	HIS
55	D8	8	ASN
56	D9	31	HIS
56	D9	33	ASN
57	D0	34	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A2	8/9 (88%)	4 (50%)	2 (25%)
22	Ab	1503/1504 (99%)	324 (21%)	0
22	Bb	1503/1504 (99%)	339 (22%)	0
23	B2	8/10 (80%)	4 (50%)	1 (12%)
25	C2	74/76 (97%)	24 (32%)	4 (5%)
25	C3	75/76 (98%)	19 (25%)	1 (1%)
25	D3	75/76 (98%)	31 (41%)	3 (4%)
26	C4	76/77 (98%)	36 (47%)	4 (5%)
58	C1	2800/2899 (96%)	802 (28%)	155 (5%)
58	D1	2800/2899 (96%)	818 (29%)	149 (5%)
59	Cs	118/119 (99%)	35 (29%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
59	Ds	118/119 (99%)	40 (33%)	0
60	D2	19/20 (95%)	8 (42%)	1 (5%)
61	D4	75/76 (98%)	23 (30%)	5 (6%)
64	DV	41/55 (74%)	14 (34%)	1 (2%)
All	All	9293/9519 (97%)	2521 (27%)	326 (3%)

All (2521) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A2	15	A
1	A2	17	U
1	A2	18	G
1	A2	19	U
22	Ab	10	G
22	Ab	23	G
22	Ab	32	G
22	Ab	33	A
22	Ab	40	G
22	Ab	48	C
22	Ab	49	C
22	Ab	51	A
22	Ab	52	A
22	Ab	60	A
22	Ab	61	A
22	Ab	62	G
22	Ab	64	C
22	Ab	75	C
22	Ab	76	G
22	Ab	79	G
22	Ab	80	U
22	Ab	81	U
22	Ab	82	U
22	Ab	83	U
22	Ab	85	C
22	Ab	86	U
22	Ab	87	C
22	Ab	89	G
22	Ab	91	G
22	Ab	95	A
22	Ab	99	G
22	Ab	109	G
22	Ab	110	A

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Mol	Chain	Res	Type
22	Ab	114	A
22	Ab	115	C
22	Ab	126	C
22	Ab	139	G
22	Ab	145	C
22	Ab	146	A
22	Ab	158	C
22	Ab	176	G
22	Ab	191	G
22	Ab	192	G
22	Ab	194	G
22	Ab	202	A
22	Ab	204	A
22	Ab	209	U
22	Ab	210	U
22	Ab	211	U
22	Ab	212	G
22	Ab	216	G
22	Ab	240	U
22	Ab	241	C
22	Ab	242	A
22	Ab	243	G
22	Ab	247	G
22	Ab	262	G
22	Ab	263	C
22	Ab	270	A
22	Ab	285	G
22	Ab	297	G
22	Ab	301	G
22	Ab	314	G
22	Ab	315	G
22	Ab	317	A
22	Ab	324	C
22	Ab	325	A
22	Ab	326	C
22	Ab	328	G
22	Ab	338	C
22	Ab	341	C
22	Ab	348	C
22	Ab	349	A
22	Ab	350	G
22	Ab	352	A

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Mol	Chain	Res	Type
22	Ab	353	G
22	Ab	362	C
22	Ab	363	U
22	Ab	368	C
22	Ab	369	A
22	Ab	380	G
22	Ab	385	A
22	Ab	393	A
22	Ab	394	C
22	Ab	402	G
22	Ab	407	A
22	Ab	408	A
22	Ab	409	G
22	Ab	410	A
22	Ab	415	C
22	Ab	418	C
22	Ab	420	G
22	Ab	425	U
22	Ab	426	A
22	Ab	431	C
22	Ab	433	U
22	Ab	434	G
22	Ab	435	A
22	Ab	436	A
22	Ab	447	A
22	Ab	455	A
22	Ab	456	C
22	Ab	457	G
22	Ab	469	G
22	Ab	470	G
22	Ab	481	A
22	Ab	482	U
22	Ab	483	A
22	Ab	487	C
22	Ab	489	G
22	Ab	493	A
22	Ab	494	A
22	Ab	495	C
22	Ab	496	U
22	Ab	502	C
22	Ab	503	C
22	Ab	505	G

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Mol	Chain	Res	Type
22	Ab	511	G
22	Ab	515	U
22	Ab	516	A
22	Ab	517	A
22	Ab	518	U
22	Ab	529	C
22	Ab	531	A
22	Ab	545	U
22	Ab	546	C
22	Ab	556	A
22	Ab	557	A
22	Ab	560	G
22	Ab	565	G
22	Ab	571	G
22	Ab	572	G
22	Ab	579	G
22	Ab	591	A
22	Ab	600	G
22	Ab	611	G
22	Ab	614	G
22	Ab	615	G
22	Ab	616	A
22	Ab	623	G
22	Ab	634	G
22	Ab	637	A
22	Ab	649	A
22	Ab	671	A
22	Ab	672	G
22	Ab	689	U
22	Ab	708	G
22	Ab	715	G
22	Ab	732	C
22	Ab	733	C
22	Ab	737	A
22	Ab	739	G
22	Ab	744	G
22	Ab	758	G
22	Ab	761	A
22	Ab	770	G
22	Ab	777	U
22	Ab	778	A
22	Ab	780	C

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Mol	Chain	Res	Type
22	Ab	800	A
22	Ab	801	C
22	Ab	802	G
22	Ab	803	A
22	Ab	804	U
22	Ab	810	C
22	Ab	812	A
22	Ab	817	U
22	Ab	823	U
22	Ab	824	C
22	Ab	825	U
22	Ab	826	C
22	Ab	829	G
22	Ab	837	A
22	Ab	865	G
22	Ab	880	G
22	Ab	887	A
22	Ab	892	A
22	Ab	894	G
22	Ab	904	G
22	Ab	905	G
22	Ab	912	C
22	Ab	913	A
22	Ab	917	G
22	Ab	938	U
22	Ab	939	U
22	Ab	944	G
22	Ab	946	A
22	Ab	947	A
22	Ab	949	G
22	Ab	952	A
22	Ab	953	A
22	Ab	954	G
22	Ab	955	A
22	Ab	956	A
22	Ab	958	C
22	Ab	960	U
22	Ab	969	U
22	Ab	970	U
22	Ab	971	G
22	Ab	980	G
22	Ab	983	A

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Mol	Chain	Res	Type
22	Ab	984	A
22	Ab	985	C
22	Ab	988	G
22	Ab	1003	G
22	Ab	1005	G
22	Ab	1006	C
22	Ab	1007	C
22	Ab	1016	G
22	Ab	1027	A
22	Ab	1033	G
22	Ab	1036	G
22	Ab	1037	C
22	Ab	1048	U
22	Ab	1049	C
22	Ab	1050	A
22	Ab	1051	G
22	Ab	1064	G
22	Ab	1069	U
22	Ab	1077	G
22	Ab	1078	U
22	Ab	1084	A
22	Ab	1091	G
22	Ab	1092	C
22	Ab	1096	C
22	Ab	1100	G
22	Ab	1107	G
22	Ab	1108	U
22	Ab	1109	U
22	Ab	1110	G
22	Ab	1112	C
22	Ab	1113	A
22	Ab	1114	G
22	Ab	1119	U
22	Ab	1120	C
22	Ab	1121	G
22	Ab	1122	G
22	Ab	1123	C
22	Ab	1129	A
22	Ab	1135	A
22	Ab	1142	U
22	Ab	1143	G
22	Ab	1144	C

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Mol	Chain	Res	Type
22	Ab	1152	A
22	Ab	1153	G
22	Ab	1166	G
22	Ab	1169	G
22	Ab	1172	G
22	Ab	1178	U
22	Ab	1179	G
22	Ab	1183	A
22	Ab	1184	G
22	Ab	1194	U
22	Ab	1195	A
22	Ab	1196	C
22	Ab	1207	A
22	Ab	1209	A
22	Ab	1220	A
22	Ab	1237	G
22	Ab	1238	A
22	Ab	1239	U
22	Ab	1240	G
22	Ab	1252	C
22	Ab	1255	G
22	Ab	1260	U
22	Ab	1262	A
22	Ab	1263	U
22	Ab	1264	C
22	Ab	1268	A
22	Ab	1269	A
22	Ab	1272	G
22	Ab	1276	G
22	Ab	1278	C
22	Ab	1279	C
22	Ab	1281	A
22	Ab	1282	G
22	Ab	1283	U
22	Ab	1284	U
22	Ab	1299	C
22	Ab	1302	C
22	Ab	1303	C
22	Ab	1304	C
22	Ab	1305	G
22	Ab	1307	C
22	Ab	1308	C

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Mol	Chain	Res	Type
22	Ab	1313	G
22	Ab	1317	C
22	Ab	1319	G
22	Ab	1320	G
22	Ab	1321	A
22	Ab	1328	A
22	Ab	1329	G
22	Ab	1335	G
22	Ab	1345	C
22	Ab	1347	U
22	Ab	1353	G
22	Ab	1362	G
22	Ab	1364	U
22	Ab	1381	A
22	Ab	1383	C
22	Ab	1384	G
22	Ab	1402	G
22	Ab	1425	G
22	Ab	1426	G
22	Ab	1427	A
22	Ab	1428	G
22	Ab	1430	C
22	Ab	1432	A
22	Ab	1433	C
22	Ab	1447	G
22	Ab	1465	G
22	Ab	1470	A
22	Ab	1475	G
22	Ab	1476	U
22	Ab	1477	A
22	Ab	1480	A
22	Ab	1481	A
22	Ab	1482	G
22	Ab	1483	G
22	Ab	1484	U
22	Ab	1485	A
22	Ab	1495	G
22	Ab	1497	A
22	Ab	1498	G
22	Ab	1503	G
22	Ab	1507	G
22	Ab	1508	G

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Mol	Chain	Res	Type
22	Ab	1509	A
23	B2	14	A
23	B2	16	A
23	B2	19	U
23	B2	20	U
22	Bb	7	G
22	Bb	8	G
22	Bb	10	G
22	Bb	31	U
22	Bb	32	G
22	Bb	33	A
22	Bb	40	G
22	Bb	48	C
22	Bb	49	C
22	Bb	52	A
22	Bb	55	C
22	Bb	60	A
22	Bb	61	A
22	Bb	62	G
22	Bb	66	U
22	Bb	67	G
22	Bb	74	G
22	Bb	76	G
22	Bb	77	G
22	Bb	78	G
22	Bb	79	G
22	Bb	80	U
22	Bb	82	U
22	Bb	83	U
22	Bb	86	U
22	Bb	91	G
22	Bb	95	A
22	Bb	102	G
22	Bb	109	G
22	Bb	110	A
22	Bb	114	A
22	Bb	115	C
22	Bb	126	C
22	Bb	132	C
22	Bb	139	G
22	Bb	141	G
22	Bb	145	C

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Mol	Chain	Res	Type
22	Bb	158	C
22	Bb	167	A
22	Bb	176	G
22	Bb	191	G
22	Bb	192	G
22	Bb	202	A
22	Bb	204	A
22	Bb	206	G
22	Bb	211	U
22	Bb	212	G
22	Bb	240	U
22	Bb	243	G
22	Bb	247	G
22	Bb	248	U
22	Bb	249	U
22	Bb	262	G
22	Bb	263	C
22	Bb	266	A
22	Bb	270	A
22	Bb	285	G
22	Bb	297	G
22	Bb	312	G
22	Bb	314	G
22	Bb	317	A
22	Bb	324	C
22	Bb	325	A
22	Bb	328	G
22	Bb	341	C
22	Bb	348	C
22	Bb	349	A
22	Bb	350	G
22	Bb	352	A
22	Bb	362	C
22	Bb	363	U
22	Bb	368	C
22	Bb	369	A
22	Bb	380	G
22	Bb	385	A
22	Bb	393	A
22	Bb	394	C
22	Bb	402	G
22	Bb	408	A

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Mol	Chain	Res	Type
22	Bb	409	G
22	Bb	410	A
22	Bb	411	A
22	Bb	417	U
22	Bb	418	C
22	Bb	420	G
22	Bb	424	G
22	Bb	425	U
22	Bb	426	A
22	Bb	431	C
22	Bb	433	U
22	Bb	435	A
22	Bb	447	A
22	Bb	455	A
22	Bb	456	C
22	Bb	463	A
22	Bb	469	G
22	Bb	470	G
22	Bb	481	A
22	Bb	482	U
22	Bb	483	A
22	Bb	489	G
22	Bb	493	A
22	Bb	494	A
22	Bb	495	C
22	Bb	496	U
22	Bb	502	C
22	Bb	511	G
22	Bb	515	U
22	Bb	516	A
22	Bb	517	A
22	Bb	518	U
22	Bb	520	C
22	Bb	529	C
22	Bb	531	A
22	Bb	545	U
22	Bb	546	C
22	Bb	554	G
22	Bb	556	A
22	Bb	557	A
22	Bb	560	G
22	Bb	568	G

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Mol	Chain	Res	Type
22	Bb	572	G
22	Bb	576	G
22	Bb	580	C
22	Bb	591	A
22	Bb	598	A
22	Bb	601	G
22	Bb	612	G
22	Bb	614	G
22	Bb	615	G
22	Bb	616	A
22	Bb	617	G
22	Bb	637	A
22	Bb	649	A
22	Bb	650	G
22	Bb	655	G
22	Bb	671	A
22	Bb	672	G
22	Bb	686	A
22	Bb	705	G
22	Bb	708	G
22	Bb	715	G
22	Bb	717	A
22	Bb	718	G
22	Bb	724	U
22	Bb	732	C
22	Bb	733	C
22	Bb	734	G
22	Bb	739	G
22	Bb	744	G
22	Bb	745	G
22	Bb	757	G
22	Bb	761	A
22	Bb	770	G
22	Bb	777	U
22	Bb	778	A
22	Bb	780	C
22	Bb	800	A
22	Bb	801	C
22	Bb	803	A
22	Bb	804	U
22	Bb	811	U
22	Bb	812	A

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Mol	Chain	Res	Type
22	Bb	817	U
22	Bb	820	G
22	Bb	823	U
22	Bb	824	C
22	Bb	825	U
22	Bb	826	C
22	Bb	837	A
22	Bb	848	U
22	Bb	852	G
22	Bb	854	G
22	Bb	862	U
22	Bb	863	G
22	Bb	865	G
22	Bb	880	G
22	Bb	892	A
22	Bb	894	G
22	Bb	898	U
22	Bb	904	G
22	Bb	905	G
22	Bb	910	C
22	Bb	912	C
22	Bb	913	A
22	Bb	917	G
22	Bb	938	U
22	Bb	939	U
22	Bb	941	G
22	Bb	944	G
22	Bb	945	C
22	Bb	946	A
22	Bb	947	A
22	Bb	949	G
22	Bb	952	A
22	Bb	953	A
22	Bb	954	G
22	Bb	955	A
22	Bb	956	A
22	Bb	958	C
22	Bb	959	U
22	Bb	960	U
22	Bb	961	A
22	Bb	969	U
22	Bb	970	U

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Mol	Chain	Res	Type
22	Bb	971	G
22	Bb	983	A
22	Bb	984	A
22	Bb	985	C
22	Bb	988	G
22	Bb	996	G
22	Bb	1003	G
22	Bb	1005	G
22	Bb	1006	C
22	Bb	1007	C
22	Bb	1013	A
22	Bb	1014	G
22	Bb	1027	A
22	Bb	1032	U
22	Bb	1033	G
22	Bb	1036	G
22	Bb	1037	C
22	Bb	1038	A
22	Bb	1048	U
22	Bb	1049	C
22	Bb	1050	A
22	Bb	1051	G
22	Bb	1064	G
22	Bb	1077	G
22	Bb	1078	U
22	Bb	1084	A
22	Bb	1091	G
22	Bb	1096	C
22	Bb	1100	G
22	Bb	1107	G
22	Bb	1108	U
22	Bb	1109	U
22	Bb	1110	G
22	Bb	1112	C
22	Bb	1113	A
22	Bb	1114	G
22	Bb	1119	U
22	Bb	1120	C
22	Bb	1121	G
22	Bb	1122	G
22	Bb	1123	C
22	Bb	1124	C

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Mol	Chain	Res	Type
22	Bb	1125	G
22	Bb	1129	A
22	Bb	1130	C
22	Bb	1135	A
22	Bb	1142	U
22	Bb	1143	G
22	Bb	1153	G
22	Bb	1165	A
22	Bb	1166	G
22	Bb	1168	G
22	Bb	1172	G
22	Bb	1178	U
22	Bb	1179	G
22	Bb	1183	A
22	Bb	1184	G
22	Bb	1193	U
22	Bb	1194	U
22	Bb	1195	A
22	Bb	1207	A
22	Bb	1220	A
22	Bb	1223	G
22	Bb	1227	A
22	Bb	1228	C
22	Bb	1237	G
22	Bb	1238	A
22	Bb	1239	U
22	Bb	1240	G
22	Bb	1245	C
22	Bb	1255	G
22	Bb	1259	C
22	Bb	1262	A
22	Bb	1263	U
22	Bb	1264	C
22	Bb	1267	A
22	Bb	1268	A
22	Bb	1269	A
22	Bb	1272	G
22	Bb	1276	G
22	Bb	1278	C
22	Bb	1279	C
22	Bb	1281	A
22	Bb	1282	G

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Mol	Chain	Res	Type
22	Bb	1283	U
22	Bb	1284	U
22	Bb	1287	G
22	Bb	1299	C
22	Bb	1302	C
22	Bb	1303	C
22	Bb	1304	C
22	Bb	1305	G
22	Bb	1313	G
22	Bb	1316	G
22	Bb	1320	G
22	Bb	1328	A
22	Bb	1329	G
22	Bb	1335	G
22	Bb	1346	A
22	Bb	1347	U
22	Bb	1351	G
22	Bb	1353	G
22	Bb	1365	C
22	Bb	1380	C
22	Bb	1381	A
22	Bb	1382	C
22	Bb	1385	C
22	Bb	1389	U
22	Bb	1402	G
22	Bb	1405	G
22	Bb	1425	G
22	Bb	1426	G
22	Bb	1427	A
22	Bb	1428	G
22	Bb	1432	A
22	Bb	1433	C
22	Bb	1434	G
22	Bb	1460	G
22	Bb	1465	G
22	Bb	1470	A
22	Bb	1472	G
22	Bb	1475	G
22	Bb	1477	A
22	Bb	1480	A
22	Bb	1481	A
22	Bb	1482	G

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Mol	Chain	Res	Type
22	Bb	1484	U
22	Bb	1485	A
22	Bb	1495	G
22	Bb	1497	A
22	Bb	1498	G
22	Bb	1503	G
22	Bb	1507	G
22	Bb	1508	G
25	C2	2	C
25	C2	4	C
25	C2	9	A
25	C2	16	U
25	C2	17	C
25	C2	18	G
25	C2	19	G
25	C2	21	A
25	C2	23	A
25	C2	30	G
25	C2	34	G
25	C2	42	C
25	C2	43	C
25	C2	46	G
25	C2	47	U
25	C2	48	C
25	C2	52	G
25	C2	53	G
25	C2	57	G
25	C2	61	C
25	C2	63	G
25	C2	73	A
25	C2	74	C
25	C2	75	C
25	C3	2	C
25	C3	16	U
25	C3	17	C
25	C3	18	G
25	C3	19	G
25	C3	20	U
25	C3	21	A
25	C3	22	G
25	C3	23	A
25	C3	39	U

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Mol	Chain	Res	Type
25	C3	40	C
25	C3	41	C
25	C3	43	C
25	C3	47	U
25	C3	48	C
25	C3	49	C
25	C3	51	U
25	C3	61	C
25	C3	74	C
26	C4	3	C
26	C4	5	G
26	C4	6	G
26	C4	7	G
26	C4	8	U
26	C4	9	G
26	C4	10	G
26	C4	11	A
26	C4	12	G
26	C4	16	C
26	C4	17	C
26	C4	18	U
26	C4	19	G
26	C4	20	G
26	C4	21	U
26	C4	22	A
26	C4	27	G
26	C4	32	G
26	C4	35	C
26	C4	36	A
26	C4	38	A
26	C4	48	U
26	C4	49	C
26	C4	50	G
26	C4	52	C
26	C4	53	G
26	C4	54	G
26	C4	60	A
26	C4	61	U
26	C4	64	G
26	C4	66	C
26	C4	69	C
26	C4	73	A

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Mol	Chain	Res	Type
26	C4	74	A
26	C4	75	C
26	C4	77	A
58	C1	8	U
58	C1	9	G
58	C1	14	G
58	C1	16	G
58	C1	33	C
58	C1	34	G
58	C1	35	G
58	C1	40	C
58	C1	44	C
58	C1	47	A
58	C1	48	U
58	C1	52	G
58	C1	53	G
58	C1	56	G
58	C1	57	U
58	C1	67	C
58	C1	69	A
58	C1	70	U
58	C1	72	A
58	C1	73	G
58	C1	81	G
58	C1	82	A
58	C1	86	G
58	C1	87	G
58	C1	88	U
58	C1	89	A
58	C1	91	C
58	C1	93	G
58	C1	98	G
58	C1	99	G
58	C1	100	A
58	C1	110	G
58	C1	115	A
58	C1	116	A
58	C1	117	U
58	C1	126	C
58	C1	132	G
58	C1	136	G
58	C1	137	G

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Mol	Chain	Res	Type
58	C1	138	A
58	C1	139	A
58	C1	140	C
58	C1	145	G
58	C1	153	G
58	C1	154	C
58	C1	158	U
58	C1	162	C
58	C1	163	G
58	C1	169	A
58	C1	184	A
58	C1	185	A
58	C1	187	A
58	C1	188	U
58	C1	192	A
58	C1	193	G
58	C1	200	G
58	C1	203	G
58	C1	204	A
58	C1	209	A
58	C1	210	A
58	C1	213	A
58	C1	216	A
58	C1	217	A
58	C1	218	U
58	C1	221	A
58	C1	236	G
58	C1	237	C
58	C1	238	G
58	C1	240	G
58	C1	248	G
58	C1	249	G
58	C1	254	G
58	C1	255	C
58	C1	256	C
58	C1	260	A
58	C1	268	G
58	C1	269	C
58	C1	270	U
58	C1	271	U
58	C1	272	G
58	C1	273	U

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Mol	Chain	Res	Type
58	C1	274	C
58	C1	275	C
58	C1	277	G
58	C1	282	G
58	C1	284	U
58	C1	285	C
58	C1	286	G
58	C1	294	C
58	C1	295	U
58	C1	296	C
58	C1	297	G
58	C1	298	G
58	C1	303	C
58	C1	321	G
58	C1	322	A
58	C1	326	U
58	C1	333	A
58	C1	334	A
58	C1	350	G
58	C1	352	G
58	C1	353	A
58	C1	355	A
58	C1	356	G
58	C1	358	C
58	C1	366	C
58	C1	375	G
58	C1	376	G
58	C1	379	G
58	C1	385	U
58	C1	386	G
58	C1	388	G
58	C1	389	G
58	C1	392	A
58	C1	393	C
58	C1	395	C
58	C1	412	G
58	C1	413	U
58	C1	414	G
58	C1	422	G
58	C1	425	G
58	C1	431	U
58	C1	432	G

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Mol	Chain	Res	Type
58	C1	433	G
58	C1	437	G
58	C1	438	A
58	C1	440	C
58	C1	444	G
58	C1	454	A
58	C1	466	U
58	C1	469	C
58	C1	473	U
58	C1	476	C
58	C1	479	A
58	C1	480	C
58	C1	481	C
58	C1	482	A
58	C1	495	A
58	C1	496	A
58	C1	497	A
58	C1	498	G
58	C1	500	U
58	C1	504	A
58	C1	506	G
58	C1	507	A
58	C1	518	G
58	C1	527	A
58	C1	528	U
58	C1	529	A
58	C1	532	G
58	C1	537	A
58	C1	550	A
58	C1	552	A
58	C1	555	C
58	C1	556	A
58	C1	557	G
58	C1	566	C
58	C1	567	C
58	C1	571	A
58	C1	572	G
58	C1	583	G
58	C1	585	G
58	C1	588	U
58	C1	595	G
58	C1	597	A

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Mol	Chain	Res	Type
58	C1	608	A
58	C1	609	C
58	C1	610	U
58	C1	624	G
58	C1	626	G
58	C1	629	U
58	C1	632	G
58	C1	635	G
58	C1	636	U
58	C1	638	G
58	C1	640	G
58	C1	644	G
58	C1	645	A
58	C1	646	G
58	C1	648	C
58	C1	650	U
58	C1	651	A
58	C1	658	C
58	C1	661	A
58	C1	669	C
58	C1	670	A
58	C1	674	C
58	C1	675	G
58	C1	676	C
58	C1	703	U
58	C1	710	C
58	C1	715	G
58	C1	716	A
58	C1	718	C
58	C1	719	C
58	C1	732	G
58	C1	753	G
58	C1	754	C
58	C1	763	G
58	C1	764	A
58	C1	768	A
58	C1	772	G
58	C1	776	C
58	C1	784	G
58	C1	785	G
58	C1	786	U
58	C1	791	G

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Mol	Chain	Res	Type
58	C1	792	A
58	C1	793	U
58	C1	799	C
58	C1	804	C
58	C1	811	G
58	C1	821	G
58	C1	822	G
58	C1	828	A
58	C1	830	A
58	C1	831	G
58	C1	836	C
58	C1	837	C
58	C1	838	G
58	C1	839	A
58	C1	840	G
58	C1	851	G
58	C1	854	G
58	C1	858	C
58	C1	859	U
58	C1	865	A
58	C1	873	U
58	C1	874	U
58	C1	876	G
58	C1	878	G
58	C1	891	G
58	C1	892	C
58	C1	894	G
58	C1	905	G
58	C1	907	A
58	C1	912	A
58	C1	924	A
58	C1	932	C
58	C1	933	A
58	C1	934	C
58	C1	936	A
58	C1	939	C
58	C1	941	A
58	C1	942	C
58	C1	946	A
58	C1	949	C
58	C1	951	G
58	C1	955	A

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Mol	Chain	Res	Type
58	C1	960	C
58	C1	962	A
58	C1	971	A
58	C1	976	G
58	C1	978	G
58	C1	982	G
58	C1	985	A
58	C1	989	A
58	C1	990	G
58	C1	1001	A
58	C1	1002	U
58	C1	1003	A
58	C1	1005	C
58	C1	1008	C
58	C1	1009	C
58	C1	1012	G
58	C1	1018	G
58	C1	1028	A
58	C1	1036	C
58	C1	1041	A
58	C1	1057	U
58	C1	1058	C
58	C1	1060	G
58	C1	1065	A
58	C1	1067	G
58	C1	1068	U
58	C1	1070	G
58	C1	1071	U
58	C1	1072	A
58	C1	1076	G
58	C1	1078	U
58	C1	1084	G
58	C1	1085	C
58	C1	1086	C
58	C1	1088	C
58	C1	1090	A
58	C1	1091	A
58	C1	1092	G
58	C1	1094	C
58	C1	1097	C
58	C1	1098	C
58	C1	1152	G

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Mol	Chain	Res	Type
58	C1	1155	G
58	C1	1157	G
58	C1	1158	U
58	C1	1159	G
58	C1	1160	G
58	C1	1161	C
58	C1	1163	C
58	C1	1167	G
58	C1	1171	A
58	C1	1174	A
58	C1	1179	C
58	C1	1180	G
58	C1	1183	G
58	C1	1184	C
58	C1	1185	U
58	C1	1186	U
58	C1	1189	G
58	C1	1200	A
58	C1	1204	U
58	C1	1205	G
58	C1	1215	G
58	C1	1216	G
58	C1	1217	G
58	C1	1218	A
58	C1	1219	U
58	C1	1220	G
58	C1	1222	C
58	C1	1223	C
58	C1	1224	C
58	C1	1239	G
58	C1	1248	A
58	C1	1249	U
58	C1	1254	A
58	C1	1255	U
58	C1	1257	A
58	C1	1262	C
58	C1	1264	A
58	C1	1265	C
58	C1	1268	G
58	C1	1287	A
58	C1	1292	A
58	C1	1293	G

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Mol	Chain	Res	Type
58	C1	1295	G
58	C1	1298	A
58	C1	1301	G
58	C1	1310	A
58	C1	1314	A
58	C1	1316	G
58	C1	1317	A
58	C1	1318	U
58	C1	1326	G
58	C1	1331	A
58	C1	1332	A
58	C1	1345	U
58	C1	1346	A
58	C1	1347	A
58	C1	1351	C
58	C1	1352	A
58	C1	1353	A
58	C1	1355	G
58	C1	1358	U
58	C1	1359	C
58	C1	1361	U
58	C1	1363	C
58	C1	1364	G
58	C1	1374	U
58	C1	1376	A
58	C1	1377	G
58	C1	1378	C
58	C1	1383	G
58	C1	1386	U
58	C1	1388	G
58	C1	1390	C
58	C1	1394	A
58	C1	1404	A
58	C1	1405	A
58	C1	1410	A
58	C1	1413	G
58	C1	1415	C
58	C1	1424	A
58	C1	1425	G
58	C1	1429	A
58	C1	1430	G
58	C1	1431	C

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Mol	Chain	Res	Type
58	C1	1436	U
58	C1	1441	U
58	C1	1442	U
58	C1	1452	C
58	C1	1453	C
58	C1	1461	G
58	C1	1462	C
58	C1	1464	A
58	C1	1465	U
58	C1	1466	G
58	C1	1472	A
58	C1	1473	C
58	C1	1474	G
58	C1	1478	U
58	C1	1482	C
58	C1	1490	A
58	C1	1491	C
58	C1	1494	G
58	C1	1495	A
58	C1	1496	G
58	C1	1498	C
58	C1	1499	A
58	C1	1501	G
58	C1	1506	A
58	C1	1507	G
58	C1	1513	C
58	C1	1517	A
58	C1	1521	G
58	C1	1524	G
58	C1	1527	U
58	C1	1528	G
58	C1	1529	G
58	C1	1530	G
58	C1	1535	A
58	C1	1536	G
58	C1	1538	C
58	C1	1539	A
58	C1	1540	A
58	C1	1541	A
58	C1	1542	U
58	C1	1543	C
58	C1	1547	C

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Mol	Chain	Res	Type
58	C1	1548	U
58	C1	1550	C
58	C1	1554	C
58	C1	1555	A
58	C1	1567	G
58	C1	1568	U
58	C1	1570	G
58	C1	1573	A
58	C1	1575	G
58	C1	1576	C
58	C1	1577	C
58	C1	1578	C
58	C1	1579	G
58	C1	1590	A
58	C1	1591	A
58	C1	1592	C
58	C1	1593	C
58	C1	1595	C
58	C1	1600	A
58	C1	1601	G
58	C1	1604	A
58	C1	1605	G
58	C1	1615	A
58	C1	1621	C
58	C1	1624	U
58	C1	1625	A
58	C1	1627	G
58	C1	1630	C
58	C1	1631	A
58	C1	1632	A
58	C1	1633	C
58	C1	1636	G
58	C1	1638	G
58	C1	1643	C
58	C1	1647	U
58	C1	1648	A
58	C1	1654	A
58	C1	1655	A
58	C1	1661	A
58	C1	1662	C
58	C1	1663	A
58	C1	1667	G

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Mol	Chain	Res	Type
58	C1	1670	C
58	C1	1676	C
58	C1	1686	C
58	C1	1693	G
58	C1	1694	C
58	C1	1698	A
58	C1	1699	G
58	C1	1700	A
58	C1	1709	C
58	C1	1713	G
58	C1	1720	G
58	C1	1724	G
58	C1	1727	G
58	C1	1732	C
58	C1	1740	C
58	C1	1741	G
58	C1	1742	G
58	C1	1744	A
58	C1	1745	G
58	C1	1747	A
58	C1	1749	G
58	C1	1766	A
58	C1	1767	U
58	C1	1769	A
58	C1	1770	G
58	C1	1775	G
58	C1	1778	G
58	C1	1780	G
58	C1	1783	G
58	C1	1792	A
58	C1	1793	G
58	C1	1794	G
58	C1	1803	A
58	C1	1806	G
58	C1	1810	A
58	C1	1821	A
58	C1	1828	U
58	C1	1829	G
58	C1	1830	C
58	C1	1831	G
58	C1	1832	A
58	C1	1846	G

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Mol	Chain	Res	Type
58	C1	1849	A
58	C1	1850	U
58	C1	1851	A
58	C1	1859	A
58	C1	1865	G
58	C1	1868	C
58	C1	1869	G
58	C1	1873	C
58	C1	1876	G
58	C1	1877	A
58	C1	1879	G
58	C1	1888	G
58	C1	1890	G
58	C1	1894	U
58	C1	1896	C
58	C1	1898	A
58	C1	1899	G
58	C1	1901	C
58	C1	1902	C
58	C1	1903	C
58	C1	1906	A
58	C1	1909	G
58	C1	1910	A
58	C1	1917	G
58	C1	1921	A
58	C1	1926	C
58	C1	1927	G
58	C1	1930	C
58	C1	1933	A
58	C1	1934	A
58	C1	1935	C
58	C1	1936	U
58	C1	1937	A
58	C1	1939	A
58	C1	1940	A
58	C1	1950	G
58	C1	1951	G
58	C1	1955	C
58	C1	1956	G
58	C1	1957	A
58	C1	1959	A
58	C1	1960	U

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Mol	Chain	Res	Type
58	C1	1961	U
58	C1	1968	C
58	C1	1976	U
58	C1	1977	U
58	C1	1983	C
58	C1	1984	U
58	C1	1985	G
58	C1	1986	C
58	C1	1988	C
58	C1	1989	G
58	C1	1990	A
58	C1	1991	A
58	C1	1992	A
58	C1	1993	A
58	C1	2003	C
58	C1	2008	G
58	C1	2012	U
58	C1	2013	G
58	C1	2014	U
58	C1	2018	G
58	C1	2044	G
58	C1	2047	C
58	C1	2052	A
58	C1	2054	A
58	C1	2055	U
58	C1	2057	C
58	C1	2060	C
58	C1	2062	U
58	C1	2064	C
58	C1	2073	G
58	C1	2076	C
58	C1	2077	G
58	C1	2080	A
58	C1	2081	A
58	C1	2082	G
58	C1	2083	A
58	C1	2084	C
58	C1	2085	C
58	C1	2086	C
58	C1	2090	G
58	C1	2091	G
58	C1	2114	G

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Mol	Chain	Res	Type
58	C1	2116	C
58	C1	2120	U
58	C1	2121	G
58	C1	2124	C
58	C1	2125	G
58	C1	2129	C
58	C1	2131	G
58	C1	2133	G
58	C1	2137	G
58	C1	2138	A
58	C1	2140	A
58	C1	2148	G
58	C1	2149	C
58	C1	2152	G
58	C1	2154	G
58	C1	2157	C
58	C1	2161	C
58	C1	2170	G
58	C1	2176	G
58	C1	2178	G
58	C1	2179	A
58	C1	2180	G
58	C1	2182	C
58	C1	2193	U
58	C1	2194	A
58	C1	2198	C
58	C1	2200	C
58	C1	2201	U
58	C1	2202	G
58	C1	2206	C
58	C1	2208	G
58	C1	2210	U
58	C1	2212	G
58	C1	2213	G
58	C1	2214	G
58	C1	2219	A
58	C1	2220	A
58	C1	2224	U
58	C1	2226	G
58	C1	2227	G
58	C1	2228	A
58	C1	2230	G

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Mol	Chain	Res	Type
58	C1	2236	A
58	C1	2237	C
58	C1	2240	C
58	C1	2246	G
58	C1	2249	G
58	C1	2250	G
58	C1	2256	U
58	C1	2257	G
58	C1	2286	C
58	C1	2291	G
58	C1	2294	C
58	C1	2297	A
58	C1	2298	A
58	C1	2299	A
58	C1	2310	G
58	C1	2314	G
58	C1	2315	G
58	C1	2316	A
58	C1	2318	G
58	C1	2319	G
58	C1	2320	A
58	C1	2322	A
58	C1	2323	U
58	C1	2324	C
58	C1	2327	C
58	C1	2329	G
58	C1	2330	G
58	C1	2331	A
58	C1	2332	G
58	C1	2336	G
58	C1	2345	G
58	C1	2346	A
58	C1	2347	A
58	C1	2351	G
58	C1	2353	C
58	C1	2357	A
58	C1	2358	C
58	C1	2361	C
58	C1	2371	A
58	C1	2394	G
58	C1	2396	C
58	C1	2409	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
58	C1	2413	C
58	C1	2417	U
58	C1	2421	G
58	C1	2434	U
58	C1	2436	A
58	C1	2440	G
58	C1	2441	A
58	C1	2442	U
58	C1	2450	A
58	C1	2451	C
58	C1	2452	C
58	C1	2459	A
58	C1	2460	U
58	C1	2463	C
58	C1	2469	G
58	C1	2475	C
58	C1	2476	C
58	C1	2480	A
58	C1	2481	G
58	C1	2485	C
58	C1	2487	A
58	C1	2488	C
58	C1	2489	A
58	C1	2493	G
58	C1	2494	C
58	C1	2495	G
58	C1	2502	U
58	C1	2508	A
58	C1	2513	G
58	C1	2516	G
58	C1	2517	U
58	C1	2518	C
58	C1	2529	A
58	C1	2532	C
58	C1	2535	G
58	C1	2540	G
58	C1	2542	A
58	C1	2554	G
58	C1	2556	G
58	C1	2558	U
58	C1	2565	U
58	C1	2566	U

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Mol	Chain	Res	Type
58	C1	2574	U
58	C1	2577	A
58	C1	2578	G
58	C1	2583	A
58	C1	2584	C
58	C1	2585	G
58	C1	2589	G
58	C1	2592	G
58	C1	2596	U
58	C1	2597	C
58	C1	2598	A
58	C1	2613	A
58	C1	2615	U
58	C1	2619	G
58	C1	2620	U
58	C1	2621	C
58	C1	2622	U
58	C1	2623	C
58	C1	2626	U
58	C1	2641	G
58	C1	2659	C
58	C1	2664	U
58	C1	2665	A
58	C1	2666	G
58	C1	2667	U
58	C1	2668	A
58	C1	2669	C
58	C1	2670	G
58	C1	2671	A
58	C1	2672	G
58	C1	2673	A
58	C1	2674	G
58	C1	2684	G
58	C1	2692	C
58	C1	2694	C
58	C1	2701	C
58	C1	2702	C
58	C1	2704	A
58	C1	2711	C
58	C1	2714	C
58	C1	2723	U
58	C1	2724	A

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Mol	Chain	Res	Type
58	C1	2725	A
58	C1	2732	U
58	C1	2738	U
58	C1	2742	C
58	C1	2745	A
58	C1	2746	A
58	C1	2760	A
58	C1	2764	C
58	C1	2770	A
58	C1	2774	G
58	C1	2776	A
58	C1	2777	A
58	C1	2778	G
58	C1	2782	G
58	C1	2787	A
58	C1	2790	A
58	C1	2791	U
58	C1	2792	G
58	C1	2801	C
58	C1	2802	A
58	C1	2803	C
58	C1	2805	G
58	C1	2806	C
58	C1	2808	U
58	C1	2809	C
58	C1	2811	A
58	C1	2812	G
58	C1	2813	C
58	C1	2814	C
58	C1	2817	U
58	C1	2827	G
58	C1	2829	A
58	C1	2830	A
58	C1	2832	A
58	C1	2839	G
58	C1	2842	G
58	C1	2843	G
58	C1	2844	A
58	C1	2853	G
58	C1	2858	U
58	C1	2859	A
58	C1	2872	C

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Mol	Chain	Res	Type
58	C1	2881	G
58	C1	2882	A
58	C1	2883	C
58	C1	2886	G
58	C1	2888	C
58	C1	2901	G
58	C1	2902	G
59	Cs	8	U
59	Cs	12	C
59	Cs	13	A
59	Cs	15	A
59	Cs	16	G
59	Cs	21	G
59	Cs	25	A
59	Cs	26	A
59	Cs	28	C
59	Cs	31	C
59	Cs	32	C
59	Cs	40	U
59	Cs	42	C
59	Cs	43	C
59	Cs	45	A
59	Cs	47	C
59	Cs	52	A
59	Cs	53	A
59	Cs	54	G
59	Cs	56	G
59	Cs	67	G
59	Cs	73	A
59	Cs	81	G
59	Cs	82	G
59	Cs	86	G
59	Cs	88	C
59	Cs	89	G
59	Cs	90	A
59	Cs	91	C
59	Cs	97	G
59	Cs	101	G
59	Cs	106	G
59	Cs	109	C
59	Cs	110	G
59	Cs	113	G

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Mol	Chain	Res	Type
60	D2	41	C
60	D2	42	C
60	D2	43	C
60	D2	47	U
60	D2	48	C
60	D2	50	U
60	D2	52	G
60	D2	53	G
25	D3	2	C
25	D3	6	G
25	D3	15	G
25	D3	16	U
25	D3	17	C
25	D3	18	G
25	D3	19	G
25	D3	20	U
25	D3	21	A
25	D3	22	G
25	D3	25	C
25	D3	29	G
25	D3	35	A
25	D3	36	A
25	D3	37	A
25	D3	39	U
25	D3	40	C
25	D3	41	C
25	D3	43	C
25	D3	46	G
25	D3	47	U
25	D3	51	U
25	D3	57	G
25	D3	59	U
25	D3	61	C
25	D3	64	A
25	D3	65	G
25	D3	67	C
25	D3	70	G
25	D3	73	A
25	D3	76	A
61	D4	3	C
61	D4	4	G
61	D4	5	G

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Mol	Chain	Res	Type
61	D4	8	U
61	D4	9	G
61	D4	12	G
61	D4	15	G
61	D4	17	C
61	D4	18	U
61	D4	19	G
61	D4	20	G
61	D4	21	U
61	D4	22	A
61	D4	26	C
61	D4	27	G
61	D4	44	A
61	D4	48	U
61	D4	49	C
61	D4	50	G
61	D4	64	G
61	D4	68	C
61	D4	74	A
61	D4	75	C
59	Ds	8	U
59	Ds	12	C
59	Ds	13	A
59	Ds	15	A
59	Ds	16	G
59	Ds	21	G
59	Ds	22	U
59	Ds	24	G
59	Ds	26	A
59	Ds	27	C
59	Ds	31	C
59	Ds	32	C
59	Ds	33	G
59	Ds	35	U
59	Ds	40	U
59	Ds	41	U
59	Ds	42	C
59	Ds	44	G
59	Ds	45	A
59	Ds	47	C
59	Ds	53	A
59	Ds	56	G

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Mol	Chain	Res	Type
59	Ds	57	A
59	Ds	67	G
59	Ds	73	A
59	Ds	75	G
59	Ds	81	G
59	Ds	82	G
59	Ds	88	C
59	Ds	89	G
59	Ds	90	A
59	Ds	91	C
59	Ds	102	A
59	Ds	106	G
59	Ds	109	C
59	Ds	110	G
59	Ds	112	U
59	Ds	113	G
59	Ds	117	G
59	Ds	118	G
58	D1	8	U
58	D1	9	G
58	D1	10	G
58	D1	33	C
58	D1	37	A
58	D1	40	C
58	D1	44	C
58	D1	47	A
58	D1	48	U
58	D1	53	G
58	D1	56	G
58	D1	57	U
58	D1	61	U
58	D1	67	C
58	D1	69	A
58	D1	70	U
58	D1	72	A
58	D1	73	G
58	D1	82	A
58	D1	84	C
58	D1	86	G
58	D1	88	U
58	D1	91	C
58	D1	92	G

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Mol	Chain	Res	Type
58	D1	93	G
58	D1	98	G
58	D1	99	G
58	D1	100	A
58	D1	107	G
58	D1	110	G
58	D1	115	A
58	D1	116	A
58	D1	117	U
58	D1	120	G
58	D1	126	C
58	D1	128	G
58	D1	136	G
58	D1	137	G
58	D1	138	A
58	D1	139	A
58	D1	142	C
58	D1	147	C
58	D1	148	A
58	D1	153	G
58	D1	154	C
58	D1	158	U
58	D1	159	G
58	D1	162	C
58	D1	163	G
58	D1	169	A
58	D1	176	G
58	D1	184	A
58	D1	185	A
58	D1	187	A
58	D1	188	U
58	D1	192	A
58	D1	193	G
58	D1	203	G
58	D1	204	A
58	D1	209	A
58	D1	210	A
58	D1	213	A
58	D1	216	A
58	D1	217	A
58	D1	218	U
58	D1	221	A

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Mol	Chain	Res	Type
58	D1	233	G
58	D1	234	C
58	D1	236	G
58	D1	237	C
58	D1	240	G
58	D1	248	G
58	D1	249	G
58	D1	255	C
58	D1	256	C
58	D1	266	C
58	D1	267	G
58	D1	269	C
58	D1	270	U
58	D1	271	U
58	D1	272	G
58	D1	273	U
58	D1	274	C
58	D1	275	C
58	D1	277	G
58	D1	282	G
58	D1	284	U
58	D1	285	C
58	D1	294	C
58	D1	295	U
58	D1	296	C
58	D1	297	G
58	D1	298	G
58	D1	303	C
58	D1	311	C
58	D1	321	G
58	D1	333	A
58	D1	334	A
58	D1	348	G
58	D1	352	G
58	D1	353	A
58	D1	354	A
58	D1	355	A
58	D1	356	G
58	D1	372	G
58	D1	375	G
58	D1	376	G
58	D1	385	U

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Mol	Chain	Res	Type
58	D1	386	G
58	D1	388	G
58	D1	391	U
58	D1	392	A
58	D1	395	C
58	D1	396	G
58	D1	398	G
58	D1	412	G
58	D1	413	U
58	D1	414	G
58	D1	417	G
58	D1	422	G
58	D1	431	U
58	D1	432	G
58	D1	433	G
58	D1	437	G
58	D1	438	A
58	D1	440	C
58	D1	442	C
58	D1	444	G
58	D1	447	U
58	D1	452	C
58	D1	454	A
58	D1	467	G
58	D1	469	C
58	D1	473	U
58	D1	479	A
58	D1	481	C
58	D1	482	A
58	D1	495	A
58	D1	496	A
58	D1	497	A
58	D1	498	G
58	D1	500	U
58	D1	504	A
58	D1	506	G
58	D1	517	G
58	D1	518	G
58	D1	529	A
58	D1	532	G
58	D1	533	C
58	D1	549	U

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Mol	Chain	Res	Type
58	D1	552	A
58	D1	553	A
58	D1	554	G
58	D1	555	C
58	D1	556	A
58	D1	557	G
58	D1	566	C
58	D1	567	C
58	D1	571	A
58	D1	583	G
58	D1	585	G
58	D1	595	G
58	D1	597	A
58	D1	608	A
58	D1	610	U
58	D1	615	G
58	D1	624	G
58	D1	626	G
58	D1	629	U
58	D1	632	G
58	D1	636	U
58	D1	638	G
58	D1	640	G
58	D1	641	G
58	D1	644	G
58	D1	645	A
58	D1	646	G
58	D1	650	U
58	D1	651	A
58	D1	653	G
58	D1	658	C
58	D1	661	A
58	D1	669	C
58	D1	670	A
58	D1	675	G
58	D1	676	C
58	D1	703	U
58	D1	705	C
58	D1	714	G
58	D1	715	G
58	D1	716	A
58	D1	732	G

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Mol	Chain	Res	Type
58	D1	733	C
58	D1	747	G
58	D1	750	G
58	D1	753	G
58	D1	754	C
58	D1	763	G
58	D1	767	C
58	D1	768	A
58	D1	775	G
58	D1	776	C
58	D1	784	G
58	D1	799	C
58	D1	805	G
58	D1	808	U
58	D1	809	G
58	D1	810	A
58	D1	811	G
58	D1	821	G
58	D1	822	G
58	D1	825	U
58	D1	828	A
58	D1	830	A
58	D1	831	G
58	D1	836	C
58	D1	837	C
58	D1	838	G
58	D1	842	C
58	D1	844	G
58	D1	851	G
58	D1	858	C
58	D1	865	A
58	D1	873	U
58	D1	874	U
58	D1	876	G
58	D1	878	G
58	D1	891	G
58	D1	894	G
58	D1	900	G
58	D1	902	C
58	D1	904	U
58	D1	905	G
58	D1	912	A

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Mol	Chain	Res	Type
58	D1	915	G
58	D1	917	U
58	D1	924	A
58	D1	928	G
58	D1	933	A
58	D1	936	A
58	D1	941	A
58	D1	942	C
58	D1	946	A
58	D1	949	C
58	D1	951	G
58	D1	952	U
58	D1	955	A
58	D1	960	C
58	D1	962	A
58	D1	972	G
58	D1	976	G
58	D1	978	G
58	D1	982	G
58	D1	985	A
58	D1	989	A
58	D1	990	G
58	D1	1002	U
58	D1	1003	A
58	D1	1005	C
58	D1	1008	C
58	D1	1009	C
58	D1	1018	G
58	D1	1019	C
58	D1	1028	A
58	D1	1036	C
58	D1	1041	A
58	D1	1047	G
58	D1	1050	C
58	D1	1057	U
58	D1	1058	C
58	D1	1060	G
58	D1	1065	A
58	D1	1067	G
58	D1	1068	U
58	D1	1070	G
58	D1	1071	U

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Mol	Chain	Res	Type
58	D1	1072	A
58	D1	1076	G
58	D1	1079	G
58	D1	1084	G
58	D1	1088	C
58	D1	1090	A
58	D1	1091	A
58	D1	1092	G
58	D1	1093	A
58	D1	1094	C
58	D1	1096	G
58	D1	1097	C
58	D1	1098	C
58	D1	1152	G
58	D1	1153	U
58	D1	1155	G
58	D1	1156	A
58	D1	1159	G
58	D1	1160	G
58	D1	1167	G
58	D1	1173	A
58	D1	1175	U
58	D1	1179	C
58	D1	1180	G
58	D1	1181	G
58	D1	1183	G
58	D1	1185	U
58	D1	1186	U
58	D1	1187	A
58	D1	1188	A
58	D1	1189	G
58	D1	1197	C
58	D1	1199	G
58	D1	1200	A
58	D1	1201	A
58	D1	1212	U
58	D1	1216	G
58	D1	1217	G
58	D1	1218	A
58	D1	1219	U
58	D1	1220	G
58	D1	1222	C

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Mol	Chain	Res	Type
58	D1	1223	C
58	D1	1224	C
58	D1	1233	A
58	D1	1239	G
58	D1	1244	C
58	D1	1248	A
58	D1	1249	U
58	D1	1252	C
58	D1	1254	A
58	D1	1255	U
58	D1	1265	C
58	D1	1268	G
58	D1	1281	G
58	D1	1287	A
58	D1	1291	A
58	D1	1292	A
58	D1	1293	G
58	D1	1295	G
58	D1	1298	A
58	D1	1299	A
58	D1	1301	G
58	D1	1310	A
58	D1	1314	A
58	D1	1316	G
58	D1	1317	A
58	D1	1318	U
58	D1	1325	G
58	D1	1326	G
58	D1	1331	A
58	D1	1332	A
58	D1	1343	C
58	D1	1345	U
58	D1	1346	A
58	D1	1347	A
58	D1	1351	C
58	D1	1352	A
58	D1	1358	U
58	D1	1359	C
58	D1	1364	G
58	D1	1366	A
58	D1	1377	G
58	D1	1383	G

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Mol	Chain	Res	Type
58	D1	1390	C
58	D1	1392	G
58	D1	1394	A
58	D1	1397	U
58	D1	1400	G
58	D1	1404	A
58	D1	1405	A
58	D1	1410	A
58	D1	1413	G
58	D1	1415	C
58	D1	1422	G
58	D1	1423	A
58	D1	1424	A
58	D1	1425	G
58	D1	1429	A
58	D1	1430	G
58	D1	1431	C
58	D1	1433	G
58	D1	1436	U
58	D1	1439	U
58	D1	1448	C
58	D1	1451	U
58	D1	1452	C
58	D1	1459	G
58	D1	1461	G
58	D1	1462	C
58	D1	1464	A
58	D1	1465	U
58	D1	1472	A
58	D1	1473	C
58	D1	1478	U
58	D1	1482	C
58	D1	1486	G
58	D1	1490	A
58	D1	1495	A
58	D1	1496	G
58	D1	1498	C
58	D1	1499	A
58	D1	1501	G
58	D1	1506	A
58	D1	1507	G
58	D1	1512	G

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Mol	Chain	Res	Type
58	D1	1513	C
58	D1	1515	A
58	D1	1517	A
58	D1	1520	C
58	D1	1521	G
58	D1	1523	A
58	D1	1524	G
58	D1	1527	U
58	D1	1528	G
58	D1	1530	G
58	D1	1535	A
58	D1	1536	G
58	D1	1538	C
58	D1	1539	A
58	D1	1540	A
58	D1	1541	A
58	D1	1542	U
58	D1	1543	C
58	D1	1544	C
58	D1	1547	C
58	D1	1548	U
58	D1	1550	C
58	D1	1551	C
58	D1	1554	C
58	D1	1555	A
58	D1	1559	U
58	D1	1573	A
58	D1	1575	G
58	D1	1576	C
58	D1	1577	C
58	D1	1578	C
58	D1	1579	G
58	D1	1590	A
58	D1	1591	A
58	D1	1593	C
58	D1	1595	C
58	D1	1600	A
58	D1	1604	A
58	D1	1605	G
58	D1	1612	A
58	D1	1615	A
58	D1	1621	C

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Mol	Chain	Res	Type
58	D1	1624	U
58	D1	1625	A
58	D1	1626	A
58	D1	1630	C
58	D1	1631	A
58	D1	1632	A
58	D1	1633	C
58	D1	1636	G
58	D1	1638	G
58	D1	1643	C
58	D1	1647	U
58	D1	1648	A
58	D1	1653	A
58	D1	1655	A
58	D1	1658	G
58	D1	1661	A
58	D1	1662	C
58	D1	1663	A
58	D1	1667	G
58	D1	1677	A
58	D1	1685	U
58	D1	1686	C
58	D1	1693	G
58	D1	1694	C
58	D1	1698	A
58	D1	1699	G
58	D1	1700	A
58	D1	1720	G
58	D1	1725	U
58	D1	1732	C
58	D1	1734	U
58	D1	1740	C
58	D1	1741	G
58	D1	1742	G
58	D1	1744	A
58	D1	1745	G
58	D1	1746	A
58	D1	1747	A
58	D1	1763	G
58	D1	1766	A
58	D1	1767	U
58	D1	1768	G

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Mol	Chain	Res	Type
58	D1	1769	A
58	D1	1770	G
58	D1	1772	C
58	D1	1773	C
58	D1	1774	C
58	D1	1775	G
58	D1	1777	G
58	D1	1778	G
58	D1	1779	A
58	D1	1780	G
58	D1	1785	A
58	D1	1792	A
58	D1	1793	G
58	D1	1794	G
58	D1	1803	A
58	D1	1810	A
58	D1	1812	C
58	D1	1817	A
58	D1	1821	A
58	D1	1829	G
58	D1	1830	C
58	D1	1831	G
58	D1	1832	A
58	D1	1842	A
58	D1	1846	G
58	D1	1849	A
58	D1	1850	U
58	D1	1851	A
58	D1	1856	G
58	D1	1865	G
58	D1	1868	C
58	D1	1869	G
58	D1	1870	G
58	D1	1873	C
58	D1	1876	G
58	D1	1877	A
58	D1	1879	G
58	D1	1888	G
58	D1	1890	G
58	D1	1894	U
58	D1	1895	G
58	D1	1896	C

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Mol	Chain	Res	Type
58	D1	1897	A
58	D1	1898	A
58	D1	1899	G
58	D1	1902	C
58	D1	1903	C
58	D1	1906	A
58	D1	1907	C
58	D1	1909	G
58	D1	1910	A
58	D1	1917	G
58	D1	1921	A
58	D1	1922	A
58	D1	1923	C
58	D1	1924	G
58	D1	1926	C
58	D1	1927	G
58	D1	1933	A
58	D1	1934	A
58	D1	1950	G
58	D1	1951	G
58	D1	1955	C
58	D1	1956	G
58	D1	1957	A
58	D1	1959	A
58	D1	1965	U
58	D1	1968	C
58	D1	1976	U
58	D1	1983	C
58	D1	1984	U
58	D1	1988	C
58	D1	1989	G
58	D1	1990	A
58	D1	1991	A
58	D1	1992	A
58	D1	1993	A
58	D1	2002	A
58	D1	2003	C
58	D1	2005	G
58	D1	2007	A
58	D1	2008	G
58	D1	2012	U
58	D1	2013	G

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Mol	Chain	Res	Type
58	D1	2014	U
58	D1	2018	G
58	D1	2044	G
58	D1	2048	G
58	D1	2052	A
58	D1	2054	A
58	D1	2055	U
58	D1	2056	G
58	D1	2057	C
58	D1	2060	C
58	D1	2064	C
58	D1	2076	C
58	D1	2077	G
58	D1	2081	A
58	D1	2082	G
58	D1	2083	A
58	D1	2084	C
58	D1	2085	C
58	D1	2087	C
58	D1	2090	G
58	D1	2107	U
58	D1	2110	U
58	D1	2114	G
58	D1	2116	C
58	D1	2120	U
58	D1	2121	G
58	D1	2123	U
58	D1	2124	C
58	D1	2125	G
58	D1	2126	C
58	D1	2128	C
58	D1	2131	G
58	D1	2133	G
58	D1	2137	G
58	D1	2138	A
58	D1	2139	U
58	D1	2142	G
58	D1	2143	U
58	D1	2144	G
58	D1	2148	G
58	D1	2152	G
58	D1	2154	G

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Mol	Chain	Res	Type
58	D1	2155	A
58	D1	2156	A
58	D1	2157	C
58	D1	2162	G
58	D1	2168	G
58	D1	2170	G
58	D1	2180	G
58	D1	2193	U
58	D1	2194	A
58	D1	2198	C
58	D1	2200	C
58	D1	2201	U
58	D1	2203	G
58	D1	2206	C
58	D1	2208	G
58	D1	2210	U
58	D1	2211	G
58	D1	2212	G
58	D1	2213	G
58	D1	2214	G
58	D1	2219	A
58	D1	2220	A
58	D1	2224	U
58	D1	2227	G
58	D1	2228	A
58	D1	2229	U
58	D1	2230	G
58	D1	2236	A
58	D1	2237	C
58	D1	2245	G
58	D1	2246	G
58	D1	2249	G
58	D1	2250	G
58	D1	2251	C
58	D1	2256	U
58	D1	2257	G
58	D1	2262	G
58	D1	2286	C
58	D1	2289	A
58	D1	2294	C
58	D1	2297	A
58	D1	2298	A

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Mol	Chain	Res	Type
58	D1	2299	A
58	D1	2313	G
58	D1	2314	G
58	D1	2316	A
58	D1	2318	G
58	D1	2319	G
58	D1	2320	A
58	D1	2323	U
58	D1	2324	C
58	D1	2329	G
58	D1	2330	G
58	D1	2331	A
58	D1	2333	A
58	D1	2336	G
58	D1	2338	A
58	D1	2345	G
58	D1	2346	A
58	D1	2347	A
58	D1	2351	G
58	D1	2356	G
58	D1	2357	A
58	D1	2358	C
58	D1	2361	C
58	D1	2388	A
58	D1	2394	G
58	D1	2396	C
58	D1	2401	U
58	D1	2404	A
58	D1	2405	C
58	D1	2413	C
58	D1	2417	U
58	D1	2421	G
58	D1	2429	A
58	D1	2433	A
58	D1	2434	U
58	D1	2435	C
58	D1	2436	A
58	D1	2440	G
58	D1	2441	A
58	D1	2446	A
58	D1	2449	U
58	D1	2450	A

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Mol	Chain	Res	Type
58	D1	2451	C
58	D1	2452	C
58	D1	2453	C
58	D1	2459	A
58	D1	2460	U
58	D1	2462	A
58	D1	2463	C
58	D1	2464	A
58	D1	2476	C
58	D1	2479	G
58	D1	2480	A
58	D1	2481	G
58	D1	2484	U
58	D1	2485	C
58	D1	2487	A
58	D1	2488	C
58	D1	2489	A
58	D1	2492	G
58	D1	2493	G
58	D1	2494	C
58	D1	2495	G
58	D1	2502	U
58	D1	2509	C
58	D1	2510	C
58	D1	2512	C
58	D1	2513	G
58	D1	2516	G
58	D1	2517	U
58	D1	2529	A
58	D1	2531	C
58	D1	2535	G
58	D1	2536	G
58	D1	2540	G
58	D1	2542	A
58	D1	2553	A
58	D1	2554	G
58	D1	2556	G
58	D1	2558	U
58	D1	2563	U
58	D1	2565	U
58	D1	2568	G
58	D1	2577	A

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Mol	Chain	Res	Type
58	D1	2578	G
58	D1	2592	G
58	D1	2595	U
58	D1	2596	U
58	D1	2598	A
58	D1	2612	C
58	D1	2613	A
58	D1	2619	G
58	D1	2620	U
58	D1	2622	U
58	D1	2623	C
58	D1	2626	U
58	D1	2641	G
58	D1	2656	G
58	D1	2664	U
58	D1	2665	A
58	D1	2666	G
58	D1	2667	U
58	D1	2668	A
58	D1	2669	C
58	D1	2671	A
58	D1	2672	G
58	D1	2673	A
58	D1	2674	G
58	D1	2677	C
58	D1	2684	G
58	D1	2690	A
58	D1	2694	C
58	D1	2701	C
58	D1	2702	C
58	D1	2713	U
58	D1	2714	C
58	D1	2722	A
58	D1	2723	U
58	D1	2724	A
58	D1	2725	A
58	D1	2732	U
58	D1	2738	U
58	D1	2739	G
58	D1	2742	C
58	D1	2745	A
58	D1	2746	A

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Mol	Chain	Res	Type
58	D1	2763	G
58	D1	2764	C
58	D1	2769	A
58	D1	2770	A
58	D1	2774	G
58	D1	2776	A
58	D1	2777	A
58	D1	2782	G
58	D1	2787	A
58	D1	2790	A
58	D1	2791	U
58	D1	2792	G
58	D1	2801	C
58	D1	2802	A
58	D1	2803	C
58	D1	2804	G
58	D1	2805	G
58	D1	2806	C
58	D1	2812	G
58	D1	2813	C
58	D1	2814	C
58	D1	2817	U
58	D1	2819	A
58	D1	2829	A
58	D1	2830	A
58	D1	2842	G
58	D1	2843	G
58	D1	2844	A
58	D1	2845	U
58	D1	2853	G
58	D1	2858	U
58	D1	2872	C
58	D1	2881	G
58	D1	2888	C
58	D1	2901	G
58	D1	2902	G
58	D1	2903	U
58	D1	2905	U
64	DV	2	C
64	DV	3	C
64	DV	12	U
64	DV	16	U

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Mol	Chain	Res	Type
64	DV	17	C
64	DV	18	G
64	DV	19	G
64	DV	30	G
64	DV	34	G
64	DV	49	G
64	DV	50	G
64	DV	51	G
64	DV	52	C
64	DV	54	C

All (326) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A2	14	A
1	A2	18	G
23	B2	13	A
25	C2	15	G
25	C2	17	C
25	C2	21	A
25	C2	47	U
25	C3	47	U
26	C4	9	G
26	C4	10	G
26	C4	16	C
26	C4	18	U
58	C1	47	A
58	C1	69	A
58	C1	72	A
58	C1	81	G
58	C1	88	U
58	C1	98	G
58	C1	99	G
58	C1	117	U
58	C1	125	C
58	C1	136	G
58	C1	187	A
58	C1	209	A
58	C1	216	A
58	C1	267	G
58	C1	284	U
58	C1	296	C

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Mol	Chain	Res	Type
58	C1	333	A
58	C1	354	A
58	C1	355	A
58	C1	375	G
58	C1	413	U
58	C1	430	C
58	C1	480	C
58	C1	495	A
58	C1	497	A
58	C1	499	G
58	C1	506	G
58	C1	527	A
58	C1	536	G
58	C1	554	G
58	C1	556	A
58	C1	566	C
58	C1	609	C
58	C1	625	A
58	C1	639	A
58	C1	715	G
58	C1	732	G
58	C1	792	A
58	C1	798	A
58	C1	810	A
58	C1	822	G
58	C1	836	C
58	C1	839	A
58	C1	873	U
58	C1	875	A
58	C1	904	U
58	C1	1018	G
58	C1	1067	G
58	C1	1071	U
58	C1	1085	C
58	C1	1151	A
58	C1	1156	A
58	C1	1254	A
58	C1	1298	A
58	C1	1331	A
58	C1	1333	U
58	C1	1345	U
58	C1	1346	A

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Mol	Chain	Res	Type
58	C1	1410	A
58	C1	1423	A
58	C1	1424	A
58	C1	1441	U
58	C1	1442	U
58	C1	1464	A
58	C1	1465	U
58	C1	1472	A
58	C1	1490	A
58	C1	1498	C
58	C1	1506	A
58	C1	1529	G
58	C1	1535	A
58	C1	1539	A
58	C1	1542	U
58	C1	1576	C
58	C1	1590	A
58	C1	1600	A
58	C1	1604	A
58	C1	1636	G
58	C1	1647	U
58	C1	1653	A
58	C1	1655	A
58	C1	1698	A
58	C1	1699	G
58	C1	1740	C
58	C1	1744	A
58	C1	1767	U
58	C1	1792	A
58	C1	1814	A
58	C1	1829	G
58	C1	1830	C
58	C1	1831	G
58	C1	1849	A
58	C1	1850	U
58	C1	1868	C
58	C1	1876	G
58	C1	1920	G
58	C1	1933	A
58	C1	1955	C
58	C1	1960	U
58	C1	1983	C

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Mol	Chain	Res	Type
58	C1	1984	U
58	C1	1991	A
58	C1	2013	G
58	C1	2018	G
58	C1	2054	A
58	C1	2056	G
58	C1	2086	C
58	C1	2147	A
58	C1	2167	C
58	C1	2178	G
58	C1	2192	A
58	C1	2193	U
58	C1	2212	G
58	C1	2227	G
58	C1	2236	A
58	C1	2260	U
58	C1	2293	G
58	C1	2319	G
58	C1	2321	A
58	C1	2322	A
58	C1	2329	G
58	C1	2330	G
58	C1	2331	A
58	C1	2346	A
58	C1	2356	G
58	C1	2357	A
58	C1	2402	G
58	C1	2416	G
58	C1	2433	A
58	C1	2450	A
58	C1	2459	A
58	C1	2475	C
58	C1	2492	G
58	C1	2517	U
58	C1	2528	C
58	C1	2553	A
58	C1	2592	G
58	C1	2596	U
58	C1	2620	U
58	C1	2622	U
58	C1	2666	G
58	C1	2673	A

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Mol	Chain	Res	Type
58	C1	2693	U
58	C1	2700	U
58	C1	2738	U
58	C1	2745	A
58	C1	2791	U
58	C1	2801	C
58	C1	2808	U
58	C1	2812	G
58	C1	2829	A
58	C1	2838	C
58	C1	2842	G
58	C1	2843	G
58	C1	2882	A
60	D2	47	U
25	D3	17	C
25	D3	35	A
25	D3	47	U
61	D4	3	C
61	D4	16	C
61	D4	17	C
61	D4	49	C
61	D4	73	A
58	D1	47	A
58	D1	56	G
58	D1	69	A
58	D1	72	A
58	D1	81	G
58	D1	98	G
58	D1	99	G
58	D1	116	A
58	D1	125	C
58	D1	136	G
58	D1	137	G
58	D1	138	A
58	D1	147	C
58	D1	158	U
58	D1	184	A
58	D1	187	A
58	D1	209	A
58	D1	284	U
58	D1	296	C
58	D1	306	A

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Mol	Chain	Res	Type
58	D1	333	A
58	D1	354	A
58	D1	355	A
58	D1	375	G
58	D1	413	U
58	D1	433	G
58	D1	495	A
58	D1	497	A
58	D1	499	G
58	D1	536	G
58	D1	552	A
58	D1	556	A
58	D1	566	C
58	D1	609	C
58	D1	625	A
58	D1	639	A
58	D1	715	G
58	D1	731	A
58	D1	792	A
58	D1	798	A
58	D1	810	A
58	D1	820	A
58	D1	836	C
58	D1	873	U
58	D1	904	U
58	D1	905	G
58	D1	912	A
58	D1	989	A
58	D1	1018	G
58	D1	1067	G
58	D1	1071	U
58	D1	1078	U
58	D1	1093	A
58	D1	1151	A
58	D1	1156	A
58	D1	1254	A
58	D1	1298	A
58	D1	1310	A
58	D1	1331	A
58	D1	1345	U
58	D1	1346	A
58	D1	1351	C

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Mol	Chain	Res	Type
58	D1	1423	A
58	D1	1424	A
58	D1	1448	C
58	D1	1464	A
58	D1	1472	A
58	D1	1498	C
58	D1	1505	G
58	D1	1529	G
58	D1	1535	A
58	D1	1538	C
58	D1	1539	A
58	D1	1542	U
58	D1	1576	C
58	D1	1590	A
58	D1	1600	A
58	D1	1604	A
58	D1	1605	G
58	D1	1630	C
58	D1	1647	U
58	D1	1653	A
58	D1	1698	A
58	D1	1699	G
58	D1	1740	C
58	D1	1792	A
58	D1	1811	C
58	D1	1814	A
58	D1	1816	A
58	D1	1829	G
58	D1	1849	A
58	D1	1850	U
58	D1	1868	C
58	D1	1876	G
58	D1	1906	A
58	D1	1920	G
58	D1	1921	A
58	D1	1933	A
58	D1	1955	C
58	D1	1983	C
58	D1	1987	A
58	D1	1991	A
58	D1	2005	G
58	D1	2013	G

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Mol	Chain	Res	Type
58	D1	2052	A
58	D1	2054	A
58	D1	2056	G
58	D1	2083	A
58	D1	2147	A
58	D1	2192	A
58	D1	2193	U
58	D1	2212	G
58	D1	2236	A
58	D1	2293	G
58	D1	2319	G
58	D1	2329	G
58	D1	2330	G
58	D1	2345	G
58	D1	2346	A
58	D1	2356	G
58	D1	2416	G
58	D1	2433	A
58	D1	2439	G
58	D1	2450	A
58	D1	2458	G
58	D1	2475	C
58	D1	2492	G
58	D1	2553	A
58	D1	2577	A
58	D1	2592	G
58	D1	2620	U
58	D1	2622	U
58	D1	2666	G
58	D1	2673	A
58	D1	2693	U
58	D1	2700	U
58	D1	2738	U
58	D1	2745	A
58	D1	2768	U
58	D1	2791	U
58	D1	2801	C
58	D1	2803	C
58	D1	2808	U
58	D1	2809	C
58	D1	2812	G
58	D1	2829	A

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Mol	Chain	Res	Type
58	D1	2842	G
58	D1	2843	G
58	D1	2858	U
64	DV	15	G

## 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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
65	PAR	Bb	1601	-	45,45,45	1.52	7 (15%)	64,67,67	2.16	20 (31%)
65	PAR	Ab	1601	-	45,45,45	1.41	5 (11%)	64,67,67	1.82	13 (20%)
66	3V6	D1	3001	67	21,25,25	2.33	9 (42%)	21,39,39	2.98	8 (38%)
66	3V6	C1	3001	67	21,25,25	2.10	8 (38%)	21,39,39	2.07	6 (28%)

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
65	PAR	Bb	1601	-	-	9/18/94/94	0/4/4/4
65	PAR	Ab	1601	-	-	7/18/94/94	2/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
66	3V6	D1	3001	67	-	4/12/53/53	0/2/2/2
66	3V6	C1	3001	67	-	2/12/53/53	0/2/2/2

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
65	Bb	1601	PAR	C41-C51	5.97	1.65	1.53
66	D1	3001	3V6	CAK-CAN	-5.26	1.42	1.49
65	Ab	1601	PAR	C34-C24	-5.17	1.47	1.53
66	C1	3001	3V6	CAK-CAS	4.31	1.64	1.53
66	D1	3001	3V6	CAS-CAU	3.99	1.59	1.52
66	C1	3001	3V6	CAV-NAL	3.71	1.50	1.45
66	D1	3001	3V6	CAV-NAL	3.39	1.50	1.45
66	C1	3001	3V6	CAK-CAN	-3.38	1.44	1.49
66	D1	3001	3V6	OAE-CAO	3.34	1.28	1.21
66	D1	3001	3V6	CAW-CAQ	-3.31	1.45	1.51
65	Ab	1601	PAR	O33-C33	-3.26	1.35	1.43
65	Bb	1601	PAR	C22-C32	-3.18	1.46	1.53
66	C1	3001	3V6	OAG-CAN	2.95	1.40	1.32
66	C1	3001	3V6	CAQ-CAN	2.94	1.42	1.37
65	Ab	1601	PAR	C11-C21	2.83	1.57	1.52
65	Bb	1601	PAR	C62-C12	-2.65	1.48	1.53
66	D1	3001	3V6	CAQ-CAN	2.61	1.42	1.37
66	D1	3001	3V6	CAT-CLJ	-2.49	1.73	1.78
66	C1	3001	3V6	CAT-CLJ	-2.43	1.73	1.78
66	D1	3001	3V6	OAM-CAX	2.28	1.53	1.47
65	Ab	1601	PAR	O23-C23	2.26	1.48	1.43
66	C1	3001	3V6	CAO-CAQ	-2.26	1.40	1.44
66	C1	3001	3V6	CAW-CAQ	-2.22	1.47	1.51
65	Bb	1601	PAR	O62-C62	2.12	1.48	1.43
65	Bb	1601	PAR	C44-C34	2.11	1.57	1.52
65	Ab	1601	PAR	C33-C43	-2.08	1.47	1.52
66	D1	3001	3V6	CAB-CAS	2.04	1.58	1.53
65	Bb	1601	PAR	C11-C21	2.02	1.56	1.52
65	Bb	1601	PAR	O11-C42	2.01	1.49	1.43

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
65	Ab	1601	PAR	O52-C13-O43	-8.43	102.30	111.43
65	Bb	1601	PAR	O54-C54-C64	-8.17	90.80	106.01
66	D1	3001	3V6	OAM-CAO-OAE	8.11	127.88	117.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
66	D1	3001	3V6	OAG-CAN-CAQ	-5.45	114.56	123.13
65	Bb	1601	PAR	O52-C13-O43	-5.39	105.59	111.43
66	D1	3001	3V6	OAE-CAO-CAQ	-4.99	118.86	125.50
65	Bb	1601	PAR	O51-C51-C41	4.66	118.16	109.69
66	D1	3001	3V6	CLJ-CAT-CLI	-4.61	100.97	108.81
66	C1	3001	3V6	CAB-CAS-CAK	4.35	116.78	110.75
66	C1	3001	3V6	OAE-CAO-CAQ	-4.28	119.80	125.50
65	Ab	1601	PAR	C13-O52-C52	-4.18	107.62	117.96
66	C1	3001	3V6	OAG-CAN-CAK	3.92	119.71	113.28
65	Bb	1601	PAR	C32-C22-C12	-3.73	103.52	111.18
65	Bb	1601	PAR	C53-C43-C33	-3.57	103.46	114.85
65	Bb	1601	PAR	C14-O54-C54	3.56	120.68	113.69
66	C1	3001	3V6	OAG-CAN-CAQ	-3.29	117.97	123.13
65	Ab	1601	PAR	C11-C21-N21	3.23	116.03	110.20
65	Bb	1601	PAR	O33-C14-O54	-3.23	101.66	110.67
66	C1	3001	3V6	CLJ-CAT-CLI	-3.15	103.45	108.81
66	D1	3001	3V6	OAG-CAN-CAK	3.13	118.41	113.28
65	Bb	1601	PAR	C13-O52-C52	-3.10	110.29	117.96
65	Bb	1601	PAR	C44-C34-C24	3.06	116.32	111.07
65	Ab	1601	PAR	C14-O33-C33	-3.05	110.42	117.96
66	C1	3001	3V6	OAM-CAO-OAE	2.91	121.28	117.58
65	Bb	1601	PAR	O41-C41-C31	-2.89	103.66	110.35
65	Bb	1601	PAR	O54-C54-C44	2.82	114.81	109.69
65	Bb	1601	PAR	O53-C53-C43	-2.67	102.14	111.29
66	D1	3001	3V6	CAK-CAN-CAQ	2.66	126.99	123.63
66	D1	3001	3V6	OAM-CAX-CAC	2.63	111.43	105.65
65	Ab	1601	PAR	C41-C31-C21	-2.59	106.61	111.07
65	Ab	1601	PAR	C64-C54-C44	-2.56	108.06	113.10
65	Bb	1601	PAR	O43-C43-C53	2.54	114.70	109.21
65	Ab	1601	PAR	C44-C34-C24	-2.44	106.88	111.07
65	Bb	1601	PAR	C11-O11-C42	2.44	124.00	117.96
65	Bb	1601	PAR	C31-C41-C51	2.41	114.54	110.24
66	D1	3001	3V6	CAB-CAS-CAU	2.37	115.65	112.44
65	Ab	1601	PAR	O51-C51-C61	2.32	112.22	106.44
65	Ab	1601	PAR	C23-C33-C43	2.30	107.30	103.22
65	Ab	1601	PAR	C53-C43-C33	-2.27	107.59	114.85
65	Bb	1601	PAR	C34-C44-C54	2.26	114.28	110.24
65	Ab	1601	PAR	O62-C62-C12	2.21	113.87	109.81
65	Bb	1601	PAR	O52-C13-C23	2.17	112.46	107.96
65	Bb	1601	PAR	O41-C41-C51	2.15	114.64	109.30
65	Bb	1601	PAR	C11-C21-C31	2.08	115.66	110.21
65	Ab	1601	PAR	O43-C13-C23	2.07	107.64	104.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
65	Bb	1601	PAR	O54-C14-C24	2.05	114.66	110.06
65	Ab	1601	PAR	C13-C23-C33	-2.03	99.66	102.10

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
66	D1	3001	3V6	O-C-CA-CB
65	Bb	1601	PAR	C21-C11-O11-C42
65	Ab	1601	PAR	C23-C13-O52-C52
65	Ab	1601	PAR	O43-C13-O52-C52
66	C1	3001	3V6	NAL-C-CA-CB
65	Bb	1601	PAR	C41-C51-C61-O61
65	Bb	1601	PAR	O43-C43-C53-O53
65	Bb	1601	PAR	C33-C43-C53-O53
65	Bb	1601	PAR	O51-C51-C61-O61
65	Bb	1601	PAR	O51-C11-O11-C42
65	Ab	1601	PAR	C52-C42-O11-C11
66	D1	3001	3V6	O-C-CA-N
65	Ab	1601	PAR	O51-C51-C61-O61
65	Bb	1601	PAR	C52-C42-O11-C11
65	Ab	1601	PAR	O54-C14-O33-C33
66	D1	3001	3V6	NAL-C-CA-N
66	D1	3001	3V6	NAL-C-CA-CB
66	C1	3001	3V6	O-C-CA-CB
65	Ab	1601	PAR	C32-C42-O11-C11
65	Bb	1601	PAR	C43-C33-O33-C14
65	Ab	1601	PAR	C44-C54-C64-N64
65	Bb	1601	PAR	C24-C14-O33-C33

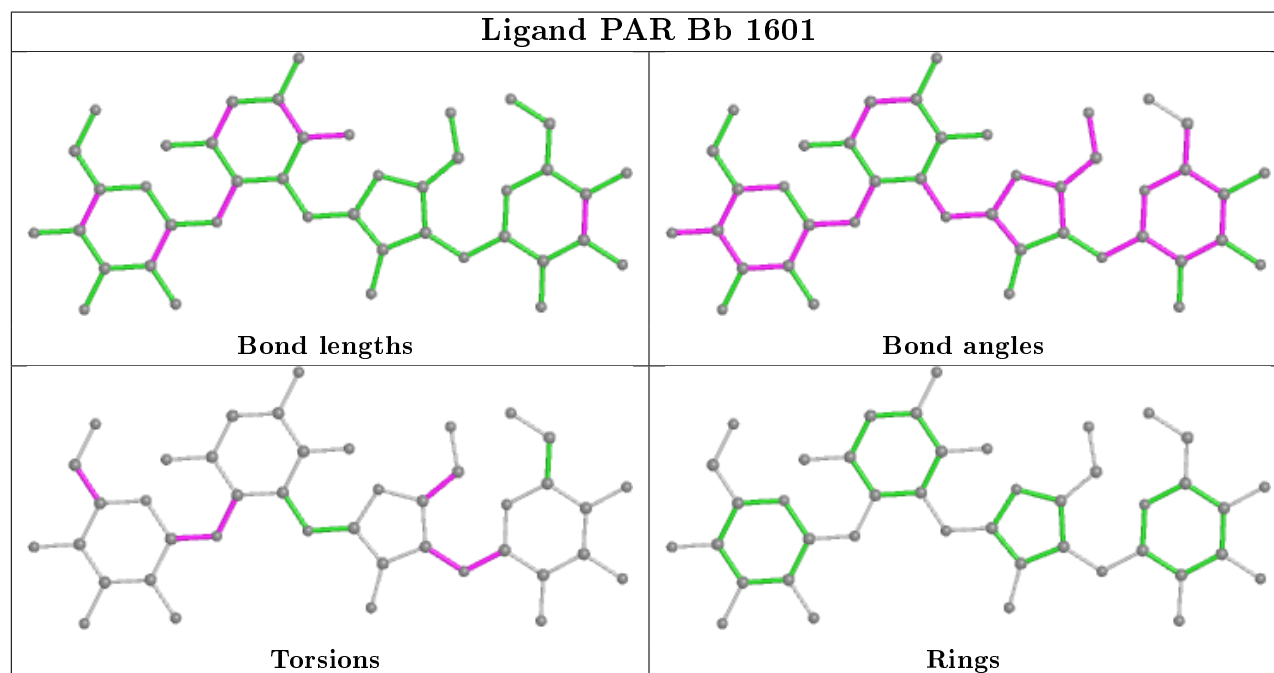
All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
65	Ab	1601	PAR	C14-C24-C34-C44-C54-O54
65	Ab	1601	PAR	C12-C22-C32-C42-C52-C62

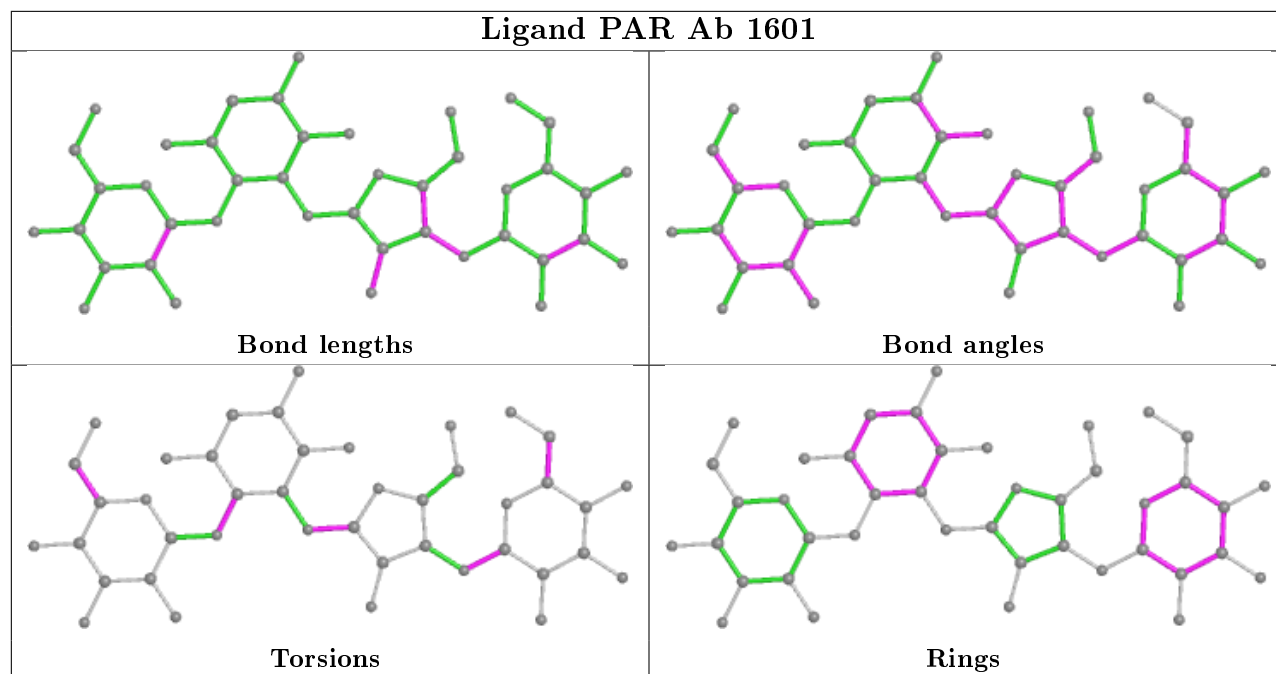
2 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
66	D1	3001	3V6	11	0
66	C1	3001	3V6	5	0

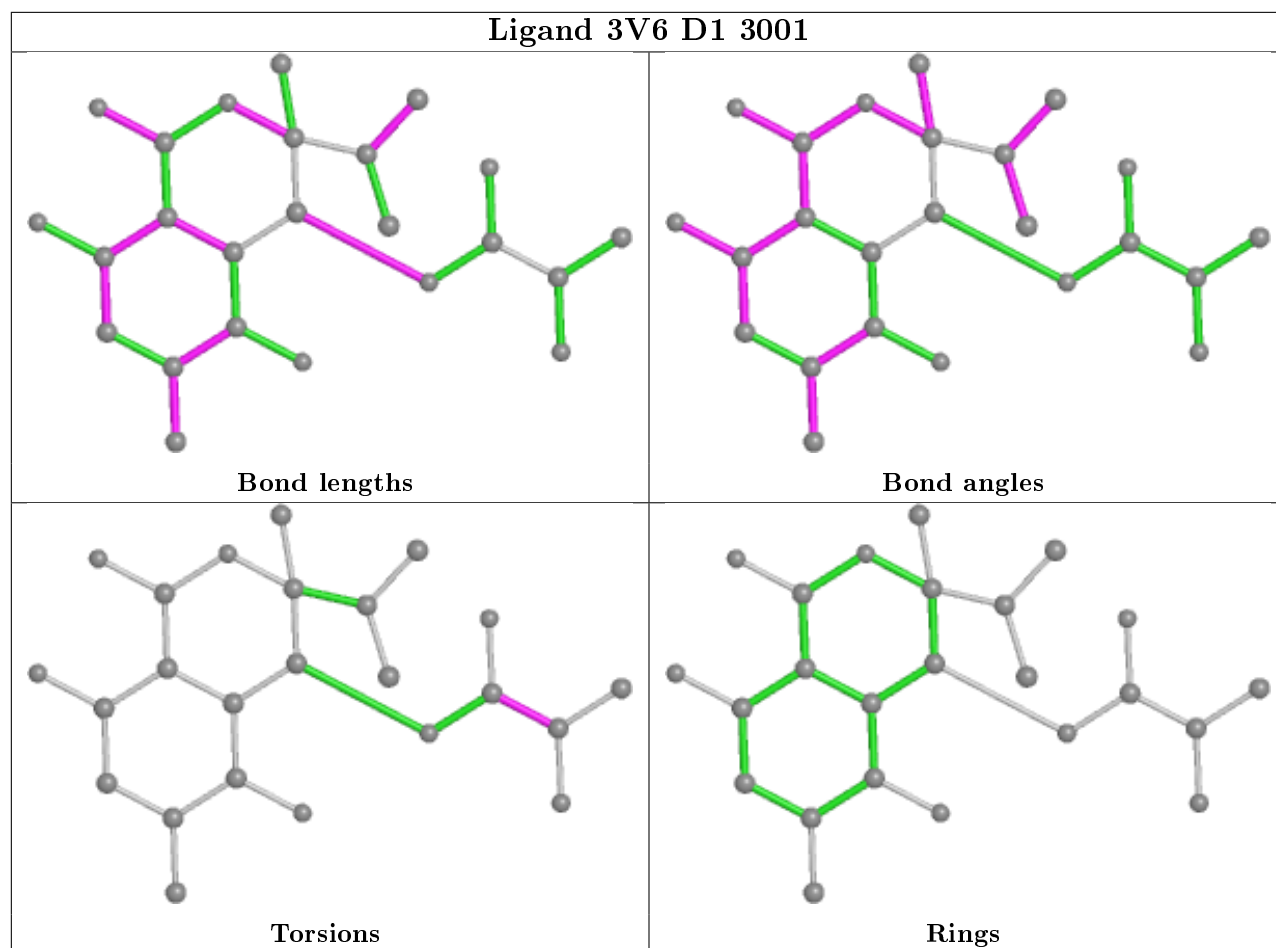
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

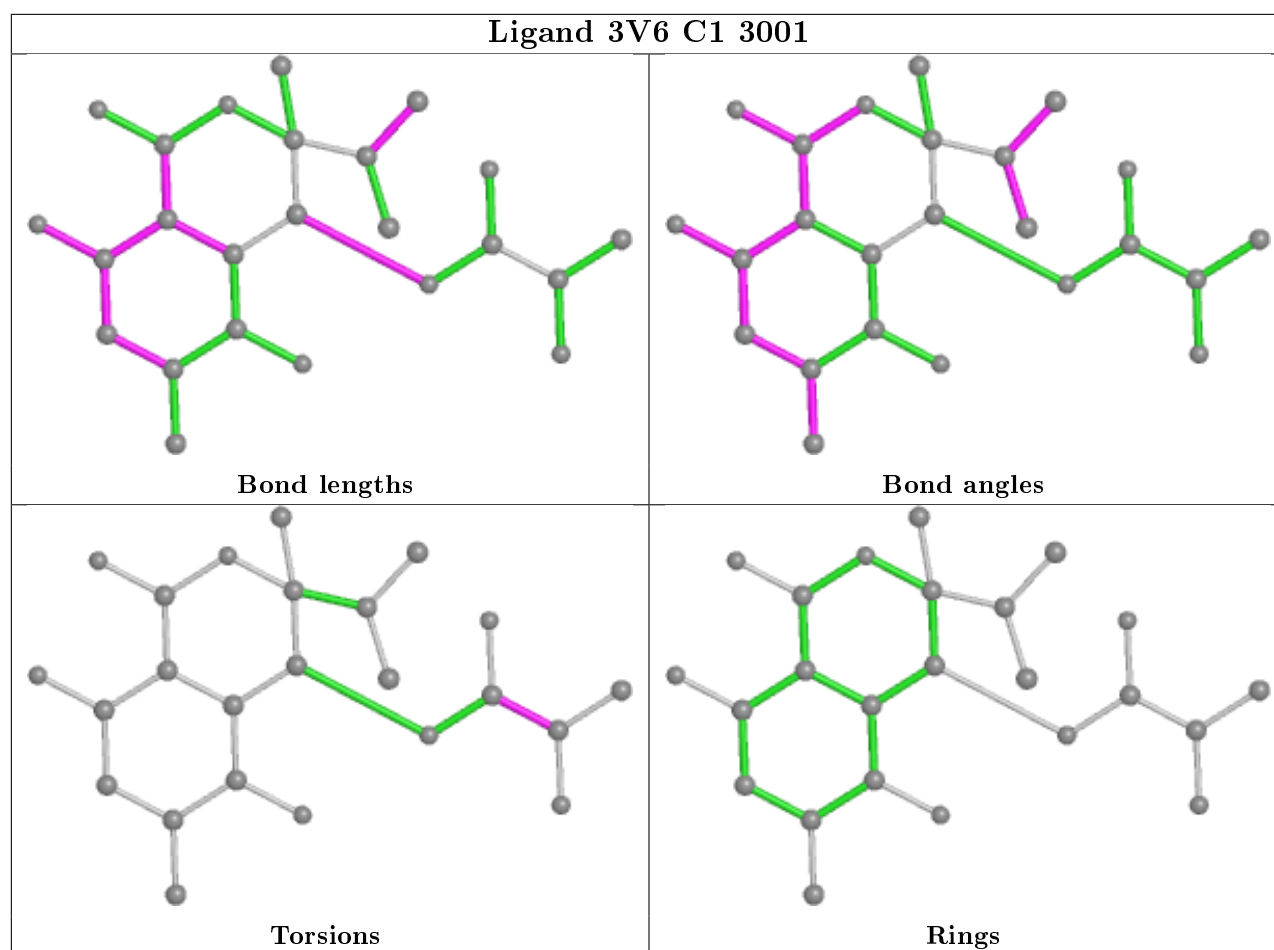


## Ligand PAR Ab 1601



## Ligand 3V6 D1 3001





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
27	CA	2
62	DA	2
58	D1	1
54	C7	1
58	C1	1
54	D7	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	DA	110:PHE	C	119:UNK	N	14.86
1	CA	110:PHE	C	119:UNK	N	12.87
1	CA	136:UNK	C	139:UNK	N	8.88
1	D7	46:HIS	C	47:THR	N	7.64
1	C7	46:HIS	C	47:THR	N	7.62
1	DA	136:UNK	C	139:UNK	N	5.70
1	D1	154:C	O3'	157:U	P	2.75
1	C1	154:C	O3'	157:U	P	2.66

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A2	9/9 (100%)	0.01	0 100 100	50, 89, 111, 114	0
2	AA	234/234 (100%)	0.24	10 (4%) 35 35	78, 124, 168, 197	0
2	BA	234/234 (100%)	0.34	17 (7%) 15 17	80, 130, 179, 209	0
3	AC	206/238 (86%)	0.23	14 (6%) 17 19	65, 108, 148, 173	0
4	AD	208/208 (100%)	-0.07	3 (1%) 75 74	51, 86, 123, 147	0
4	BD	208/208 (100%)	-0.15	1 (0%) 91 90	48, 78, 117, 144	0
5	AE	150/150 (100%)	-0.00	3 (2%) 65 64	66, 91, 124, 144	0
5	BE	150/150 (100%)	0.03	0 100 100	57, 83, 122, 141	0
6	AF	101/101 (100%)	-0.29	2 (1%) 65 64	55, 85, 109, 170	0
6	BF	101/101 (100%)	-0.17	1 (0%) 82 81	52, 96, 130, 158	0
7	AG	155/155 (100%)	0.06	13 (8%) 11 13	58, 86, 125, 181	0
7	BG	155/155 (100%)	0.46	10 (6%) 18 20	78, 112, 154, 184	0
8	AH	138/138 (100%)	-0.00	0 100 100	60, 90, 117, 184	0
8	BH	138/138 (100%)	0.27	2 (1%) 75 74	63, 95, 123, 145	0
9	AI	127/127 (100%)	0.46	7 (5%) 25 25	62, 108, 150, 175	0
9	BI	127/127 (100%)	0.88	17 (13%) 3 4	77, 131, 179, 215	0
10	AJ	98/98 (100%)	0.78	13 (13%) 3 4	77, 121, 176, 188	0
10	BJ	98/98 (100%)	1.15	22 (22%) 0 1	65, 134, 173, 202	0
11	AK	119/119 (100%)	-0.02	5 (4%) 36 35	39, 76, 110, 158	0
11	BK	119/119 (100%)	0.49	6 (5%) 28 29	47, 94, 141, 193	0
12	AL	124/124 (100%)	0.34	9 (7%) 15 17	49, 82, 125, 180	0
12	BL	124/124 (100%)	0.07	5 (4%) 38 37	41, 60, 105, 158	0
13	AM	124/124 (100%)	0.30	7 (5%) 24 25	66, 98, 144, 197	0
13	BM	124/124 (100%)	0.73	10 (8%) 12 13	66, 113, 164, 204	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
14	AN	60/60 (100%)	0.25	1 (1%) 70 68	65, 103, 130, 142	0
14	BN	60/60 (100%)	0.30	1 (1%) 70 68	59, 94, 119, 134	0
15	AO	88/88 (100%)	-0.07	0 100 100	46, 76, 112, 123	0
15	BO	88/88 (100%)	0.06	1 (1%) 80 79	55, 94, 120, 132	0
16	AP	83/83 (100%)	0.11	2 (2%) 59 57	52, 73, 101, 136	0
16	BP	83/83 (100%)	0.40	3 (3%) 42 42	59, 89, 135, 152	0
17	AR	99/99 (100%)	0.03	1 (1%) 82 81	59, 80, 108, 115	0
17	BR	99/99 (100%)	0.16	2 (2%) 65 64	65, 94, 126, 135	0
18	AS	70/70 (100%)	0.26	2 (2%) 51 50	56, 88, 119, 156	0
18	BS	70/70 (100%)	0.58	5 (7%) 16 18	66, 94, 142, 180	0
19	AT	78/78 (100%)	0.85	12 (15%) 2 2	67, 110, 164, 180	0
19	BT	78/78 (100%)	1.04	11 (14%) 2 3	79, 118, 161, 184	0
20	AU	99/99 (100%)	0.29	3 (3%) 50 49	62, 86, 125, 146	0
20	BU	99/99 (100%)	0.60	8 (8%) 12 13	64, 107, 146, 154	0
21	AW	24/24 (100%)	1.67	7 (29%) 0 0	63, 80, 112, 138	0
21	BW	24/24 (100%)	1.22	4 (16%) 1 2	64, 91, 132, 163	0
22	Ab	1504/1504 (100%)	-0.17	24 (1%) 72 70	30, 75, 154, 300	0
22	Bb	1504/1504 (100%)	-0.04	39 (2%) 56 54	31, 81, 165, 318	0
23	B2	10/10 (100%)	0.29	0 100 100	60, 107, 138, 172	0
24	BC	206/206 (100%)	0.13	7 (3%) 45 44	64, 105, 149, 169	0
25	C2	75/76 (98%)	7.29	69 (92%) 0 0	99, 250, 345, 377	0
25	C3	76/76 (100%)	0.33	6 (7%) 12 14	60, 130, 198, 227	0
25	D3	76/76 (100%)	0.49	3 (3%) 39 38	59, 147, 212, 228	0
26	C4	77/77 (100%)	-0.31	0 100 100	44, 79, 132, 159	0
27	CA	87/206 (42%)	3.10	49 (56%) 0 0	98, 186, 221, 241	0
28	CB	271/271 (100%)	-0.33	0 100 100	23, 48, 83, 150	0
28	DB	271/271 (100%)	-0.24	4 (1%) 73 72	20, 52, 86, 159	0
29	CC	204/204 (100%)	0.11	6 (2%) 51 50	31, 68, 123, 150	0
29	DC	204/204 (100%)	-0.00	3 (1%) 73 72	24, 61, 124, 169	0
30	CD	207/207 (100%)	-0.27	4 (1%) 66 65	29, 64, 133, 194	0
30	DD	207/207 (100%)	-0.09	5 (2%) 59 57	20, 65, 146, 223	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
31	CE	181/181 (100%)	0.04	7 (3%) 39 38	59, 92, 137, 213	0
31	DE	181/181 (100%)	0.50	14 (7%) 13 15	76, 117, 154, 198	0
32	CF	159/159 (100%)	1.10	34 (21%) 0 1	82, 134, 175, 219	0
32	DF	159/159 (100%)	0.11	7 (4%) 34 34	45, 85, 126, 178	0
33	CI	145/145 (100%)	0.28	4 (2%) 53 51	40, 88, 128, 150	0
33	DI	145/145 (100%)	0.29	8 (5%) 25 25	60, 108, 139, 165	0
34	CJ	0/130	-	-	-	-
34	DJ	0/130	-	-	-	-
35	CM	138/138 (100%)	0.04	1 (0%) 87 87	47, 78, 118, 130	0
35	DM	138/138 (100%)	-0.05	0 100 100	36, 73, 121, 151	0
36	CN	122/122 (100%)	-0.11	1 (0%) 86 85	35, 66, 89, 111	0
36	DN	122/122 (100%)	-0.35	0 100 100	27, 51, 75, 107	0
37	CO	146/146 (100%)	0.25	4 (2%) 54 53	34, 77, 127, 168	0
37	DO	146/146 (100%)	0.28	5 (3%) 45 44	31, 87, 123, 165	0
38	CP	141/141 (100%)	-0.03	2 (1%) 75 74	44, 75, 111, 192	0
38	DP	141/141 (100%)	-0.10	2 (1%) 75 74	42, 71, 106, 219	0
39	CQ	117/117 (100%)	-0.20	0 100 100	38, 63, 94, 127	0
39	DQ	117/117 (100%)	-0.05	0 100 100	27, 61, 99, 130	0
40	CR	98/98 (100%)	0.39	3 (3%) 49 48	47, 89, 130, 176	0
40	DR	98/98 (100%)	1.24	21 (21%) 0 1	68, 113, 143, 163	0
41	CS	137/137 (100%)	0.04	5 (3%) 42 42	45, 79, 142, 200	0
41	DS	137/137 (100%)	0.04	4 (2%) 51 50	43, 71, 148, 192	0
42	CT	117/117 (100%)	-0.10	2 (1%) 70 68	37, 66, 116, 138	0
42	DT	117/117 (100%)	-0.16	1 (0%) 84 83	31, 68, 111, 153	0
43	CU	101/101 (100%)	0.05	2 (1%) 65 64	35, 92, 122, 134	0
43	DU	101/101 (100%)	0.22	5 (4%) 28 29	26, 86, 123, 196	0
44	CW	113/113 (100%)	-0.15	2 (1%) 68 67	38, 54, 90, 182	0
45	CX	92/92 (100%)	-0.28	0 100 100	39, 65, 89, 109	0
45	DX	92/92 (100%)	-0.28	0 100 100	33, 55, 88, 115	0
46	CY	100/100 (100%)	1.16	23 (23%) 0 1	58, 94, 168, 214	0
46	DY	100/100 (100%)	0.83	13 (13%) 3 4	48, 81, 193, 251	0
47	CZ	176/176 (100%)	0.33	9 (5%) 28 28	76, 118, 157, 233	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
47	DZ	176/176 (100%)	0.47	15 (8%) 10 12	69, 119, 173, 203	0
48	Ca	84/84 (100%)	0.62	8 (9%) 8 10	44, 67, 127, 170	0
48	Da	84/84 (100%)	0.60	9 (10%) 6 7	49, 82, 137, 167	0
49	CH	93/93 (100%)	-0.10	1 (1%) 80 79	30, 54, 102, 140	0
49	DH	93/93 (100%)	0.08	1 (1%) 80 79	29, 66, 121, 179	0
50	CK	71/71 (100%)	0.00	2 (2%) 53 51	42, 85, 125, 180	0
50	DK	71/71 (100%)	-0.02	2 (2%) 53 51	37, 68, 124, 179	0
51	CL	59/59 (100%)	0.62	4 (6%) 17 19	45, 72, 111, 223	0
51	DL	59/59 (100%)	0.35	5 (8%) 10 12	48, 79, 120, 213	0
52	C5	30/30 (100%)	-0.31	0 100 100	76, 99, 130, 155	0
52	D5	30/30 (100%)	0.39	2 (6%) 17 19	99, 128, 155, 167	0
53	C6	59/59 (100%)	0.33	5 (8%) 10 12	34, 63, 160, 206	0
53	D6	59/59 (100%)	0.06	4 (6%) 17 19	28, 65, 172, 205	0
54	C7	44/44 (100%)	1.55	13 (29%) 0 0	54, 101, 146, 183	0
54	D7	44/44 (100%)	2.16	18 (40%) 0 0	84, 125, 165, 181	0
55	C8	48/48 (100%)	-0.13	2 (4%) 36 35	26, 40, 79, 139	0
55	D8	48/48 (100%)	-0.17	2 (4%) 36 35	21, 34, 77, 135	0
56	C9	63/63 (100%)	-0.01	1 (1%) 72 70	34, 54, 90, 123	0
56	D9	63/63 (100%)	0.08	2 (3%) 47 46	39, 66, 102, 136	0
57	C0	36/36 (100%)	3.05	21 (58%) 0 0	93, 125, 175, 177	0
57	D0	36/36 (100%)	2.88	25 (69%) 0 0	73, 106, 141, 145	0
58	C1	2807/2899 (96%)	-0.25	30 (1%) 80 79	21, 54, 148, 279	0
58	D1	2807/2899 (96%)	-0.22	44 (1%) 72 70	16, 52, 155, 267	0
59	Cs	119/119 (100%)	-0.25	2 (1%) 70 68	58, 83, 138, 197	0
59	Ds	119/119 (100%)	0.20	5 (4%) 36 35	62, 104, 147, 172	0
60	D2	20/20 (100%)	3.87	18 (90%) 0 0	133, 235, 281, 283	0
61	D4	76/76 (100%)	-0.24	0 100 100	37, 79, 120, 201	0
62	DA	87/206 (42%)	3.23	60 (68%) 0 0	118, 190, 257, 309	0
63	DW	113/113 (100%)	-0.17	2 (1%) 68 67	33, 51, 100, 159	0
64	DV	55/55 (100%)	6.54	50 (90%) 0 0	110, 248, 297, 345	0
All	All	20982/21697 (96%)	0.11	991 (4%) 31 31	16, 77, 159, 377	0

All (991) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
25	C2	70	G	23.4
64	DV	50	G	21.8
25	C2	71	G	21.6
25	C2	17	C	20.5
25	C2	3	C	20.1
25	C2	73	A	19.2
46	DY	59	GLY	17.9
25	C2	5	G	17.8
25	C2	2	C	16.1
25	C2	58	A	16.1
25	C2	1	G	15.7
64	DV	17	C	15.3
27	CA	90	GLY	15.0
64	DV	51	G	14.1
22	Bb	85	C	13.8
25	C2	23	A	13.8
25	C2	16	U	13.8
64	DV	16	U	13.7
64	DV	49	G	13.4
64	DV	3	C	13.4
25	C2	72	C	13.2
31	CE	2	PRO	12.5
62	DA	52	ARG	12.3
22	Bb	84	A	12.3
58	C1	2812	G	12.2
25	C2	18	G	12.1
62	DA	107	TRP	11.6
25	C2	15	G	11.6
25	C2	22	G	11.2
25	C2	4	C	11.2
64	DV	15	G	11.1
64	DV	52	C	11.1
64	DV	2	C	10.9
46	DY	51	VAL	10.7
25	C2	52	G	10.4
22	Ab	82	U	10.2
51	CL	1	MET	10.2
22	Ab	81	U	10.2
62	DA	51	PRO	10.1
58	D1	2812	G	10.1
64	DV	20	U	9.7
25	C2	69	G	9.7

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Mol	Chain	Res	Type	RSRZ
13	BM	124	PRO	9.7
25	C2	19	G	9.5
48	Ca	6	GLY	9.5
57	C0	12	ASP	9.4
64	DV	5	G	9.3
25	C2	60	U	9.1
25	C2	74	C	9.1
47	CZ	114	GLY	9.0
64	DV	23	A	9.0
27	CA	70	LYS	9.0
25	C2	6	G	9.0
64	DV	14	A	8.9
13	AM	123	ALA	8.8
25	C2	20	U	8.7
64	DV	53	A	8.7
25	C2	61	C	8.7
64	DV	22	G	8.6
62	DA	85	GLU	8.5
42	CT	118	GLY	8.5
48	Ca	5	LYS	8.1
27	CA	91	ALA	7.9
27	CA	57	ASN	7.9
48	Ca	7	LEU	7.9
62	DA	84	LYS	7.9
48	Da	8	GLY	7.8
22	Ab	85	C	7.8
58	D1	2807	G	7.8
60	D2	55	U	7.7
57	C0	13	LYS	7.7
22	Bb	79	G	7.7
57	C0	14	CYS	7.6
44	CW	113	LYS	7.6
22	Bb	86	U	7.6
64	DV	4	C	7.6
13	AM	124	PRO	7.6
27	CA	95	GLY	7.6
38	DP	141	GLN	7.5
12	AL	128	ALA	7.5
64	DV	38	A	7.3
25	C2	66	U	7.3
64	DV	18	G	7.3
46	CY	45	VAL	7.2

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Mol	Chain	Res	Type	RSRZ
64	DV	41	C	7.2
27	CA	105	ASP	7.2
48	Ca	8	GLY	7.2
25	C2	63	G	7.1
64	DV	1	G	7.1
48	Ca	4	LYS	7.0
53	C6	60	VAL	7.0
64	DV	13	C	7.0
62	DA	89	ALA	6.9
27	CA	107	TRP	6.9
46	CY	59	GLY	6.9
53	C6	59	GLU	6.9
25	C2	57	G	6.8
58	C1	2807	G	6.8
32	CF	170	ARG	6.7
57	D0	29	ASN	6.7
10	AJ	33	GLN	6.7
22	Ab	980	G	6.7
25	C2	64	A	6.7
25	C2	55	U	6.6
11	AK	129	SER	6.6
25	C2	7	A	6.6
50	CK	72	ALA	6.5
46	CY	50	ARG	6.5
53	D6	60	VAL	6.5
22	Bb	80	U	6.5
51	DL	1	MET	6.5
7	AG	83	ALA	6.3
54	D7	20	ASN	6.3
60	D2	52	G	6.3
64	DV	40	U	6.2
29	DC	204	ALA	6.2
25	C2	67	C	6.2
43	DU	36	PRO	6.2
50	DK	70	GLN	6.2
64	DV	46	U	6.2
57	C0	11	CYS	6.2
41	DS	1	MET	6.1
25	C2	24	G	6.1
28	DB	26	LYS	6.1
62	DA	109	ASP	6.1
7	BG	84	ASN	6.0

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Mol	Chain	Res	Type	RSRZ
25	C2	14	A	6.0
25	C2	48	C	6.0
62	DA	92	ASP	6.0
27	CA	51	PRO	6.0
53	C6	54	GLY	6.0
62	DA	18	LYS	6.0
22	Bb	83	U	6.0
64	DV	45	G	6.0
57	D0	12	ASP	5.9
27	CA	59	ARG	5.9
27	CA	69	GLY	5.9
32	DF	44	VAL	5.9
58	D1	2809	C	5.9
25	C2	75	C	5.9
25	C2	59	U	5.8
57	C0	29	ASN	5.8
47	DZ	113	ALA	5.8
46	CY	60	PHE	5.8
64	DV	47	C	5.8
58	D1	2808	U	5.8
38	CP	141	GLN	5.8
27	CA	89	ALA	5.8
57	C0	10	ILE	5.8
58	C1	2813	C	5.7
57	C0	37	GLY	5.7
25	C2	68	C	5.7
64	DV	48	C	5.7
20	BU	106	ALA	5.7
41	DS	39	ARG	5.7
31	DE	86	MET	5.6
64	DV	42	C	5.6
27	CA	108	MET	5.6
48	Da	7	LEU	5.6
60	D2	47	U	5.6
25	C2	65	G	5.6
27	CA	110	PHE	5.6
25	C2	56	C	5.6
25	C2	21	A	5.6
27	CA	106	ALA	5.6
18	BS	88	LYS	5.6
62	DA	77	ILE	5.6
64	DV	27	G	5.5

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Mol	Chain	Res	Type	RSRZ
27	CA	71	GLN	5.5
10	BJ	98	ILE	5.5
11	BK	128	ALA	5.5
58	C1	217	A	5.5
22	Ab	1011	C	5.5
57	D0	11	CYS	5.4
62	DA	72	VAL	5.4
40	CR	54	LEU	5.4
10	BJ	4	ILE	5.4
13	BM	125	ARG	5.4
22	Bb	1006	C	5.4
60	D2	40	C	5.4
48	Da	4	LYS	5.4
62	DA	71	GLN	5.4
13	AM	84	ILE	5.4
37	CO	149	GLU	5.3
58	C1	2806	C	5.3
22	Bb	980	G	5.3
22	Bb	981	G	5.3
46	CY	44	ILE	5.3
9	BI	101	PHE	5.3
27	CA	19	VAL	5.3
62	DA	108	MET	5.2
64	DV	6	G	5.2
25	C2	31	A	5.2
46	DY	61	ILE	5.2
57	D0	36	GLN	5.2
57	D0	37	GLY	5.2
58	C1	2815	G	5.2
11	BK	129	SER	5.2
40	DR	82	ILE	5.2
27	CA	52	ARG	5.2
10	BJ	99	LYS	5.1
27	CA	68	LEU	5.1
30	DD	1	MET	5.1
64	DV	54	C	5.1
25	C2	8	U	5.1
9	BI	102	LEU	5.1
47	DZ	167	PRO	5.1
25	C2	13	C	5.1
27	CA	56	GLN	5.1
62	DA	83	ILE	5.0

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Mol	Chain	Res	Type	RSRZ
64	DV	29	G	5.0
54	D7	19	ARG	5.0
22	Bb	1268	A	5.0
58	C1	2808	U	5.0
50	DK	72	ALA	5.0
64	DV	55	C	5.0
58	C1	2809	C	4.9
64	DV	43	G	4.9
7	AG	84	ASN	4.9
31	CE	50	ALA	4.9
32	CF	168	PRO	4.9
58	C1	2811	A	4.9
64	DV	7	A	4.9
13	AM	125	ARG	4.8
3	AC	160	ALA	4.8
64	DV	31	A	4.8
32	DF	42	ARG	4.8
27	CA	80	GLY	4.8
31	CE	48	GLU	4.8
46	CY	51	VAL	4.8
40	DR	24	LEU	4.8
22	Bb	1239	U	4.8
12	AL	64	TYR	4.7
62	DA	23	ASP	4.7
32	CF	158	HIS	4.7
58	D1	2805	G	4.7
62	DA	57	ASN	4.7
27	CA	109	ASP	4.7
42	DT	118	GLY	4.7
64	DV	19	G	4.7
22	Bb	209	U	4.7
46	CY	46	LYS	4.7
58	D1	2810	A	4.7
64	DV	32	U	4.7
3	AC	155	GLY	4.7
25	C2	45	U	4.7
13	BM	121	LYS	4.6
58	D1	2815	G	4.6
10	BJ	34	VAL	4.6
48	Da	3	HIS	4.6
40	DR	54	LEU	4.6
22	Bb	1014	G	4.6

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Mol	Chain	Res	Type	RSRZ
46	DY	52	SER	4.6
32	CF	83	TYR	4.6
60	D2	57	G	4.6
10	AJ	34	VAL	4.6
25	C2	41	C	4.5
58	D1	2814	C	4.5
12	BL	127	GLU	4.5
7	BG	85	TYR	4.5
54	D7	49	HIS	4.5
62	DA	61	THR	4.5
58	D1	2813	C	4.5
64	DV	30	G	4.5
37	DO	149	GLU	4.5
25	D3	20	U	4.5
46	DY	58	GLY	4.5
58	D1	2200	C	4.5
57	D0	10	ILE	4.4
25	C2	27	G	4.4
11	AK	128	ALA	4.4
62	DA	86	ALA	4.4
64	DV	12	U	4.4
13	AM	122	LYS	4.4
22	Ab	981	G	4.3
25	C2	10	G	4.3
57	C0	30	PRO	4.3
46	CY	61	ILE	4.3
60	D2	56	C	4.3
57	D0	30	PRO	4.3
32	CF	169	VAL	4.3
9	BI	85	LEU	4.3
53	D6	58	LEU	4.3
25	C2	12	U	4.3
57	D0	32	HIS	4.3
27	CA	102	LYS	4.3
64	DV	39	U	4.3
51	CL	2	PRO	4.3
25	C2	42	C	4.2
62	DA	68	LEU	4.2
64	DV	24	G	4.2
64	DV	8	U	4.2
22	Bb	1016	G	4.2
25	C2	28	G	4.2

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Mol	Chain	Res	Type	RSRZ
11	BK	17	GLY	4.2
7	BG	5	ARG	4.2
21	AW	18	TYR	4.2
57	D0	34	GLN	4.2
24	BC	207	VAL	4.2
54	D7	42	TRP	4.2
12	BL	128	ALA	4.2
25	C2	47	U	4.2
32	CF	56	SER	4.2
54	D7	26	ASN	4.2
22	Bb	87	C	4.2
9	BI	96	LEU	4.2
40	DR	23	ARG	4.2
32	CF	44	VAL	4.2
30	CD	1	MET	4.1
46	DY	60	PHE	4.1
58	D1	2806	C	4.1
58	D1	2905	U	4.1
25	C2	62	C	4.1
54	C7	13	CYS	4.1
48	Da	6	GLY	4.1
54	C7	50	ARG	4.1
58	D1	2904	C	4.1
31	DE	2	PRO	4.1
10	BJ	33	GLN	4.1
47	CZ	113	ALA	4.1
22	Ab	84	A	4.1
54	C7	14	THR	4.0
22	Bb	211	U	4.0
25	C2	30	G	4.0
60	D2	42	C	4.0
30	CD	24	LEU	4.0
60	D2	54	U	4.0
58	D1	2811	A	4.0
9	BI	99	LEU	4.0
62	DA	38	ASP	4.0
27	CA	83	ILE	4.0
57	C0	25	VAL	3.9
59	Ds	87	G	3.9
62	DA	110	PHE	3.9
54	D7	13	CYS	3.9
25	C2	46	G	3.9

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Mol	Chain	Res	Type	RSRZ
33	CI	12	LEU	3.9
27	CA	58	VAL	3.9
32	CF	45	VAL	3.9
64	DV	44	A	3.9
47	DZ	63	ASP	3.9
58	C1	2814	C	3.9
17	BR	100	LYS	3.9
19	BT	38	SER	3.9
60	D2	44	G	3.9
62	DA	45	ALA	3.9
10	BJ	97	GLU	3.8
27	CA	34	THR	3.8
40	DR	53	SER	3.8
47	DZ	149	SER	3.8
62	DA	95	GLY	3.8
62	DA	87	GLU	3.8
27	CA	41	VAL	3.8
27	CA	76	ALA	3.8
46	CY	49	VAL	3.8
13	BM	123	ALA	3.8
58	D1	1554	C	3.8
46	DY	2	ARG	3.8
27	CA	75	LEU	3.8
7	AG	5	ARG	3.7
27	CA	78	ALA	3.7
47	DZ	168	GLU	3.7
60	D2	41	C	3.7
25	C2	40	C	3.7
64	DV	21	A	3.7
57	C0	28	GLU	3.7
40	DR	94	TYR	3.7
49	DH	85	LEU	3.7
2	BA	133	LYS	3.7
62	DA	56	GLN	3.7
32	DF	45	VAL	3.7
24	BC	206	GLU	3.7
27	CA	103	ILE	3.7
13	BM	122	LYS	3.7
25	C2	32	U	3.7
62	DA	70	LYS	3.6
11	BK	127	LYS	3.6
53	C6	58	LEU	3.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
46	DY	55	TYR	3.6
40	DR	48	LEU	3.6
2	BA	123	ALA	3.6
25	C2	54	U	3.6
58	C1	2200	C	3.6
22	Ab	79	G	3.6
6	AF	101	ALA	3.6
60	D2	39	U	3.6
62	DA	91	ALA	3.6
63	DW	113	ALA	3.6
18	AS	85	LEU	3.6
58	D1	2137	G	3.6
52	D5	51	TYR	3.6
47	CZ	112	ARG	3.6
21	AW	24	ARG	3.6
27	CA	53	ARG	3.6
21	AW	25	LYS	3.6
22	Bb	88	C	3.6
19	AT	29	ARG	3.6
37	CO	150	ALA	3.6
22	Bb	1121	G	3.5
22	Ab	1239	U	3.5
62	DA	19	VAL	3.5
27	CA	55	ASP	3.5
44	CW	112	GLY	3.5
54	C7	16	CYS	3.5
57	D0	28	GLU	3.5
58	C1	2167	C	3.5
20	BU	101	GLY	3.5
60	D2	48	C	3.5
22	Ab	1268	A	3.5
46	CY	62	GLU	3.5
13	BM	98	VAL	3.5
62	DA	43	VAL	3.5
58	D1	2160	C	3.5
30	DD	25	PRO	3.5
54	D7	12	GLU	3.5
12	AL	28	LYS	3.5
57	C0	32	HIS	3.5
33	CI	20	ASP	3.5
19	BT	66	MET	3.5
58	C1	2902	G	3.4

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Mol	Chain	Res	Type	RSRZ
60	D2	46	G	3.4
18	AS	88	LYS	3.4
46	CY	63	LYS	3.4
41	CS	1	MET	3.4
62	DA	106	GLY	3.4
25	C3	20	U	3.4
51	DL	4	LEU	3.4
7	AG	6	ARG	3.4
25	C3	17	C	3.4
50	CK	71	ASN	3.4
47	DZ	114	GLY	3.4
2	AA	21	ARG	3.4
19	BT	47	HIS	3.4
46	CY	28	LYS	3.4
62	DA	88	GLU	3.4
62	DA	47	LEU	3.4
62	DA	104	LEU	3.4
64	DV	10	G	3.4
60	D2	49	C	3.4
46	CY	48	ALA	3.4
62	DA	90	GLY	3.4
58	D1	934	C	3.4
7	AG	82	GLY	3.4
47	DZ	169	GLU	3.4
13	BM	7	VAL	3.4
27	CA	45	ALA	3.4
54	D7	51	GLU	3.4
62	DA	73	ARG	3.4
20	BU	45	GLN	3.3
54	C7	26	ASN	3.3
30	DD	24	LEU	3.3
25	C2	49	C	3.3
58	D1	2158	C	3.3
40	DR	60	GLY	3.3
58	D1	2902	G	3.3
22	Ab	1432	A	3.3
10	AJ	32	ALA	3.3
19	BT	81	ARG	3.3
31	CE	49	ASP	3.3
62	DA	50	ASP	3.3
22	Bb	1015	G	3.3
3	AC	189	ALA	3.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
40	CR	104	GLY	3.3
56	D9	64	TYR	3.3
21	AW	17	THR	3.3
10	BJ	36	GLY	3.3
27	CA	77	ILE	3.3
32	CF	52	VAL	3.2
57	C0	15	LYS	3.2
47	DZ	166	SER	3.2
62	DA	76	ALA	3.2
29	CC	76	ARG	3.2
46	CY	3	VAL	3.2
22	Ab	1005	G	3.2
22	Ab	1016	G	3.2
25	C2	44	G	3.2
27	CA	60	GLY	3.2
58	C1	2805	G	3.2
57	D0	9	ARG	3.2
3	AC	207	VAL	3.2
57	D0	14	CYS	3.2
2	AA	135	GLN	3.2
57	C0	24	TYR	3.2
48	Ca	9	SER	3.2
41	CS	39	ARG	3.2
47	DZ	96	VAL	3.2
21	BW	23	PRO	3.2
27	CA	93	TYR	3.2
58	D1	2180	G	3.2
27	CA	96	GLY	3.1
54	D7	43	CYS	3.1
58	D1	2161	C	3.1
32	CF	32	GLU	3.1
9	AI	4	TYR	3.1
40	DR	52	SER	3.1
62	DA	63	SER	3.1
19	AT	28	LYS	3.1
53	D6	59	GLU	3.1
57	C0	31	LYS	3.1
16	BP	46	PRO	3.1
18	BS	54	ARG	3.1
57	C0	34	GLN	3.1
58	D1	2900	A	3.1
10	BJ	8	LEU	3.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
27	CA	104	LEU	3.1
62	DA	53	ARG	3.1
9	AI	56	LEU	3.1
29	CC	69	LYS	3.1
31	DE	4	ASP	3.1
37	CO	110	TYR	3.1
46	CY	2	ARG	3.1
58	C1	2810	A	3.1
2	BA	130	ARG	3.0
25	C3	19	G	3.0
58	C1	2816	G	3.0
12	AL	19	ARG	3.0
32	DF	169	VAL	3.0
22	Bb	1120	C	3.0
32	CF	33	LEU	3.0
22	Bb	1432	A	3.0
40	DR	108	GLY	3.0
21	AW	23	PRO	3.0
51	CL	59	VAL	3.0
2	AA	130	ARG	3.0
7	BG	154	TYR	3.0
8	BH	62	TYR	3.0
38	DP	140	ALA	3.0
54	C7	52	VAL	3.0
54	D7	11	LEU	3.0
3	AC	154	SER	3.0
62	DA	20	TYR	3.0
40	DR	80	LEU	3.0
58	C1	532	G	3.0
2	BA	152	PHE	3.0
32	DF	168	PRO	3.0
62	DA	96	GLY	3.0
25	C3	16	U	3.0
9	BI	2	GLU	3.0
48	Da	9	SER	3.0
37	CO	91	PHE	3.0
57	D0	13	LYS	3.0
22	Bb	1009	C	3.0
32	CF	157	TYR	3.0
40	DR	49	VAL	3.0
59	Ds	88	C	3.0
9	BI	29	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
46	CY	43	ASN	2.9
53	D6	54	GLY	2.9
25	C2	51	U	2.9
2	BA	129	GLU	2.9
62	DA	69	GLY	2.9
22	Bb	1013	A	2.9
32	CF	105	LEU	2.9
40	DR	36	TYR	2.9
43	DU	101	GLY	2.9
62	DA	39	GLU	2.9
54	C7	42	TRP	2.9
9	BI	100	GLY	2.9
32	CF	111	HIS	2.9
25	C2	29	G	2.9
2	AA	156	LYS	2.9
22	Bb	1011	C	2.9
25	C2	38	A	2.9
40	DR	68	GLN	2.9
47	DZ	153	SER	2.9
60	D2	50	U	2.9
46	DY	47	LYS	2.9
32	CF	159	GLU	2.9
64	DV	11	C	2.9
7	AG	80	VAL	2.9
21	BW	25	LYS	2.9
25	C2	50	U	2.9
29	DC	69	LYS	2.9
53	C6	2	ALA	2.9
54	D7	39	TYR	2.9
10	AJ	5	ARG	2.9
13	AM	7	VAL	2.9
58	D1	944	A	2.9
60	D2	45	U	2.9
2	AA	70	PHE	2.9
56	C9	64	TYR	2.9
54	C7	51	GLU	2.9
57	C0	4	ARG	2.9
3	AC	196	LEU	2.9
58	C1	2168	G	2.9
62	DA	105	ASP	2.9
30	DD	133	ASN	2.9
32	CF	129	THR	2.9

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Mol	Chain	Res	Type	RSRZ
38	CP	140	ALA	2.9
58	D1	2804	G	2.9
2	AA	128	GLU	2.9
6	BF	101	ALA	2.8
37	DO	110	TYR	2.8
40	DR	84	GLN	2.8
6	AF	55	ASP	2.8
59	Ds	52	A	2.8
9	AI	90	PRO	2.8
59	Ds	89	G	2.8
25	C2	43	C	2.8
58	D1	2157	C	2.8
57	C0	35	ARG	2.8
55	D8	48	LYS	2.8
22	Bb	1010	G	2.8
41	CS	136	GLN	2.8
42	CT	117	GLN	2.8
62	DA	93	TYR	2.8
3	AC	159	GLY	2.8
57	D0	22	ARG	2.8
58	D1	2185	C	2.8
64	DV	28	G	2.8
29	DC	76	ARG	2.8
58	D1	217	A	2.8
2	BA	127	ILE	2.8
19	BT	43	GLU	2.8
25	D3	44	G	2.8
9	AI	30	GLY	2.8
54	D7	14	THR	2.8
40	DR	107	GLU	2.8
64	DV	36	A	2.8
9	BI	95	LYS	2.8
12	AL	60	LEU	2.8
25	C2	9	A	2.8
10	AJ	99	LYS	2.8
2	BA	131	PRO	2.8
10	AJ	22	LYS	2.8
47	DZ	112	ARG	2.8
57	D0	16	VAL	2.8
46	CY	58	GLY	2.7
58	C1	1553	A	2.7
9	BI	19	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
64	DV	25	C	2.7
32	CF	96	ALA	2.7
46	CY	64	GLU	2.7
51	CL	3	ARG	2.7
57	D0	27	CYS	2.7
47	DZ	97	GLU	2.7
11	AK	127	LYS	2.7
46	DY	50	ARG	2.7
22	Bb	1012	G	2.7
29	CC	204	ALA	2.7
7	BG	78	ARG	2.7
19	BT	36	ARG	2.7
60	D2	43	C	2.7
19	AT	12	ASP	2.7
54	D7	50	ARG	2.7
31	DE	26	GLN	2.7
62	DA	60	GLY	2.7
57	D0	5	ALA	2.7
27	CA	79	LYS	2.7
40	DR	81	GLY	2.7
62	DA	80	GLY	2.7
3	AC	153	VAL	2.7
22	Ab	1509	A	2.7
21	BW	5	ASP	2.7
31	DE	103	LEU	2.7
12	BL	64	TYR	2.7
57	C0	26	ILE	2.7
57	D0	26	ILE	2.7
20	BU	99	LEU	2.7
49	CH	85	LEU	2.7
10	BJ	77	PRO	2.7
32	CF	58	GLU	2.7
19	AT	47	HIS	2.7
22	Ab	80	U	2.6
12	BL	29	GLY	2.6
9	BI	36	TYR	2.6
27	CA	87	GLU	2.6
22	Ab	1012	G	2.6
7	BG	4	ARG	2.6
24	BC	166	GLU	2.6
20	BU	100	ILE	2.6
58	C1	1218	A	2.6

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Mol	Chain	Res	Type	RSRZ
58	D1	2321	A	2.6
17	AR	75	ARG	2.6
55	C8	47	ARG	2.6
10	AJ	87	THR	2.6
32	CF	21	PRO	2.6
10	BJ	76	ASN	2.6
3	AC	194	GLY	2.6
37	DO	104	GLY	2.6
57	D0	25	VAL	2.6
20	BU	42	GLN	2.6
29	CC	54	GLN	2.6
31	DE	76	SER	2.6
58	D1	2901	G	2.6
2	BA	134	GLU	2.6
22	Bb	1112	C	2.6
33	DI	138	ILE	2.6
2	BA	122	PHE	2.6
2	BA	136	VAL	2.6
31	DE	35	GLU	2.6
33	DI	117	GLU	2.6
46	DY	53	PRO	2.6
9	AI	29	ASN	2.6
10	BJ	10	GLY	2.6
22	Bb	1019	G	2.6
40	DR	37	ALA	2.6
41	DS	135	ALA	2.6
31	CE	75	LYS	2.6
57	D0	33	LYS	2.6
47	DZ	62	PRO	2.6
54	D7	9	LEU	2.6
62	DA	65	PRO	2.6
54	C7	49	HIS	2.6
62	DA	34	THR	2.6
32	CF	18	GLU	2.5
57	D0	18	ARG	2.5
57	D0	17	ILE	2.5
51	DL	2	PRO	2.5
58	D1	2159	C	2.5
54	D7	16	CYS	2.5
18	BS	51	LEU	2.5
2	AA	123	ALA	2.5
14	BN	2	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
7	BG	156	TRP	2.5
19	AT	41	VAL	2.5
62	DA	55	ASP	2.5
7	AG	2	ALA	2.5
9	BI	8	GLY	2.5
25	C2	11	C	2.5
16	AP	19	ILE	2.5
41	DS	29	ARG	2.5
25	C3	44	G	2.5
22	Bb	82	U	2.5
58	D1	2190	A	2.5
7	AG	86	GLN	2.5
22	Bb	1005	G	2.5
31	DE	78	SER	2.5
24	BC	179	ARG	2.5
27	CA	88	GLU	2.5
55	C8	48	LYS	2.5
62	DA	67	GLY	2.5
25	C2	53	G	2.5
48	Da	5	LYS	2.5
12	AL	127	GLU	2.5
32	CF	43	VAL	2.5
22	Ab	1022	C	2.5
46	CY	57	GLN	2.5
58	D1	2156	A	2.5
10	AJ	74	ILE	2.5
2	BA	96	ARG	2.5
47	CZ	156	LYS	2.5
28	DB	271	ILE	2.5
58	D1	2164	C	2.4
10	AJ	4	ILE	2.4
46	CY	52	SER	2.4
9	AI	65	VAL	2.4
33	CI	3	VAL	2.4
58	D1	2175	G	2.4
18	BS	29	PHE	2.4
19	BT	69	HIS	2.4
15	BO	87	ILE	2.4
22	Bb	89	G	2.4
46	CY	53	PRO	2.4
9	AI	20	ARG	2.4
55	D8	47	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
58	C1	1554	C	2.4
59	Cs	88	C	2.4
2	BA	15	VAL	2.4
48	Da	42	GLY	2.4
10	BJ	47	PHE	2.4
7	AG	156	TRP	2.4
32	CF	57	ASP	2.4
32	CF	94	TYR	2.4
43	CU	93	GLU	2.4
21	AW	22	ARG	2.4
28	DB	270	ILE	2.4
22	Ab	1019	G	2.4
59	Ds	86	G	2.4
27	CA	92	ASP	2.4
46	CY	6	HIS	2.4
10	BJ	35	SER	2.4
57	D0	7	VAL	2.4
2	AA	131	PRO	2.4
22	Bb	157	A	2.4
47	CZ	95	PRO	2.4
2	BA	128	GLU	2.4
10	BJ	64	GLU	2.4
19	AT	43	GLU	2.4
19	AT	81	ARG	2.4
13	BM	84	ILE	2.4
58	D1	298	G	2.4
30	CD	10	PRO	2.4
19	BT	63	THR	2.4
32	CF	95	ARG	2.3
32	CF	113	VAL	2.3
11	AK	11	LYS	2.3
46	DY	28	LYS	2.3
19	AT	31	ILE	2.3
36	CN	51	ALA	2.3
62	DA	27	ARG	2.3
4	AD	23	GLY	2.3
10	BJ	71	LEU	2.3
46	CY	47	LYS	2.3
27	CA	85	GLU	2.3
13	BM	94	ARG	2.3
64	DV	35	A	2.3
2	AA	132	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
10	BJ	7	LYS	2.3
3	AC	98	ASN	2.3
3	AC	206	GLU	2.3
4	BD	26	CYS	2.3
32	CF	167	GLU	2.3
22	Bb	212	G	2.3
57	D0	24	TYR	2.3
58	C1	2166	C	2.3
9	BI	126	SER	2.3
62	DA	37	PHE	2.3
19	BT	29	ARG	2.3
54	C7	12	GLU	2.3
58	D1	1218	A	2.3
31	DE	49	ASP	2.3
62	DA	100	ILE	2.3
32	CF	26	VAL	2.3
47	CZ	115	GLY	2.3
22	Bb	341	C	2.3
10	BJ	24	VAL	2.3
32	CF	40	GLU	2.3
19	AT	35	SER	2.3
5	AE	16	THR	2.3
10	AJ	31	GLY	2.3
40	CR	57	LYS	2.3
43	DU	97	LYS	2.3
58	C1	2175	G	2.3
58	D1	2816	G	2.3
7	AG	4	ARG	2.3
7	AG	7	ALA	2.3
24	BC	189	ALA	2.3
7	AG	8	GLU	2.3
33	DI	85	GLU	2.3
22	Bb	1509	A	2.3
58	C1	2321	A	2.3
7	BG	91	VAL	2.3
2	BA	126	GLU	2.3
58	C1	2904	C	2.3
40	DR	57	LYS	2.3
24	BC	76	VAL	2.3
62	DA	24	GLU	2.2
10	BJ	28	ARG	2.2
32	CF	88	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
28	DB	35	LYS	2.2
54	D7	48	VAL	2.2
16	AP	37	GLY	2.2
4	AD	49	ARG	2.2
19	BT	74	PHE	2.2
20	AU	46	GLU	2.2
47	CZ	162	GLU	2.2
10	AJ	35	SER	2.2
48	Ca	3	HIS	2.2
22	Ab	979	A	2.2
51	DL	39	ASP	2.2
58	D1	2802	A	2.2
57	D0	23	VAL	2.2
25	C2	39	U	2.2
31	CE	25	TYR	2.2
25	D3	17	C	2.2
9	BI	65	VAL	2.2
10	BJ	38	ILE	2.2
32	CF	89	ILE	2.2
16	BP	47	ASP	2.2
21	AW	6	ARG	2.2
2	AA	133	LYS	2.2
12	AL	20	LYS	2.2
12	AL	125	PRO	2.2
33	DI	84	GLY	2.2
22	Bb	71	G	2.2
31	CE	28	VAL	2.2
10	BJ	22	LYS	2.2
60	D2	38	A	2.2
56	D9	48	PHE	2.2
14	AN	17	LYS	2.2
25	C3	18	G	2.2
20	BU	98	PRO	2.2
40	DR	41	ASP	2.2
27	CA	73	ARG	2.2
47	DZ	80	ARG	2.2
17	BR	99	SER	2.2
22	Ab	1013	A	2.2
62	DA	49	ILE	2.2
40	DR	104	GLY	2.2
10	BJ	69	ASN	2.2
22	Ab	977	C	2.2

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Mol	Chain	Res	Type	RSRZ
27	CA	82	LYS	2.2
58	D1	2330	G	2.2
7	BG	8	GLU	2.2
22	Bb	81	U	2.2
32	CF	46	GLU	2.2
27	CA	63	SER	2.2
41	CS	92	GLY	2.2
19	AT	62	ILE	2.2
20	AU	101	GLY	2.2
3	AC	193	TYR	2.2
12	AL	27	LEU	2.2
27	CA	40	THR	2.2
32	DF	43	VAL	2.2
37	DO	118	GLY	2.2
22	Ab	86	U	2.2
32	CF	123	PHE	2.1
41	CS	106	SER	2.1
19	BT	40	ILE	2.1
16	BP	35	LYS	2.1
32	CF	81	GLU	2.1
62	DA	94	VAL	2.1
31	DE	85	GLY	2.1
3	AC	191	THR	2.1
7	BG	83	ALA	2.1
58	D1	2671	A	2.1
54	C7	31	PRO	2.1
8	BH	59	LEU	2.1
31	DE	25	TYR	2.1
33	DI	139	GLN	2.1
57	C0	21	GLY	2.1
58	C1	2134	U	2.1
58	C1	2161	C	2.1
58	D1	2199	C	2.1
5	AE	13	ILE	2.1
19	AT	27	GLU	2.1
47	DZ	144	LEU	2.1
62	DA	48	GLY	2.1
21	BW	24	ARG	2.1
57	C0	9	ARG	2.1
11	BK	117	ASN	2.1
9	BI	81	ILE	2.1
63	DW	112	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
2	BA	132	LYS	2.1
30	DD	14	PRO	2.1
27	CA	50	ASP	2.1
31	DE	54	GLU	2.1
20	AU	54	LYS	2.1
3	AC	161	GLU	2.1
27	CA	43	VAL	2.1
51	DL	59	VAL	2.1
2	BA	36	ARG	2.1
59	Cs	11	C	2.1
35	CM	68	GLU	2.1
29	CC	75	VAL	2.1
2	BA	59	GLU	2.1
22	Ab	1010	G	2.1
58	D1	2166	C	2.1
32	DF	167	GLU	2.1
37	DO	134	ALA	2.1
52	D5	52	SER	2.1
29	CC	66	HIS	2.1
4	AD	161	ASN	2.1
9	BI	35	GLU	2.1
9	BI	93	ARG	2.1
20	BU	50	GLU	2.1
33	DI	123	LEU	2.1
62	DA	54	SER	2.1
54	C7	43	CYS	2.1
13	BM	15	VAL	2.1
5	AE	31	LEU	2.1
33	CI	9	LEU	2.1
46	DY	4	LYS	2.0
58	C1	298	G	2.0
58	C1	375	G	2.0
58	D1	532	G	2.0
30	CD	133	ASN	2.0
31	DE	50	ALA	2.0
11	BK	98	LEU	2.0
33	DI	6	LEU	2.0
54	D7	17	LYS	2.0
10	AJ	28	ARG	2.0
18	BS	32	ARG	2.0
22	Bb	1021	C	2.0
22	Bb	1226	C	2.0

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Mol	Chain	Res	Type	RSRZ
10	AJ	100	THR	2.0
31	DE	75	LYS	2.0
10	BJ	21	GLN	2.0
11	AK	13	GLN	2.0
7	AG	85	TYR	2.0
19	AT	71	LEU	2.0
33	DI	118	LYS	2.0
22	Ab	470	G	2.0
24	BC	161	GLU	2.0
47	CZ	92	SER	2.0
62	DA	74	VAL	2.0
13	AM	2	ALA	2.0
25	C2	36	A	2.0
48	Ca	76	GLY	2.0
54	D7	37	ARG	2.0
58	C1	2194	A	2.0
32	CF	128	PRO	2.0
43	CU	36	PRO	2.0
43	DU	37	VAL	2.0
12	BL	33	ARG	2.0
47	CZ	28	MET	2.0
48	Da	70	GLN	2.0
54	C7	17	LYS	2.0
57	C0	27	CYS	2.0
43	DU	95	LEU	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

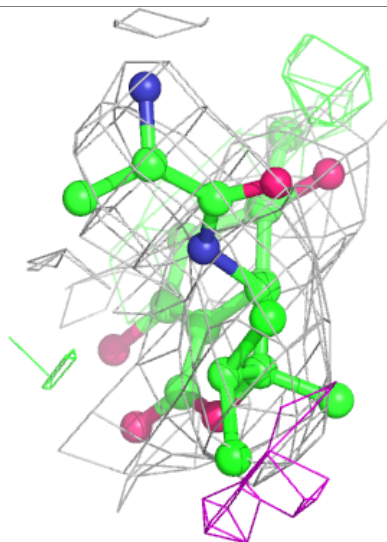
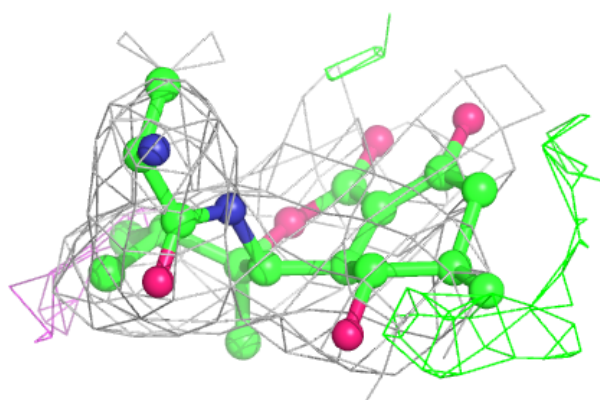
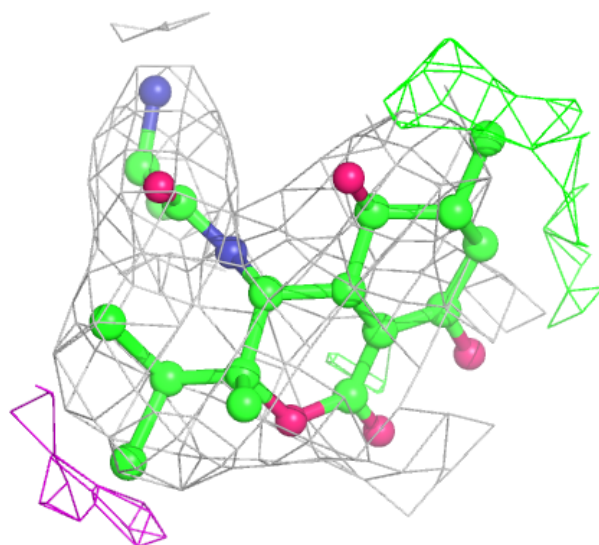
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
66	3V6	C1	3001	24/24	0.92	0.25	46,63,76,91	0
65	PAR	Ab	1601	42/42	0.93	0.20	51,65,75,91	0
67	MG	D1	3002	1/1	0.93	0.24	40,40,40,40	0
66	3V6	D1	3001	24/24	0.94	0.24	32,55,75,86	0
67	MG	C1	3002	1/1	0.95	0.22	41,41,41,41	0
65	PAR	Bb	1601	42/42	0.96	0.20	42,50,56,67	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.

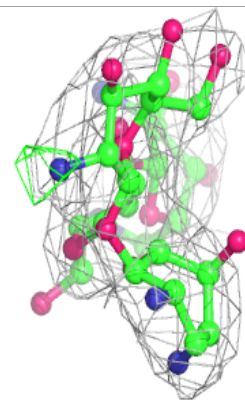
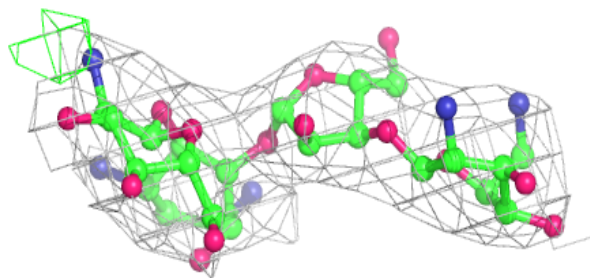
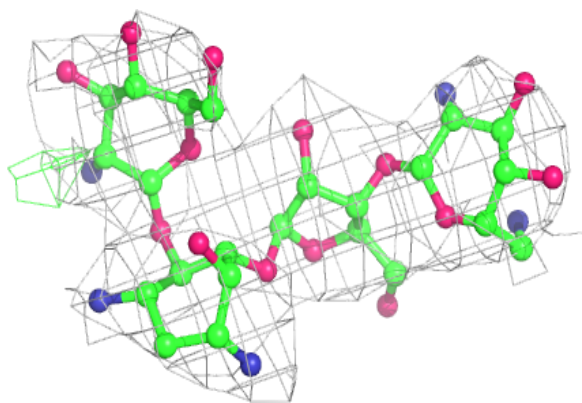
**Electron density around 3V6 C1 3001:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



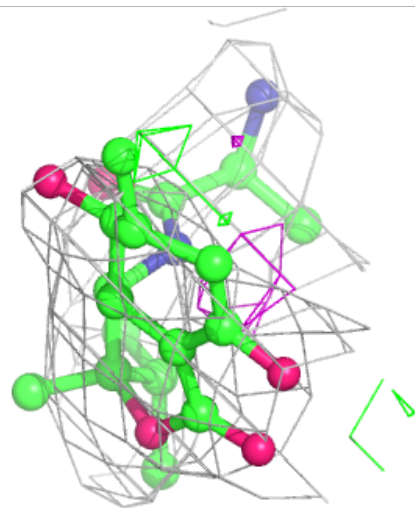
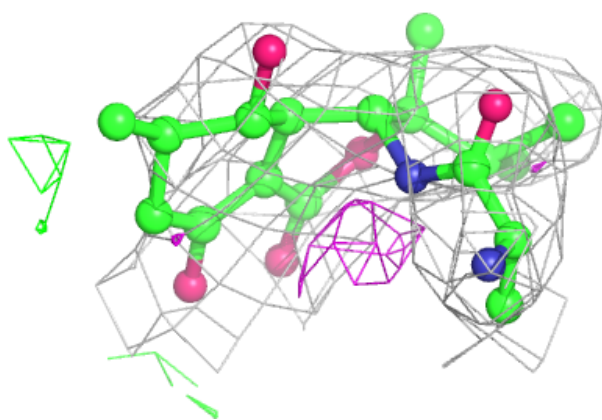
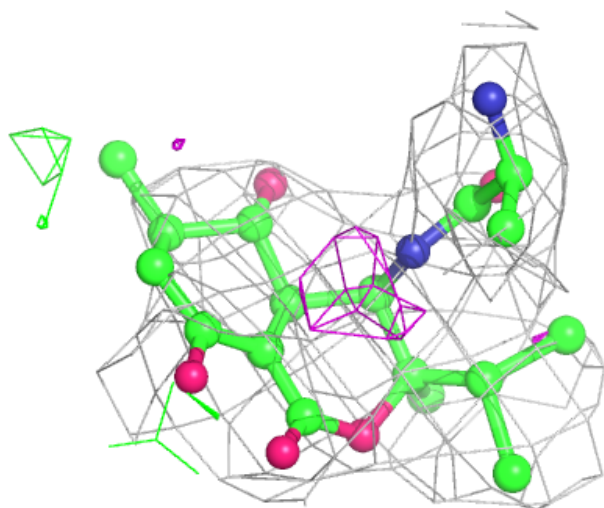
**Electron density around PAR Ab 1601:**

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



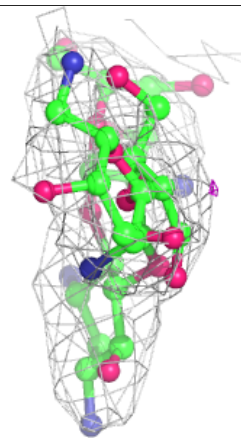
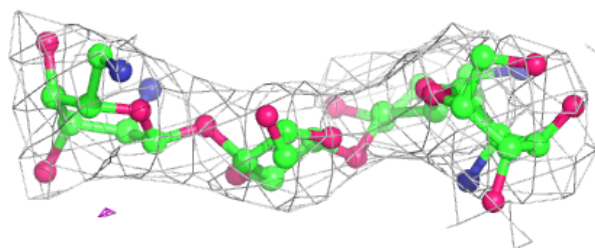
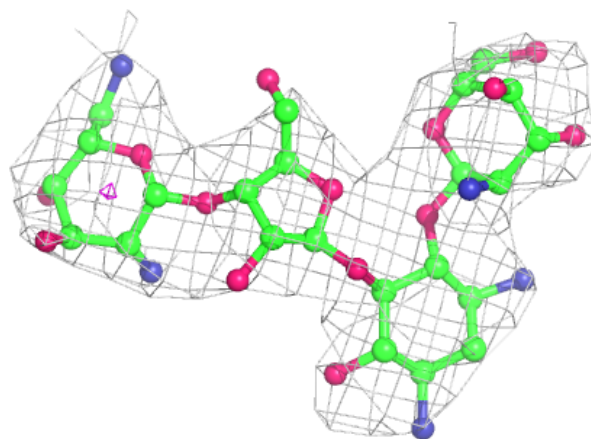
**Electron density around 3V6 D1 3001:**

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



**Electron density around PAR Bb 1601:**

$2mF_o-DF_c$  (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.