



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 29, 2026 – 12:09 PM UTC

PDB ID : 4WT8 / pdb_00004wt8
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

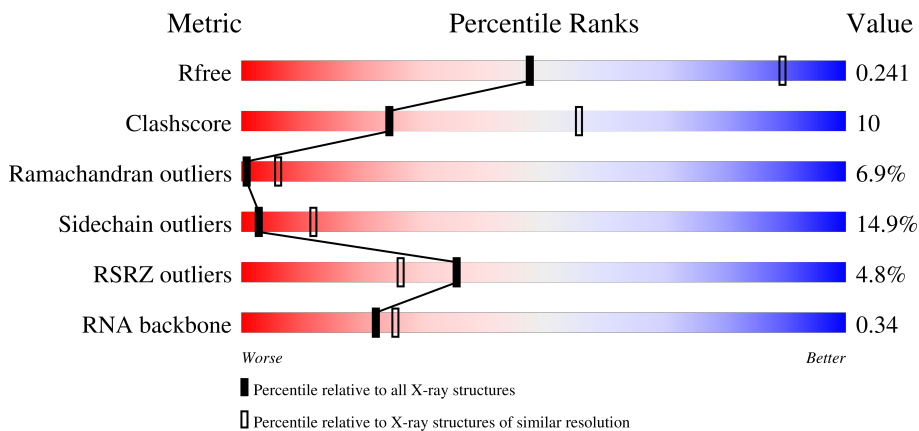
1 Overall quality at a glance i

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.



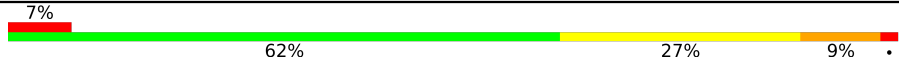
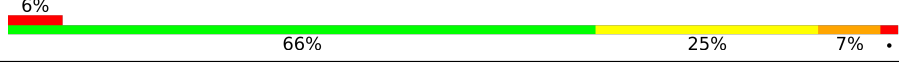
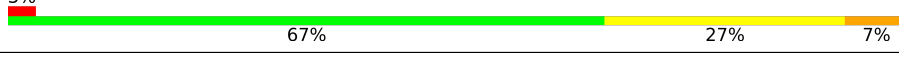


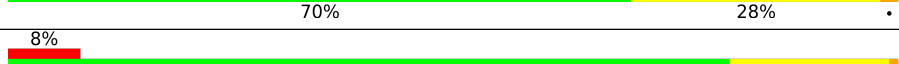
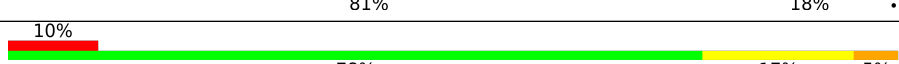
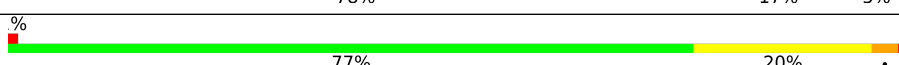
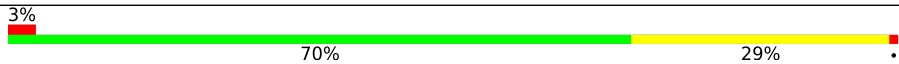


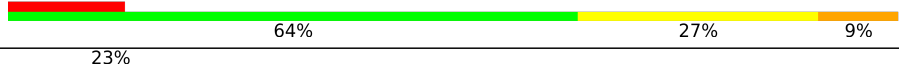
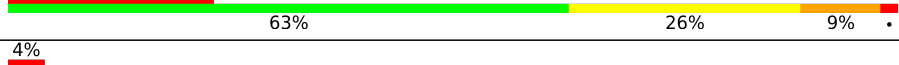

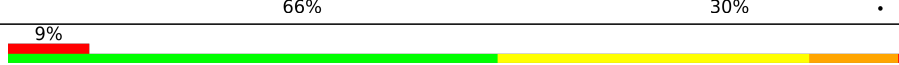










Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)
RNA backbone	3983	1157 (3.80-3.00)

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

Mol	Chain	Length	Quality of chain
1	A2	9	
2	AA	234	
2	BA	234	
3	AC	238	

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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	5% 63% 34% .
17	AR	99	% 74% 25% .
17	BR	99	3% 67% 29% ..
18	AS	70	% 60% 31% 7% .
18	BS	70	% 61% 30% 6% .
19	AT	78	12% 44% 47% 8% .
19	BT	78	18% 42% 42% 14% .
20	AU	99	12% 65% 27% 6% .
20	BU	99	15% 63% 31% 6% .
21	AW	24	8% 75% 25%
21	BW	24	38% 58% 38% .
22	Ab	1504	% 55% 33% 10% .
22	Bb	1504	% 57% 32% 10% .
23	B2	10	20% 20% 50% 30%
24	BC	206	7% 70% 25% 5%
25	C2	76	11% 53% 32% 14% .
25	C3	76	4% 42% 46% 12%
25	D3	76	39% 36% 24% .
26	C4	77	% 32% 34% 27% 6%
27	CA	206	14% 75% 15% . 8%
28	CB	271	% 58% 29% 10% .
28	DB	271	2% 55% 30% 11% .
29	CC	204	5% 54% 34% 10% .
29	DC	204	5% 47% 36% 15% .
30	CD	207	% 57% 33% 9% .



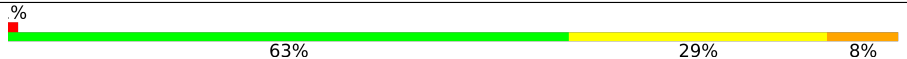
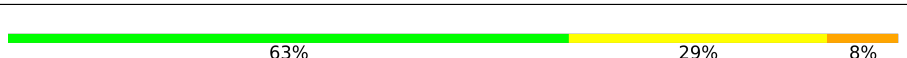
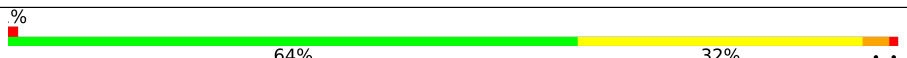
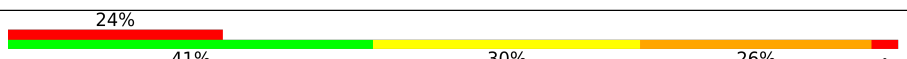
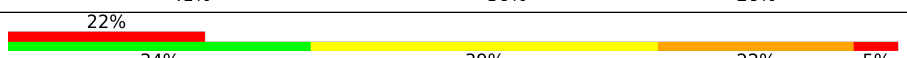
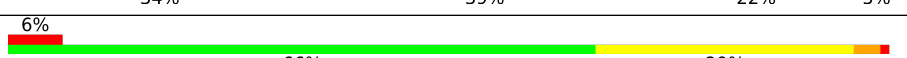
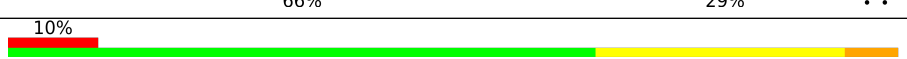

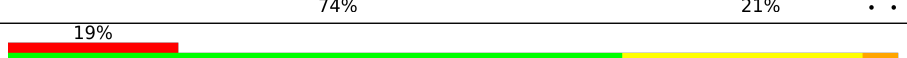







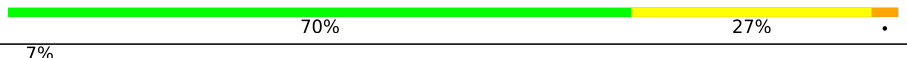
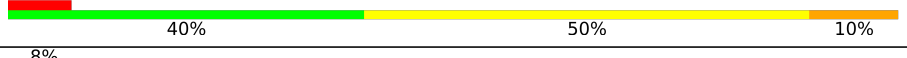

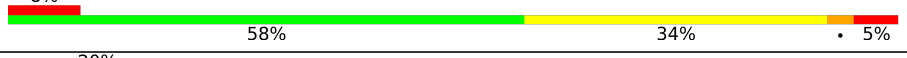
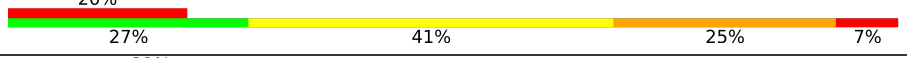
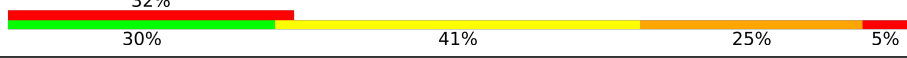

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Mol	Chain	Length	Quality of chain
30	DD	207	
31	CE	181	
31	DE	181	
32	CF	159	
32	DF	159	
33	CI	145	
33	DI	145	
34	CJ	130	
34	DJ	130	
35	CM	138	
35	DM	138	
36	CN	122	
36	DN	122	
37	CO	146	
37	DO	146	
38	CP	141	
38	DP	141	
39	CQ	117	
39	DQ	117	
40	CR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

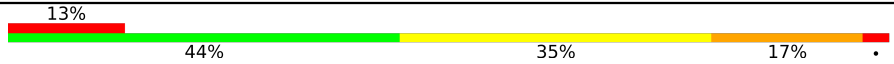

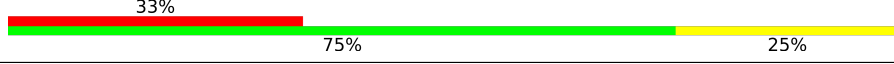
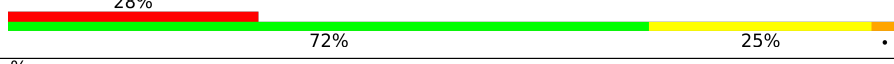

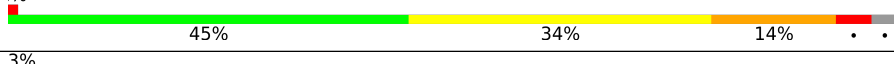

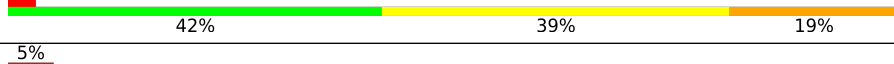
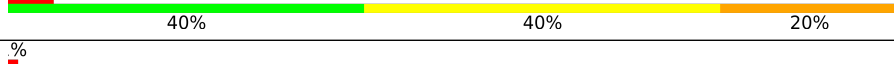
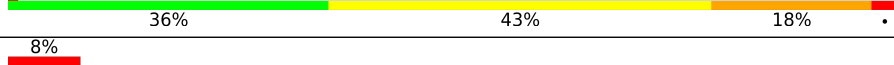



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Mol	Chain	Length	Quality of chain
43	CU	101	
43	DU	101	
44	CW	113	
45	CX	92	
45	DX	92	
46	CY	100	
46	DY	100	
47	CZ	176	
47	DZ	176	
48	Ca	84	
48	Da	84	
49	CH	93	
49	DH	93	
50	CK	71	
50	DK	71	
51	CL	59	
51	DL	59	
52	C5	30	
52	D5	30	
53	C6	59	
53	D6	59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

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
			Total	C	N	O	P			
1	A2	9	173	76	29	59	9	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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
			Total	C	N	O	S			
10	AJ	98	Total 795	C 499	N 156	O 139	S 1	0	0	0
10	BJ	98	Total 795	C 499	N 156	O 139	S 1	0	0	0

- 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
			Total	C	N	O			
21	BW	24	209	128	50	31	0	0	0

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

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

- Molecule 23 is a RNA chain called mRNA.

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

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

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

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

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

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

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

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

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

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
			Total	C	N	O	S			
28	CB	271	2105	1329	416	357	3	0	0	0
28	DB	271	2105	1329	416	357	3	0	0	0

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

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

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

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

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

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

- 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
			Total	C	N	O	S			
37	DO	146	1114	692	227	193	2	0	0	0

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

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

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

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

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

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

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

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

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

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

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
			Total	C	N	O	P			
58	C1	2807	60459	26907	11311	19435	2806	0	0	0
58	D1	2807	60459	26907	11311	19435	2806	0	0	0

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

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

- 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
			Total	C	N	O	P			
60	D2	20	416	186	65	146	19	0	0	0

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

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

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

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

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

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

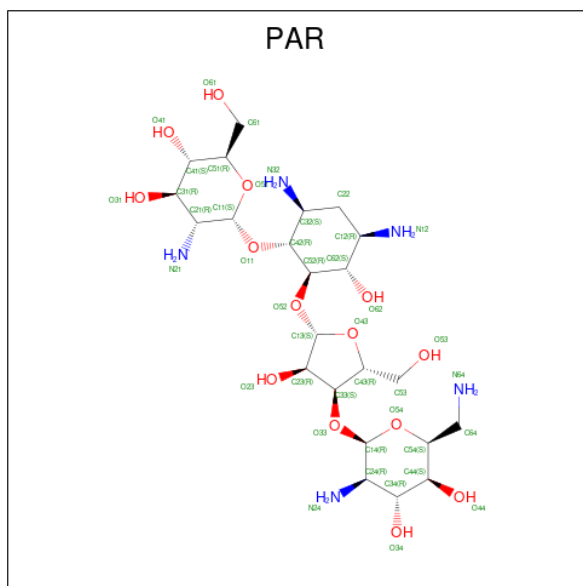
There is a discrepancy between the modelled and reference sequences:

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

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

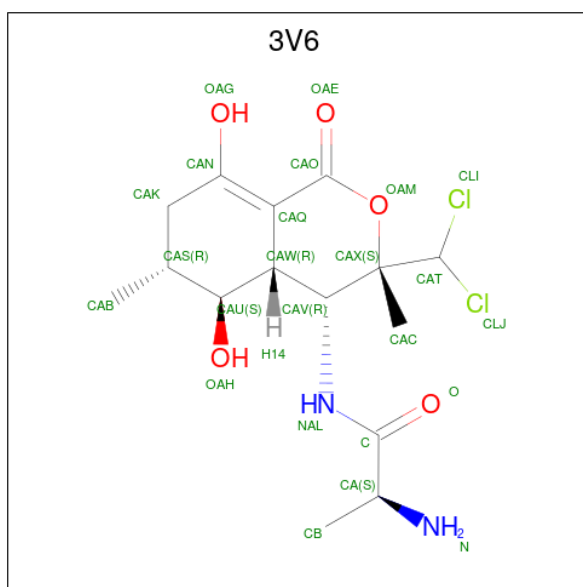
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
64	DV	55	1167	527	220	379	41	0	0	0

- Molecule 65 is PAROMOMYCIN (CCD ID: PAR) (formula: C₂₃H₄₅N₅O₁₄).



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

- Molecule 66 is Bactobolin A (CCD ID: 3V6) (formula: C₁₅H₂₂Cl₂N₂O₅).



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

- Molecule 67 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

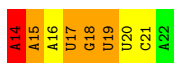
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
67	C1	1	Total	Mg	0	0
			1	1		
67	D1	1	Total	Mg	0	0
			1	1		

3 Residue-property plots

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

- Molecule 1: mRNA

Chain A2: 



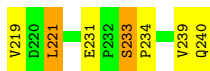
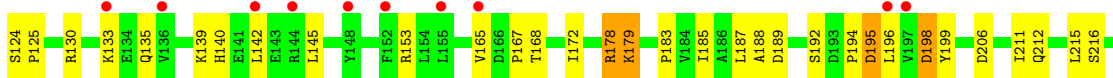
- Molecule 2: 30S ribosomal protein S2

Chain AA: 



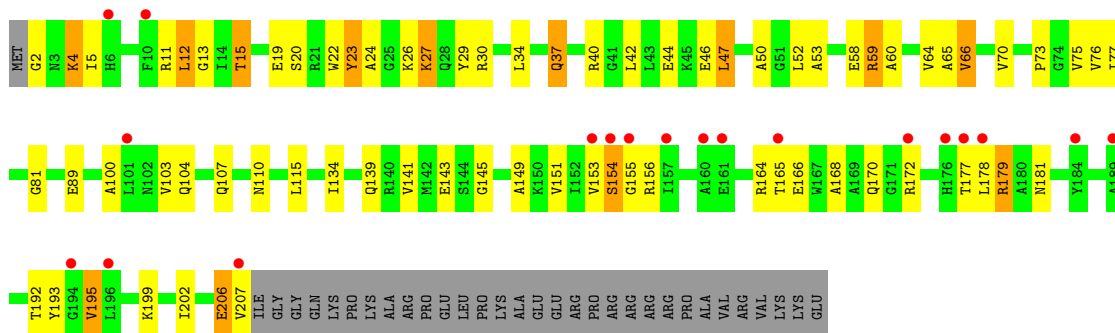
- Molecule 2: 30S ribosomal protein S2

Chain BA: 

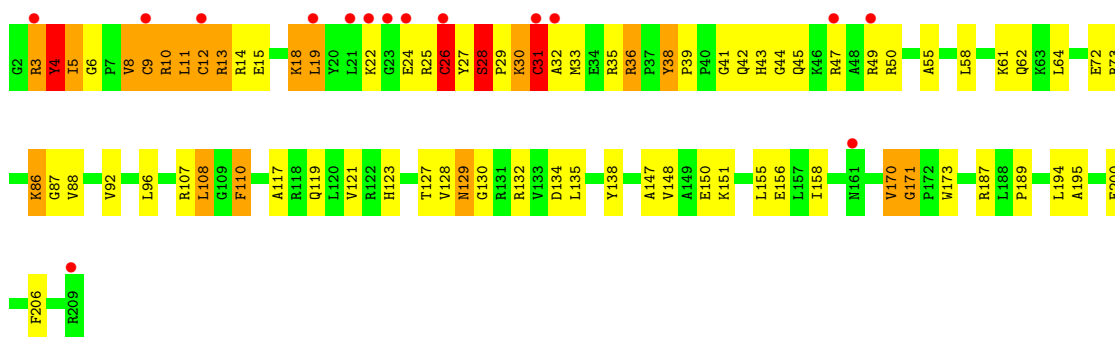


- Molecule 3: 30S ribosomal protein S3

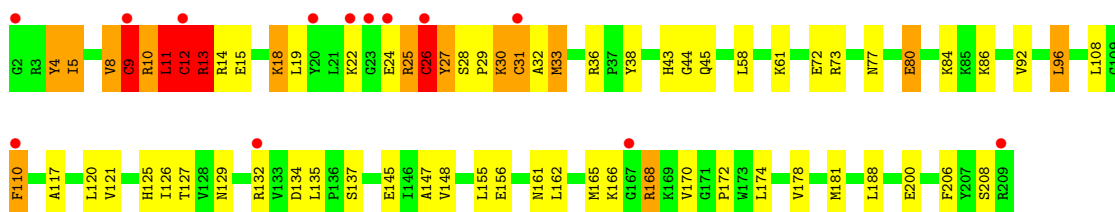
Chain AC: 



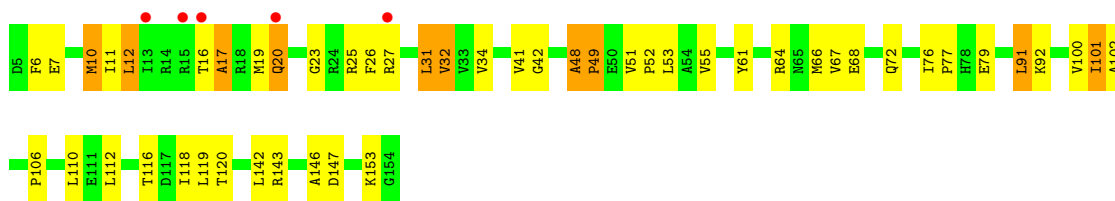
• Molecule 4: 30S ribosomal protein S4



• Molecule 4: 30S ribosomal protein S4

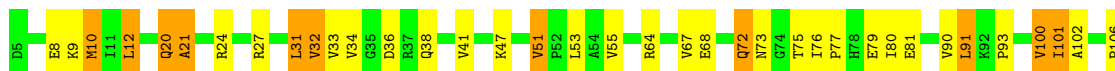


• Molecule 5: 30S ribosomal protein S5

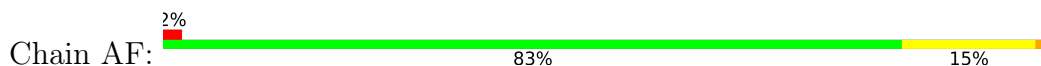


• Molecule 5: 30S ribosomal protein S5

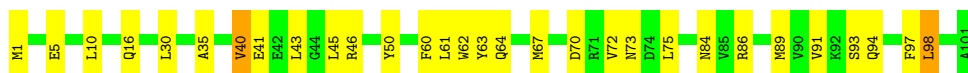




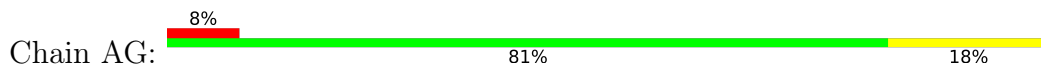
• Molecule 6: 30S ribosomal protein S6



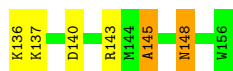
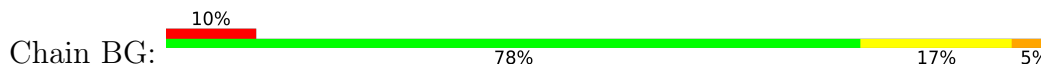
• Molecule 6: 30S ribosomal protein S6



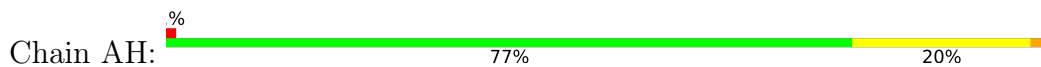
• Molecule 7: 30S ribosomal protein S7



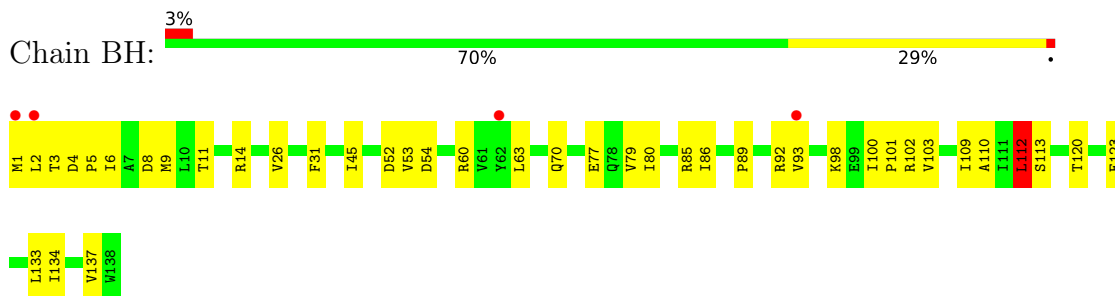
• Molecule 7: 30S ribosomal protein S7



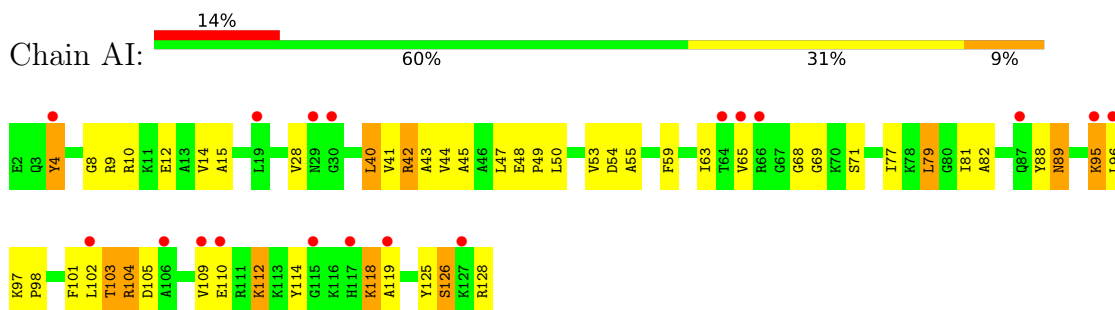
• Molecule 8: 30S ribosomal protein S8



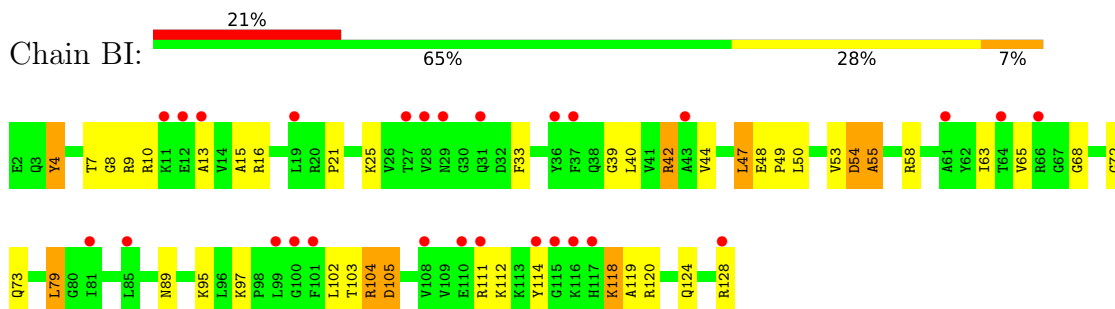
- Molecule 8: 30S ribosomal protein S8



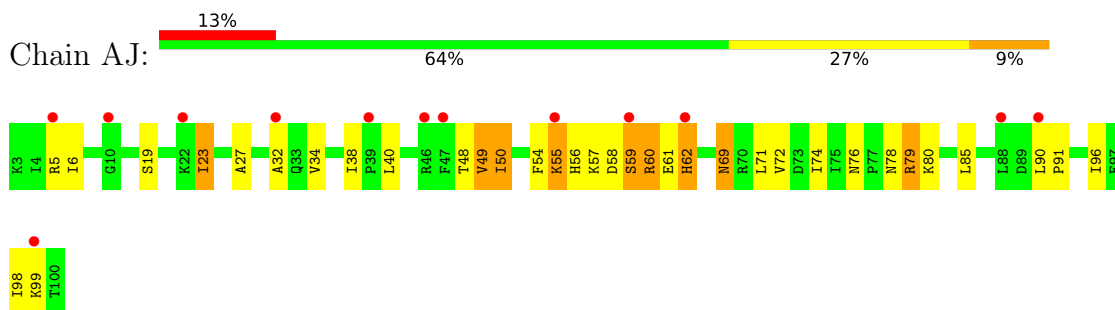
- Molecule 9: 30S ribosomal protein S9



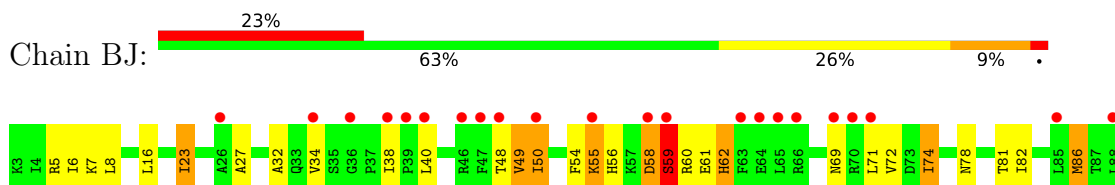
- Molecule 9: 30S ribosomal protein S9

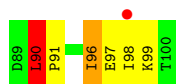


- Molecule 10: 30S ribosomal protein S10

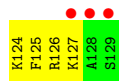


- Molecule 10: 30S ribosomal protein S10

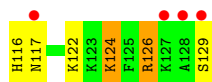
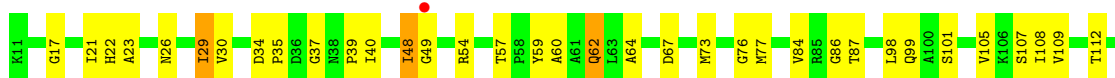




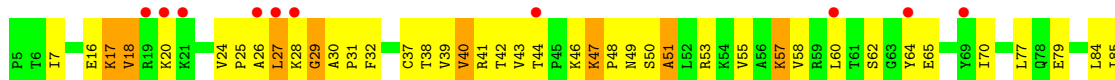
- Molecule 11: 30S ribosomal protein S11



- Molecule 11: 30S ribosomal protein S11



- Molecule 12: 30S ribosomal protein S12

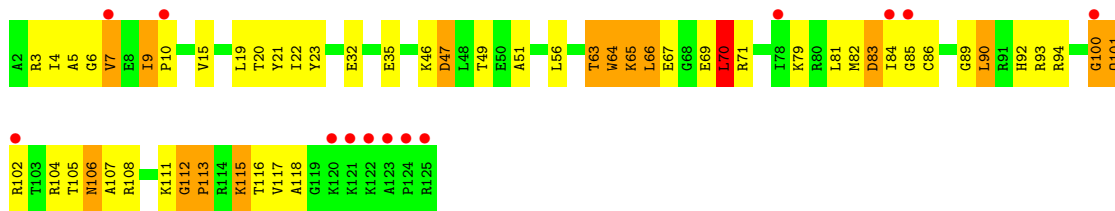


- Molecule 12: 30S ribosomal protein S12

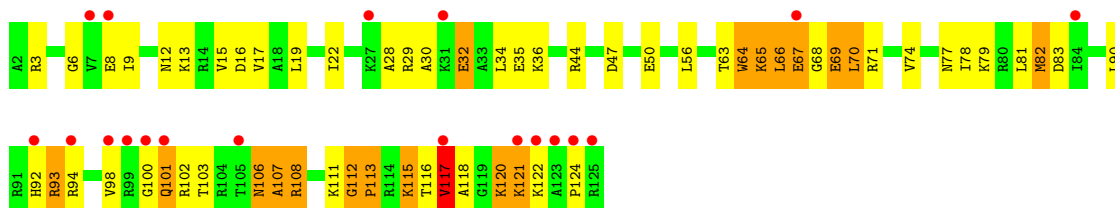


- Molecule 13: 30S ribosomal protein S13

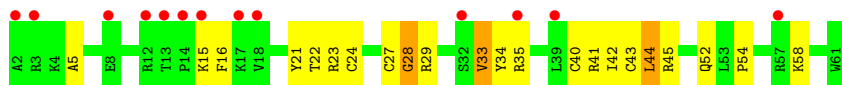




- Molecule 13: 30S ribosomal protein S13



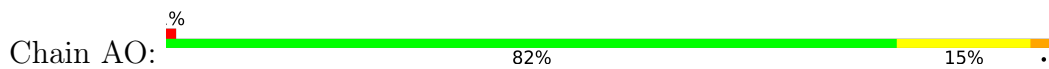
- Molecule 14: 30S ribosomal protein S14 type Z



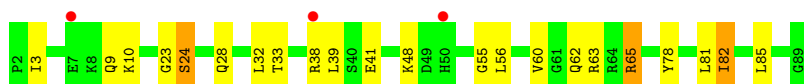
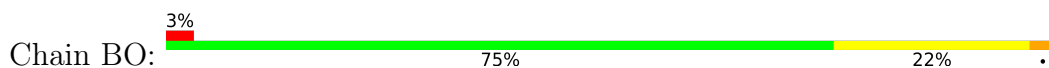
- Molecule 14: 30S ribosomal protein S14 type Z



- Molecule 15: 30S ribosomal protein S15

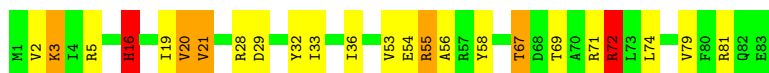


- Molecule 15: 30S ribosomal protein S15



- Molecule 16: 30S ribosomal protein S16

Chain AP:  71% 20% 6%




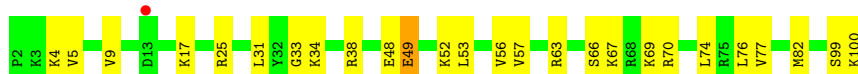
• Molecule 16: 30S ribosomal protein S16

Chain BP:  5% 63% 34%



• Molecule 17: 30S ribosomal protein S17

Chain AR:  74% 25%



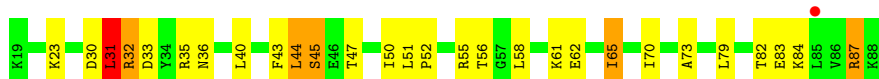
• Molecule 17: 30S ribosomal protein S17

Chain BR:  3% 67% 29%



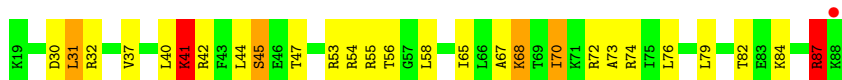
• Molecule 18: 30S ribosomal protein S18

Chain AS:  60% 31% 7%



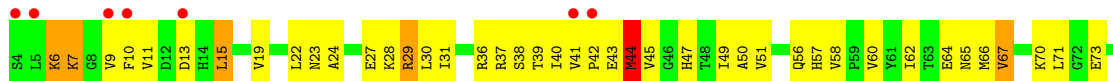
• Molecule 18: 30S ribosomal protein S18

Chain BS:  61% 30% 6%



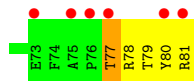
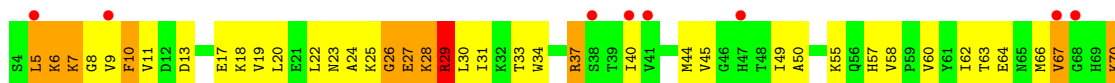
• Molecule 19: 30S ribosomal protein S19

Chain AT:  12% 44% 47% 8%

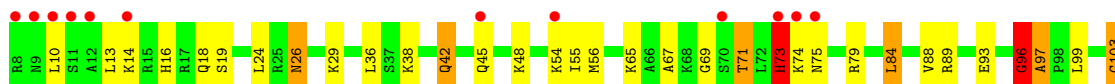




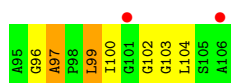
- Molecule 19: 30S ribosomal protein S19



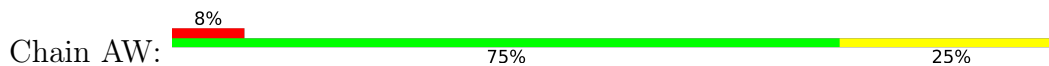
- Molecule 20: 30S ribosomal protein S20



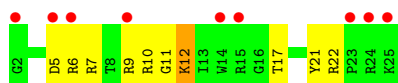
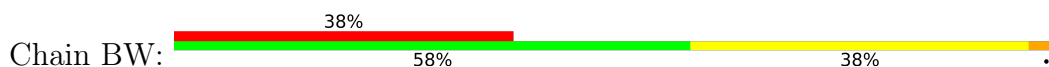
- Molecule 20: 30S ribosomal protein S20



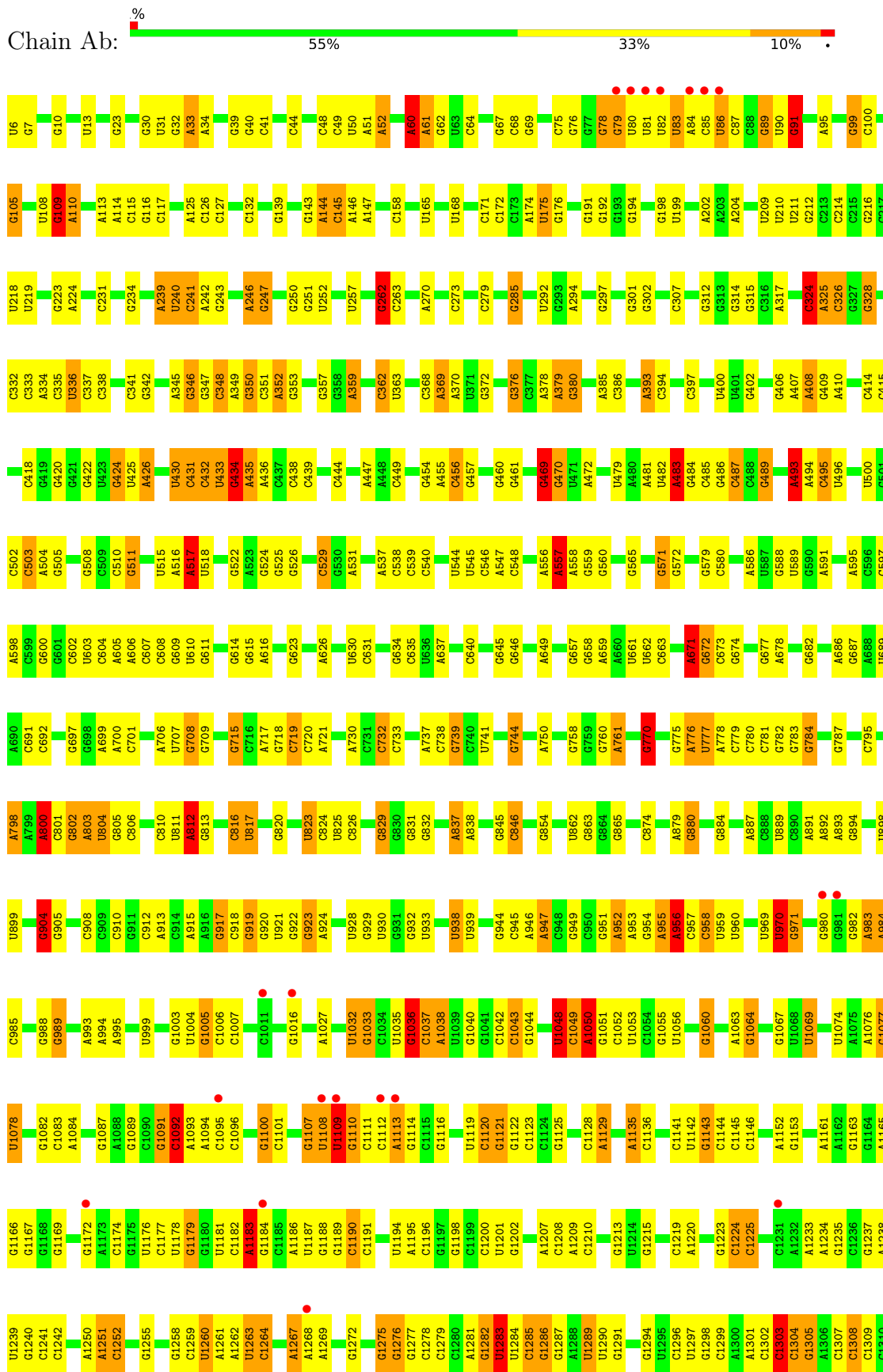
- Molecule 21: 30S ribosomal protein Thx

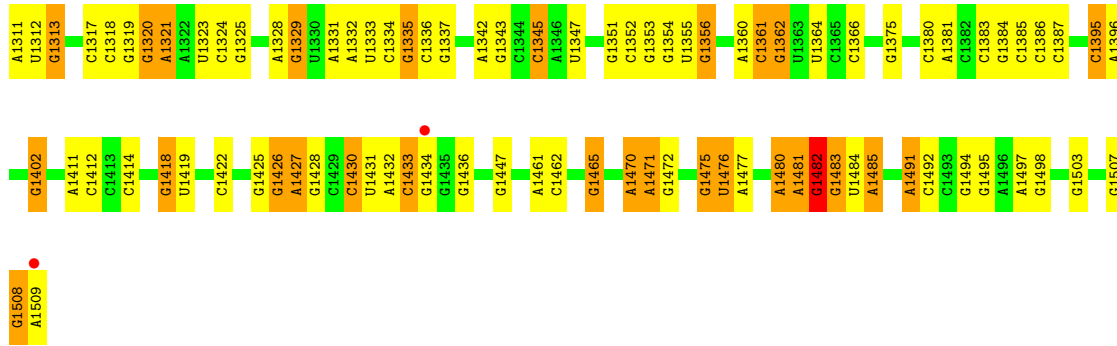


- Molecule 21: 30S ribosomal protein Thx

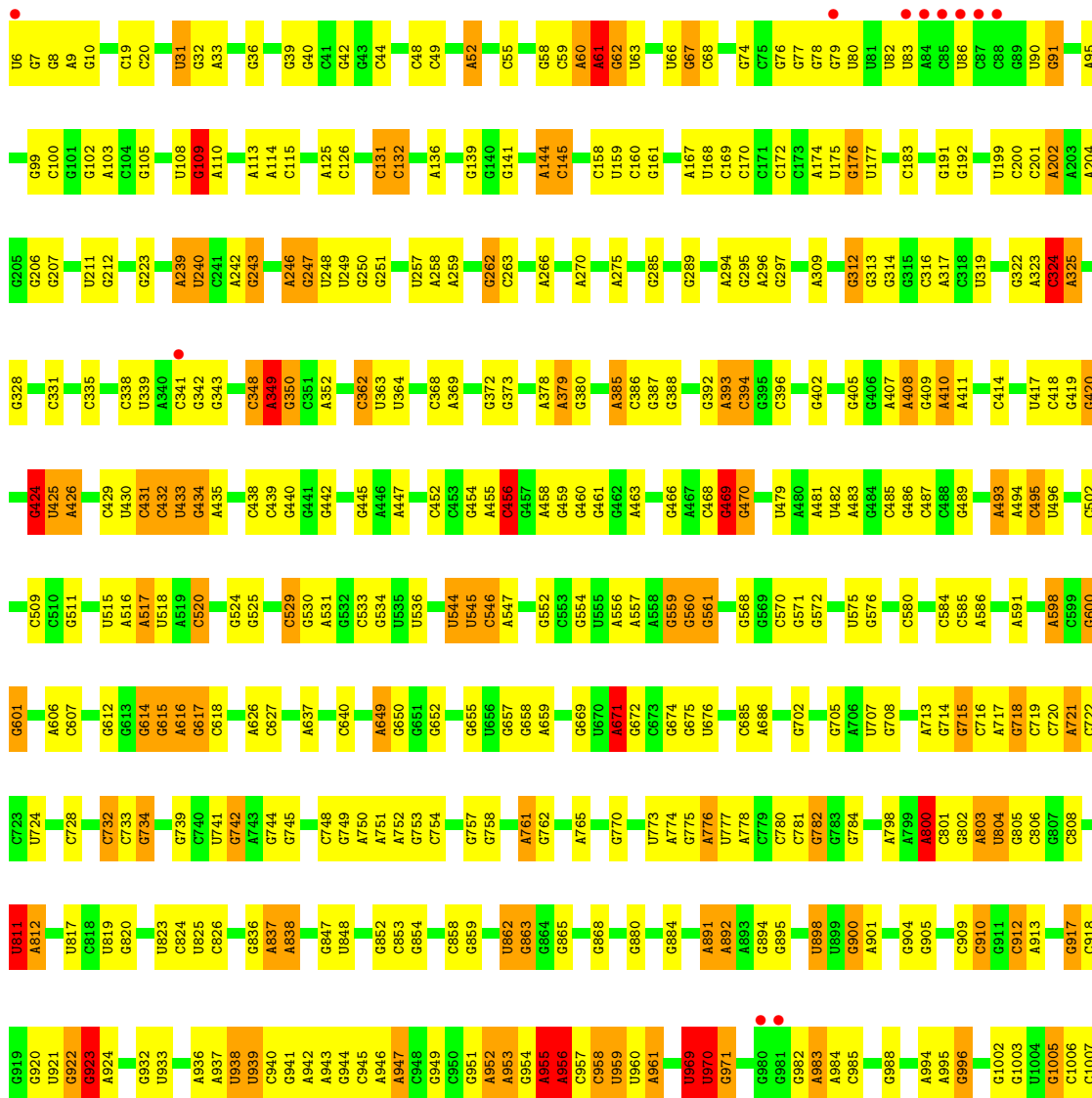


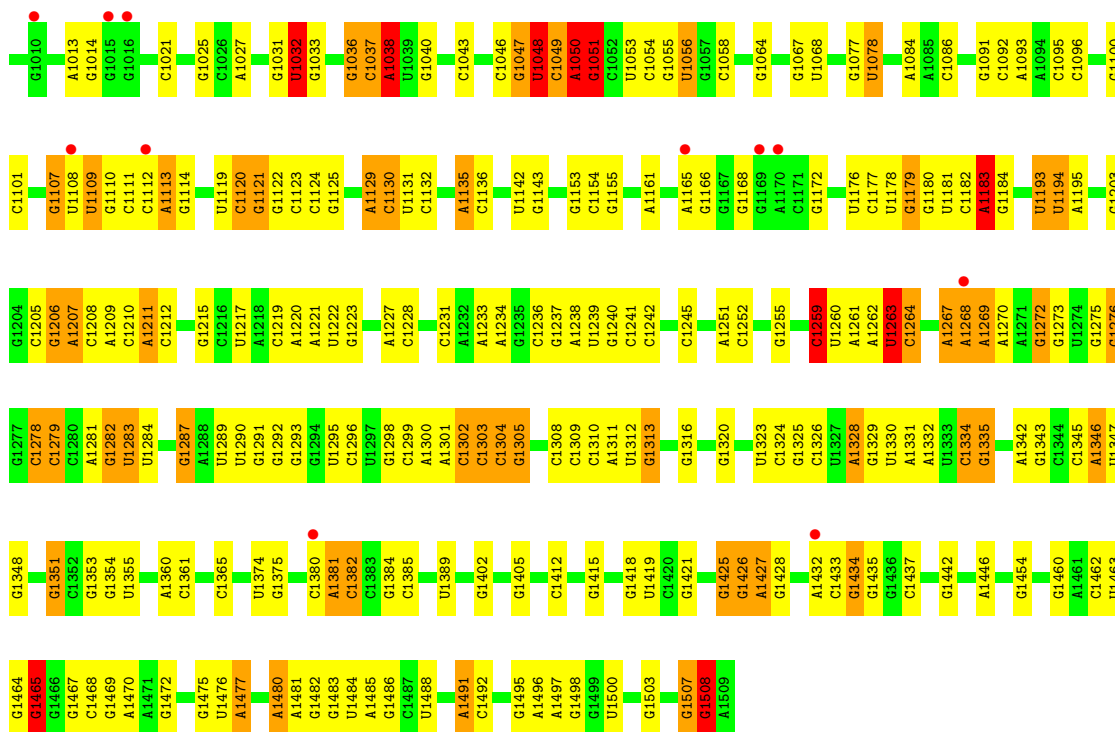
• Molecule 22: RNA (1504-MER)



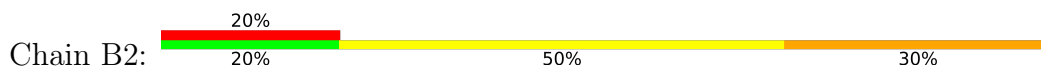


• Molecule 22: RNA (1504-MER)

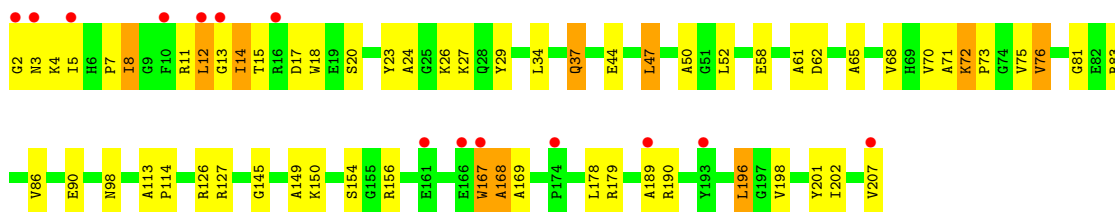




• Molecule 23: mRNA



• Molecule 24: 30S ribosomal protein S3

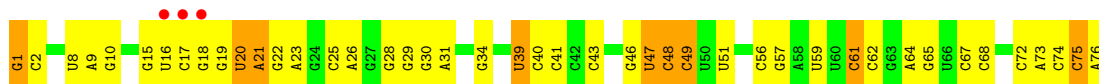


• Molecule 25: A site tNA, E site tNA

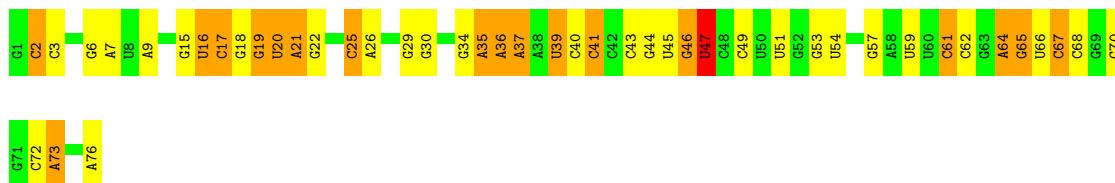


• Molecule 25: A site tNA, E site tNA

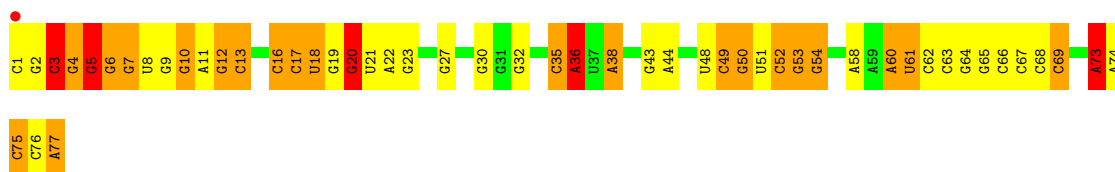




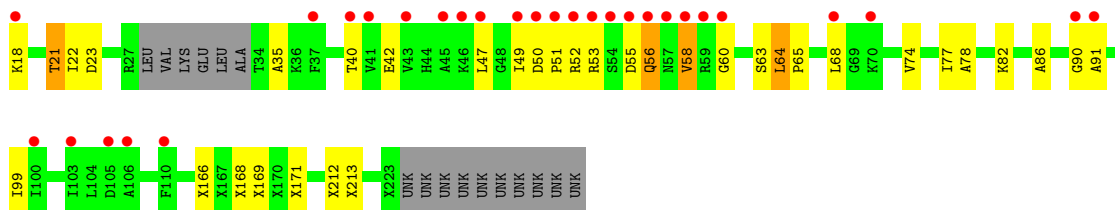
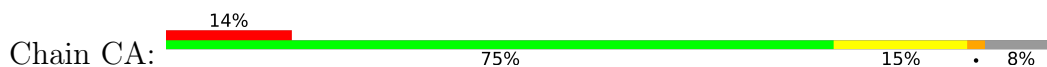
• Molecule 25: A site tNA, E site tNA



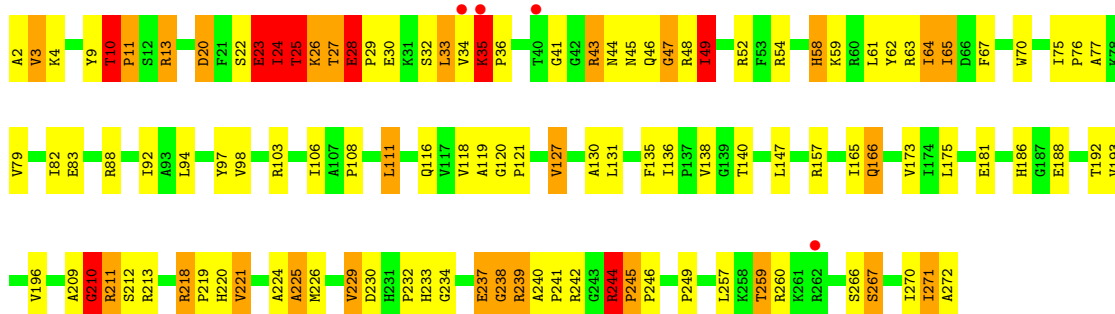
• Molecule 26: P site trNA



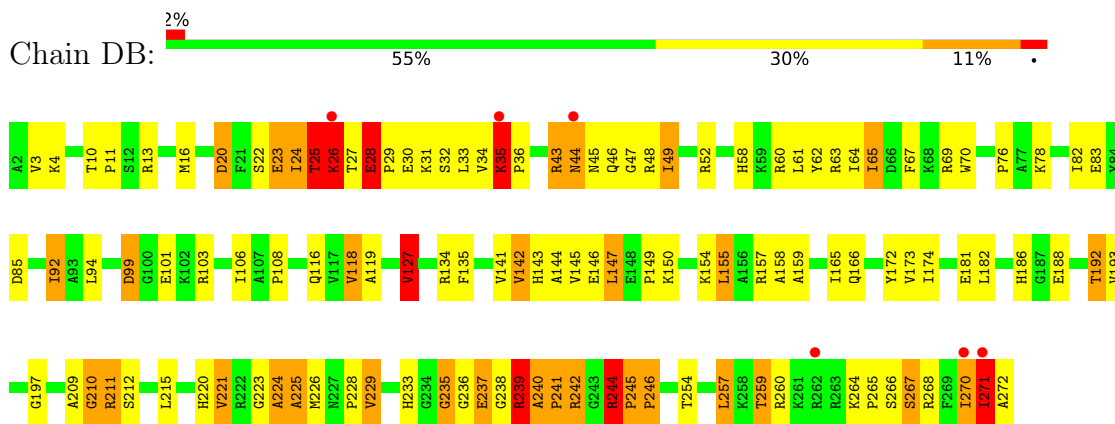
• Molecule 27: 50S ribosomal protein L1



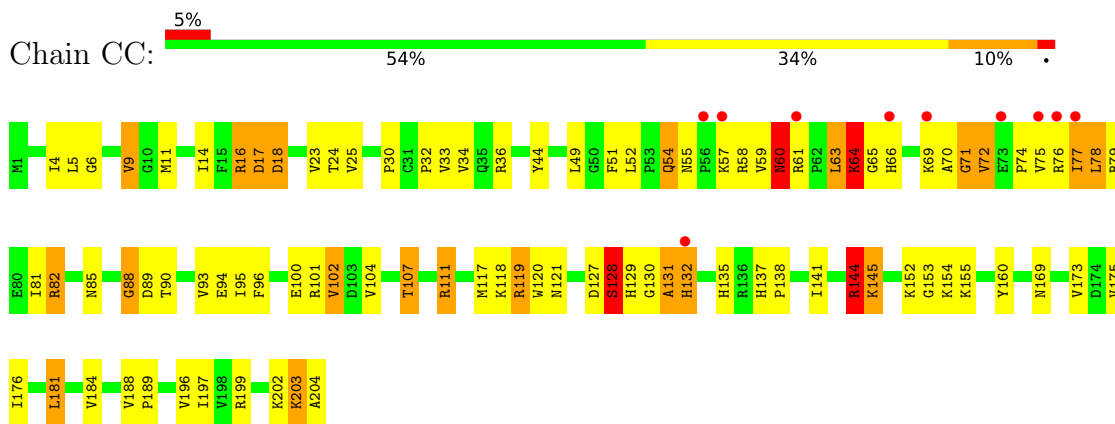
• Molecule 28: 50S ribosomal protein L2



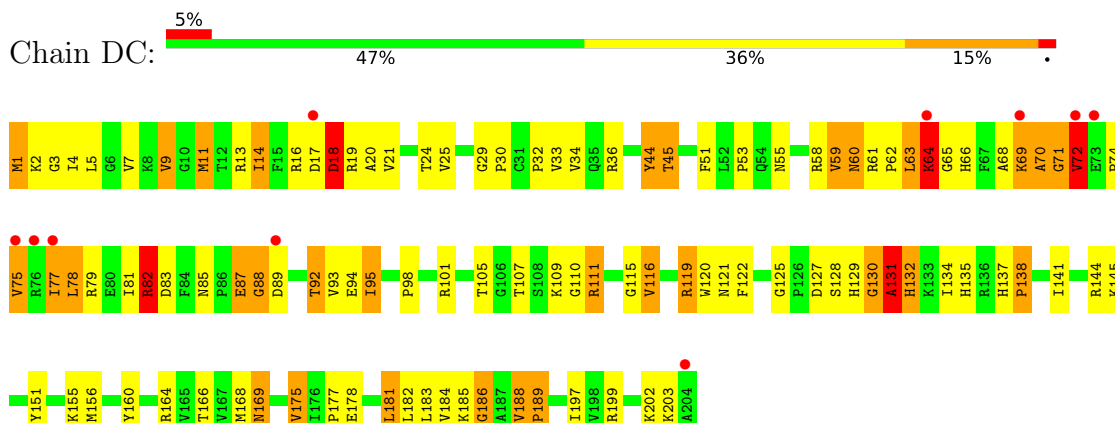
• Molecule 28: 50S ribosomal protein L2



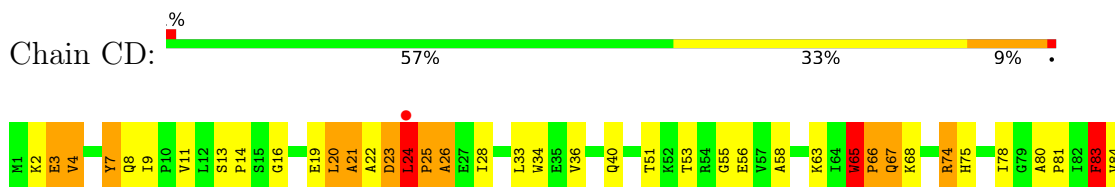
• Molecule 29: 50S ribosomal protein L3

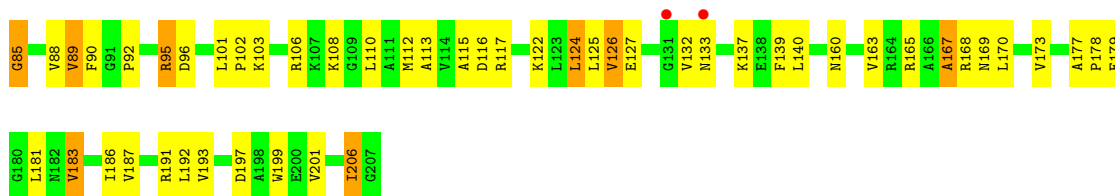


• Molecule 29: 50S ribosomal protein L3

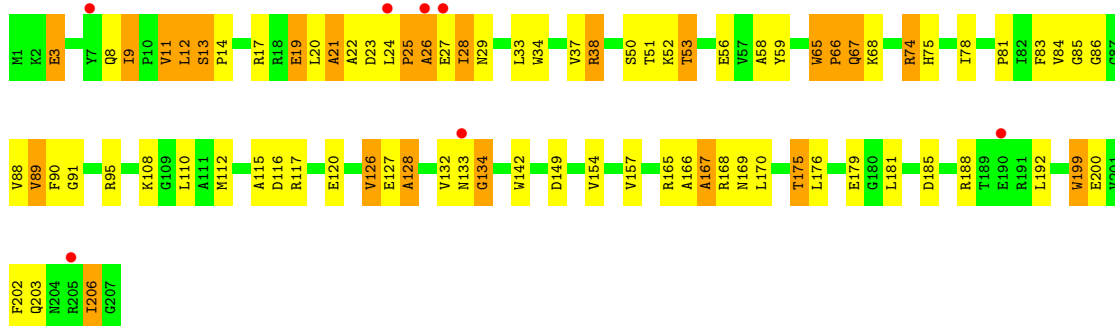


• Molecule 30: 50S ribosomal protein L4

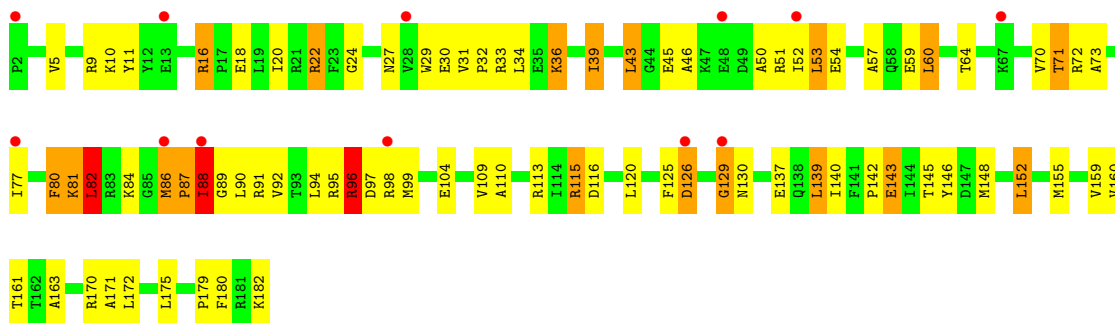




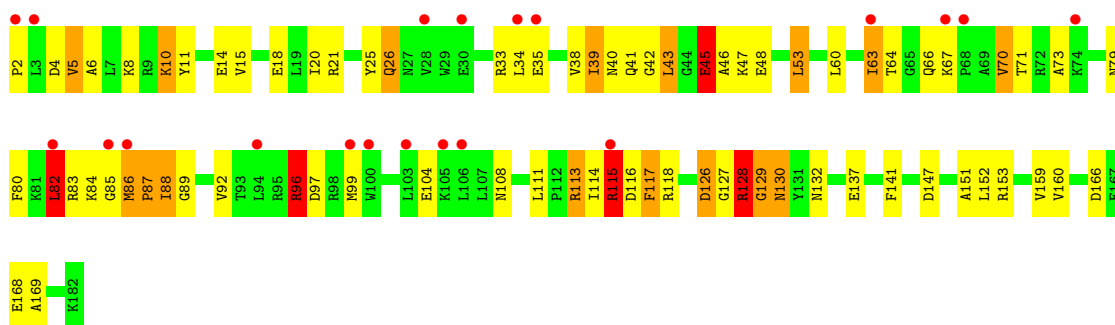
- Molecule 30: 50S ribosomal protein L4



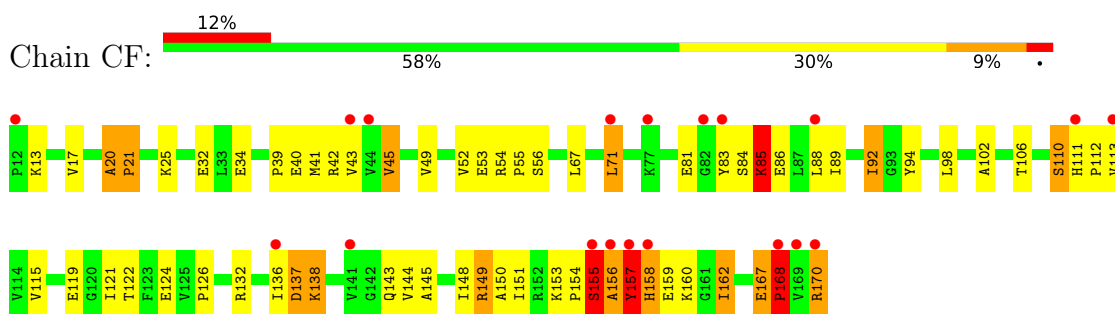
- Molecule 31: 50S ribosomal protein L5



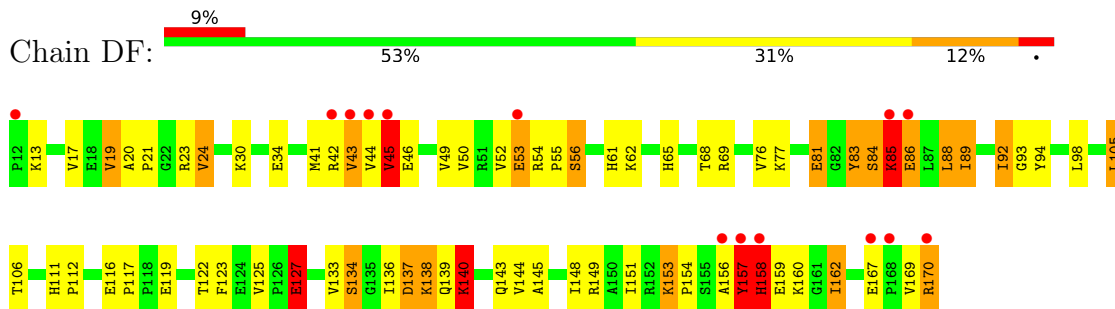
- Molecule 31: 50S ribosomal protein L5



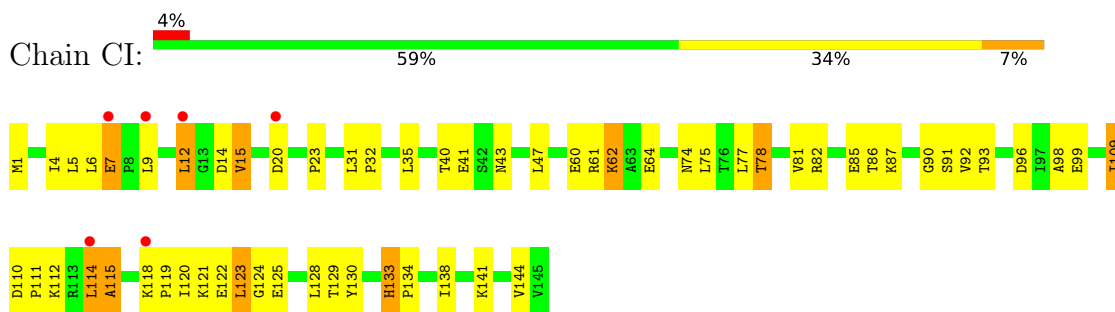
- Molecule 32: 50S ribosomal protein L6



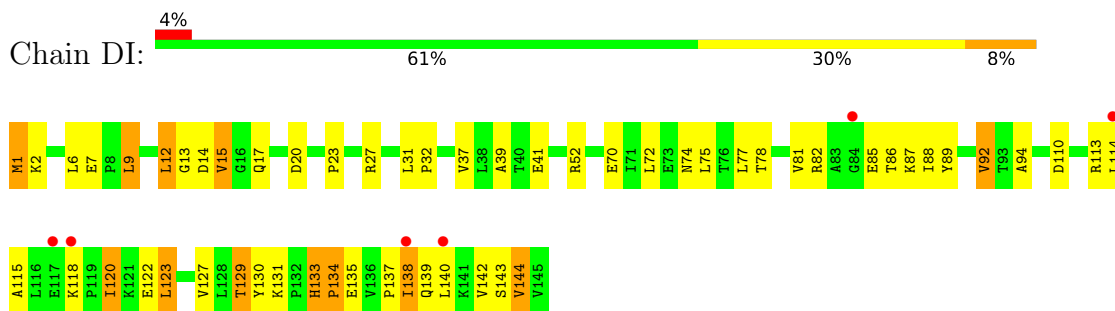
- Molecule 32: 50S ribosomal protein L6



- 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

Chain DJ:  95% 5%



- Molecule 35: 50S ribosomal protein L13

Chain CM:  5% 61% 24% 13%



- Molecule 35: 50S ribosomal protein L13

Chain DM:  7% 57% 30% 11%



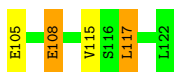
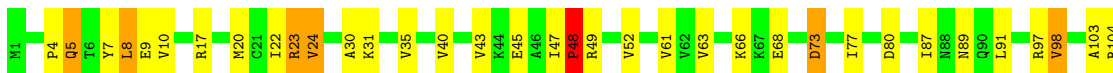
- Molecule 36: 50S ribosomal protein L14

Chain CN:  2% 61% 32% 7%

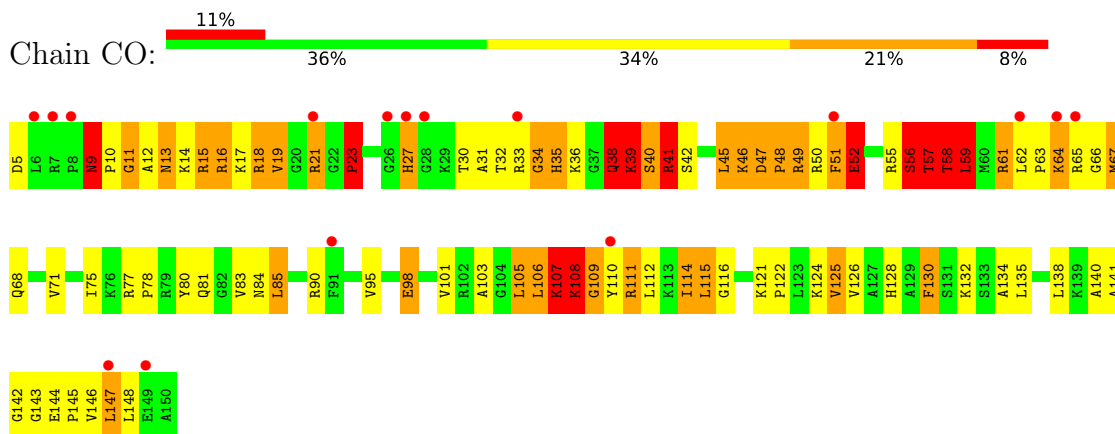


- Molecule 36: 50S ribosomal protein L14

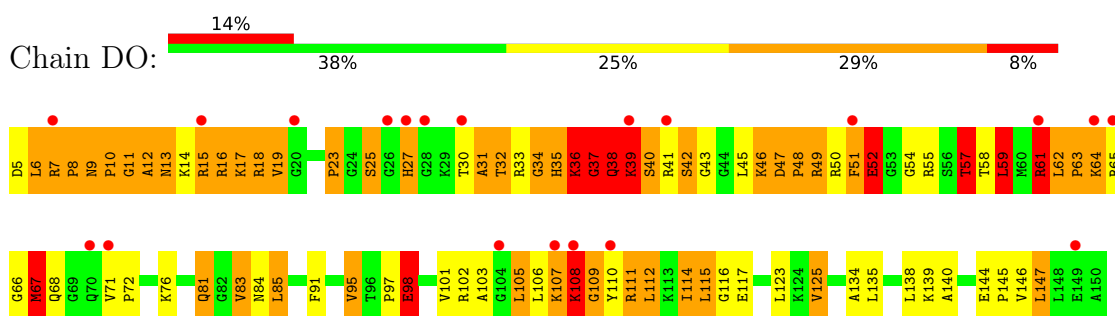
Chain DN:  68% 25% 7%



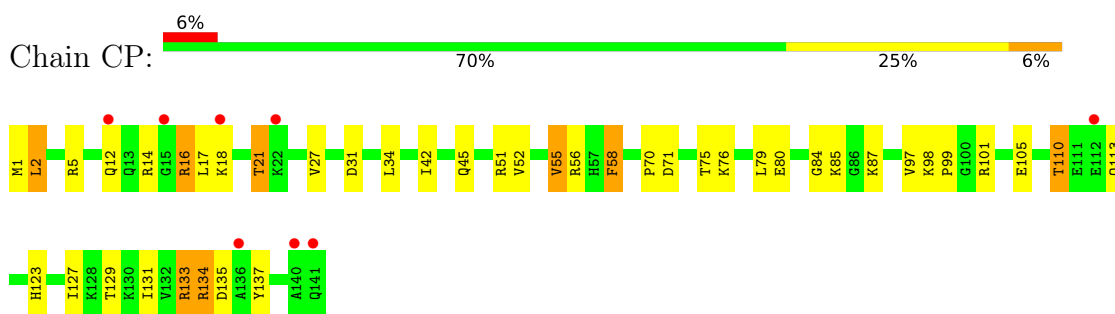
- Molecule 37: 50S ribosomal protein L15



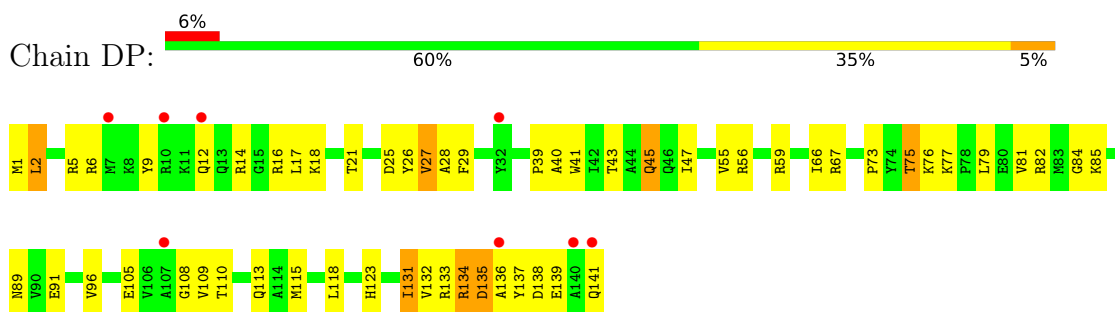
- Molecule 37: 50S ribosomal protein L15



- Molecule 38: 50S ribosomal protein L16

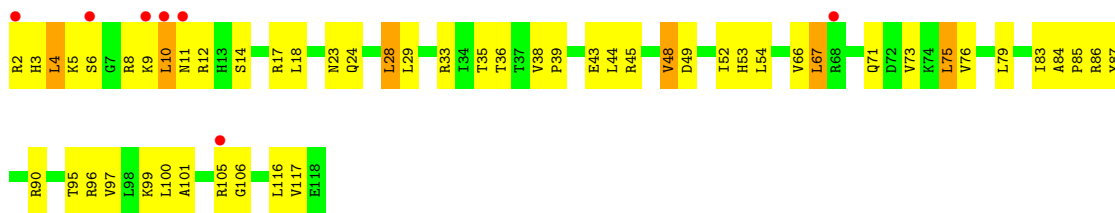


- Molecule 38: 50S ribosomal protein L16

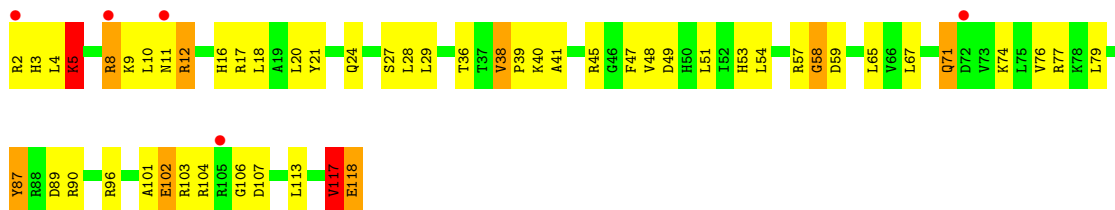


- Molecule 39: 50S ribosomal protein L17

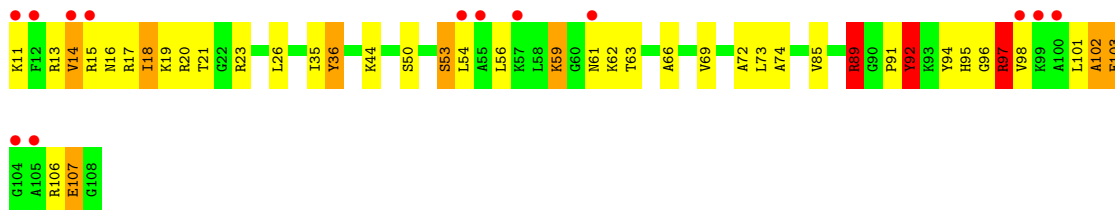




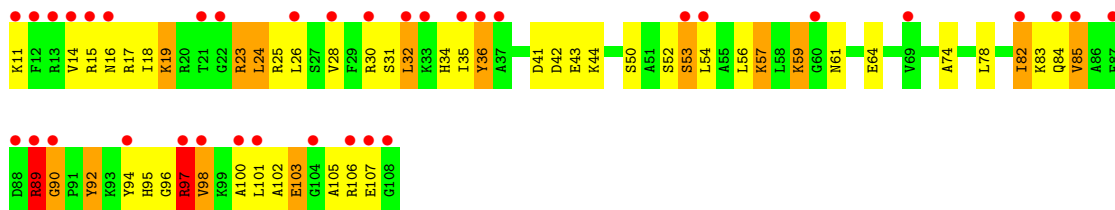
• Molecule 39: 50S ribosomal protein L17



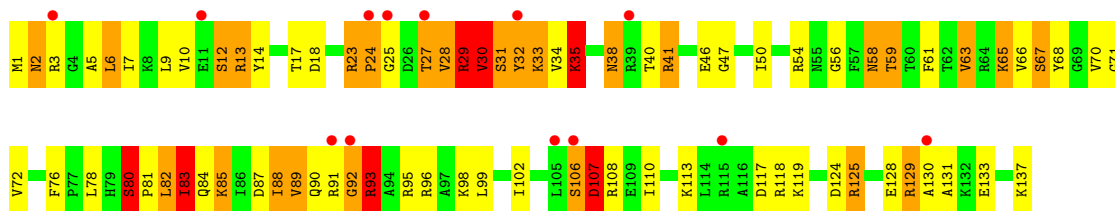
• Molecule 40: 50S ribosomal protein L18



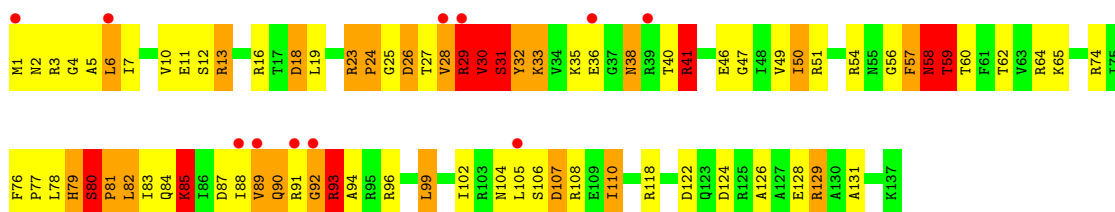
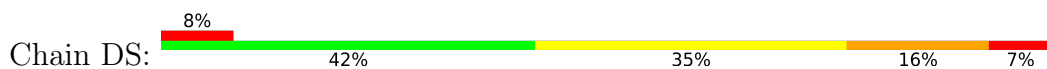
• Molecule 40: 50S ribosomal protein L18



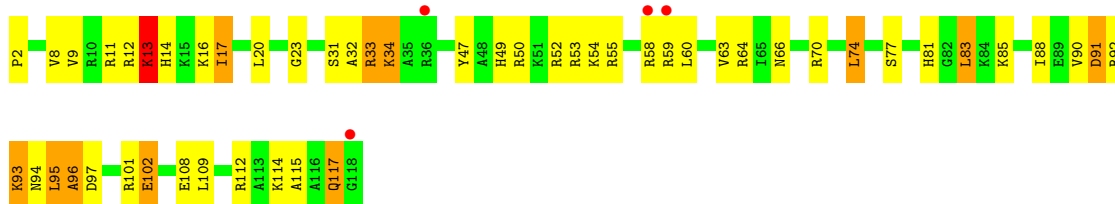
• Molecule 41: 50S ribosomal protein L19



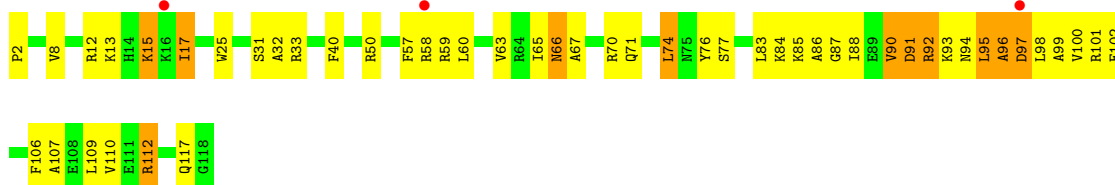
- Molecule 41: 50S ribosomal protein L19



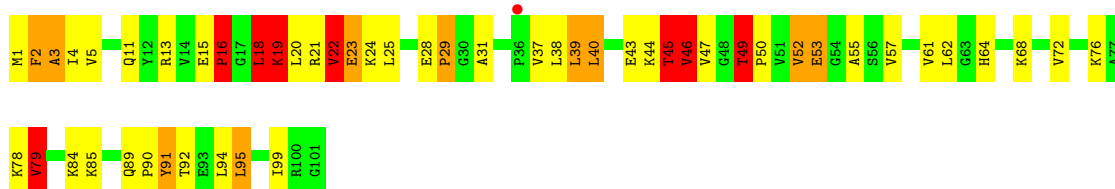
- Molecule 42: 50S ribosomal protein L20



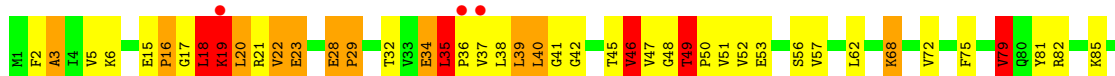
- Molecule 42: 50S ribosomal protein L20

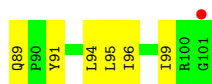


- Molecule 43: 50S ribosomal protein L21

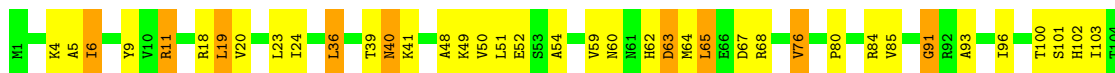


- Molecule 43: 50S ribosomal protein L21

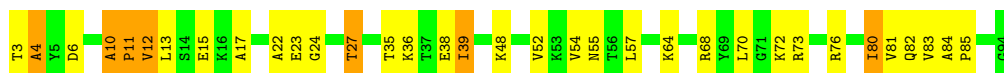




- Molecule 44: 50S ribosomal protein L22



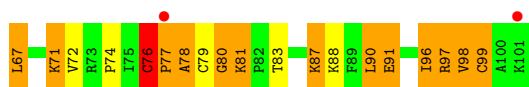
- Molecule 45: 50S ribosomal protein L23



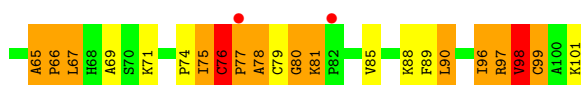
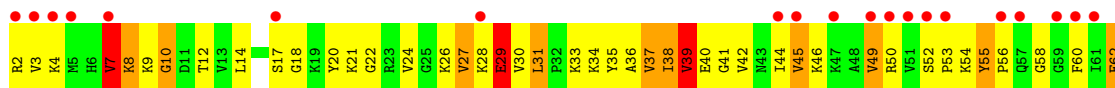
- Molecule 45: 50S ribosomal protein L23



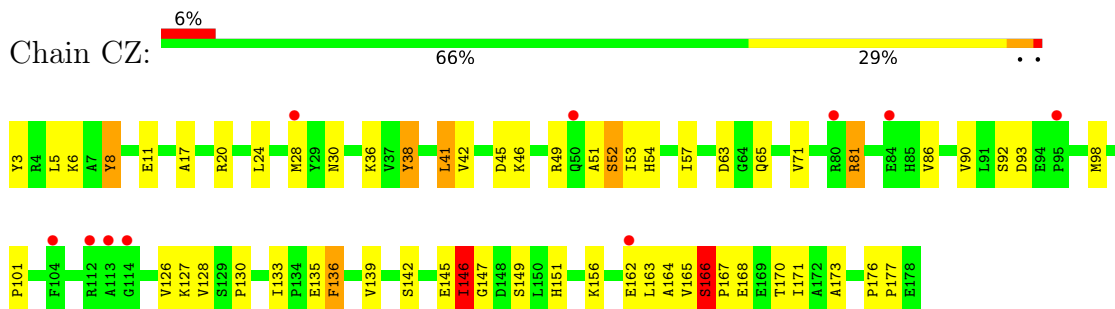
- Molecule 46: 50S ribosomal protein L24



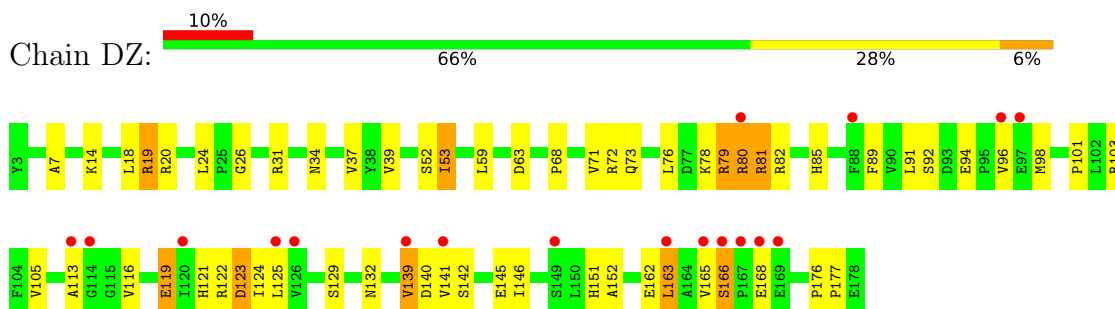
- Molecule 46: 50S ribosomal protein L24



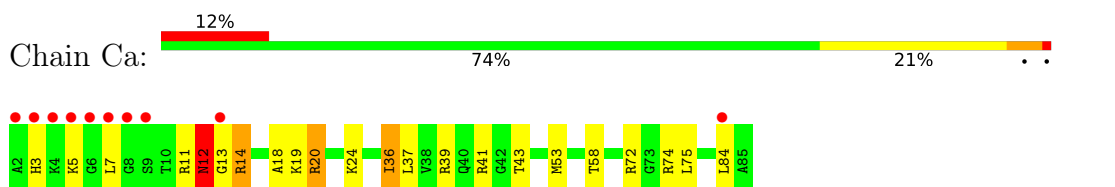
- Molecule 47: 50S ribosomal protein L25



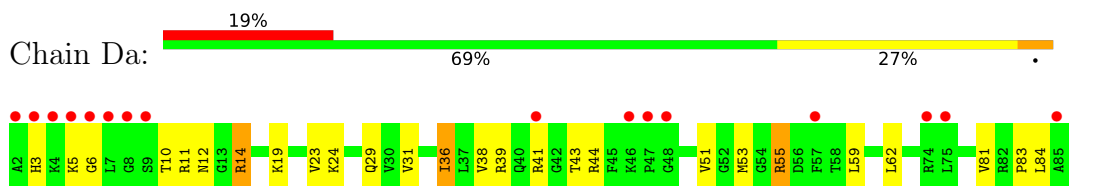
- Molecule 47: 50S ribosomal protein L25



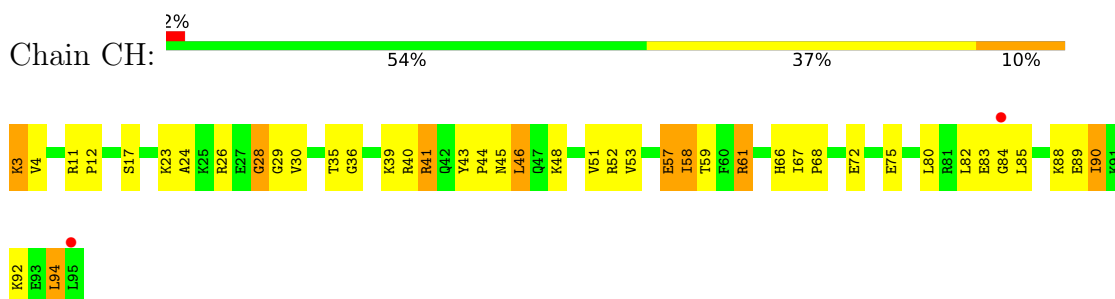
- Molecule 48: 50S ribosomal protein L27



- Molecule 48: 50S ribosomal protein L27

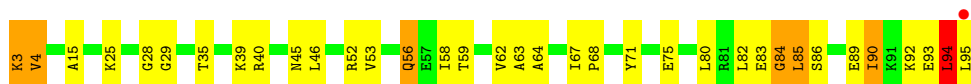


- Molecule 49: 50S ribosomal protein L28

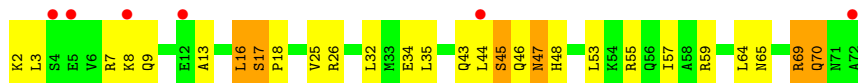


- Molecule 49: 50S ribosomal protein L28

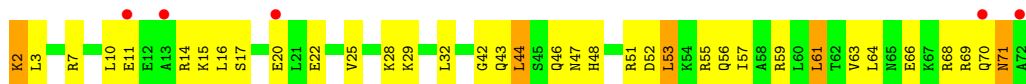




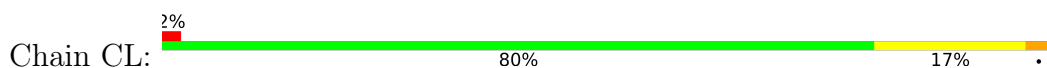
- Molecule 50: 50S ribosomal protein L29



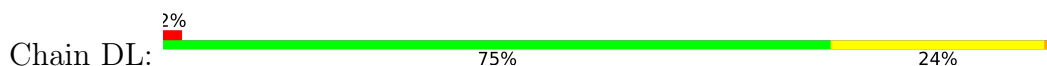
- Molecule 50: 50S ribosomal protein L29



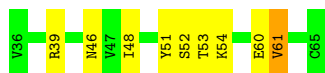
- Molecule 51: 50S ribosomal protein L30



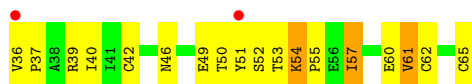
- Molecule 51: 50S ribosomal protein L30



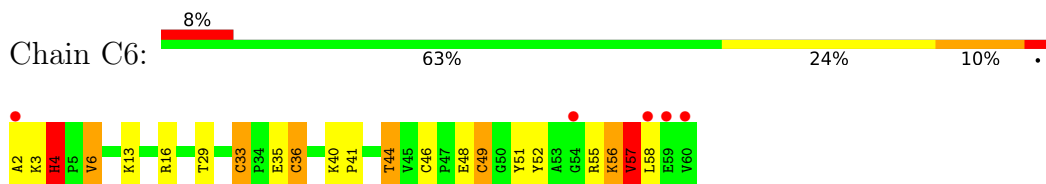
- Molecule 52: 50S ribosomal protein L31



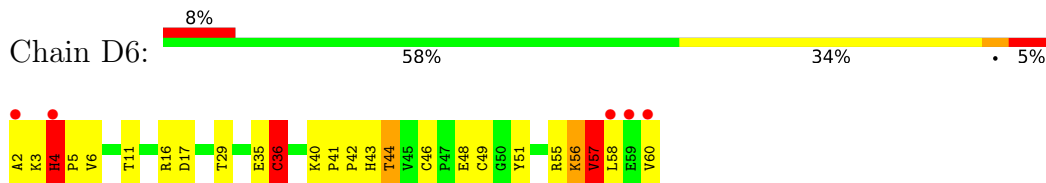
- Molecule 52: 50S ribosomal protein L31



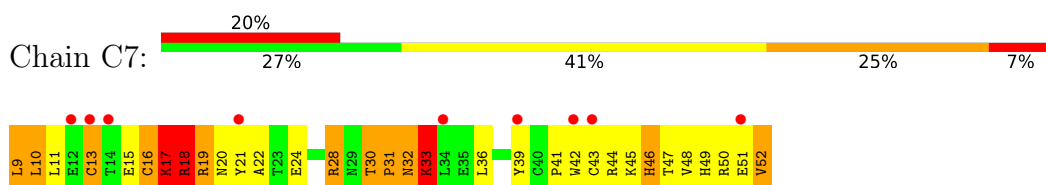
- Molecule 53: 50S ribosomal protein L32



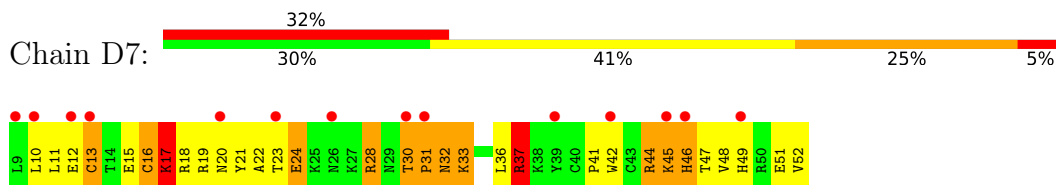
- Molecule 53: 50S ribosomal protein L32



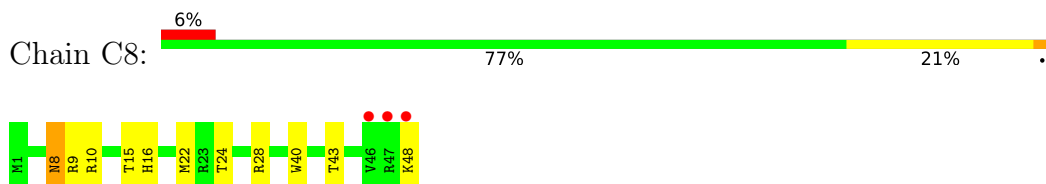
- Molecule 54: 50S ribosomal protein L33



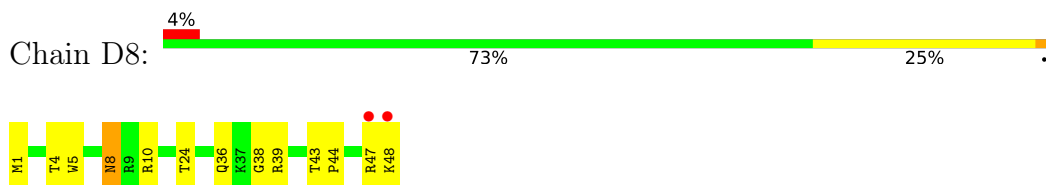
- Molecule 54: 50S ribosomal protein L33



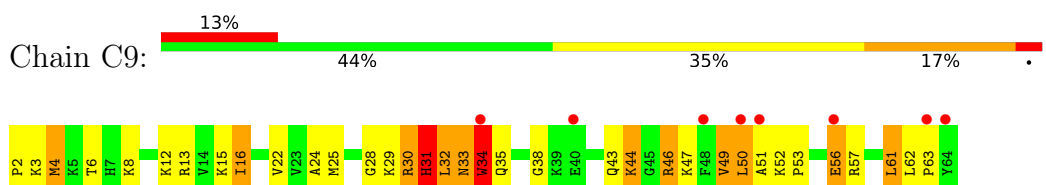
- Molecule 55: 50S ribosomal protein L34



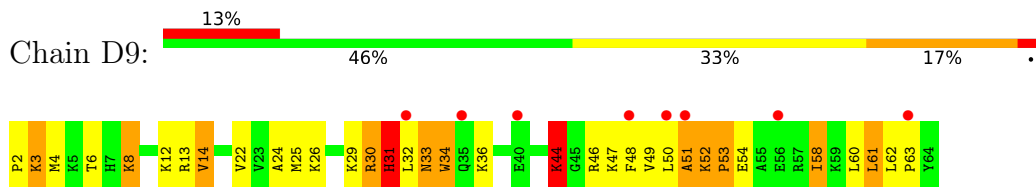
- Molecule 55: 50S ribosomal protein L34



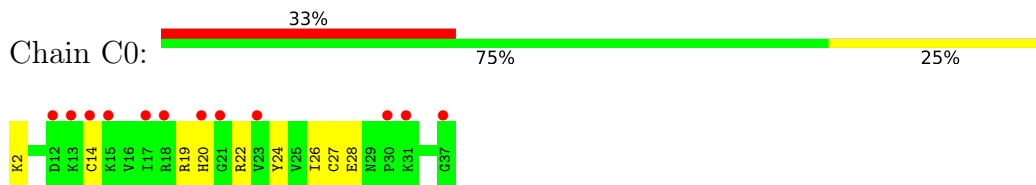
- Molecule 56: 50S ribosomal protein L35



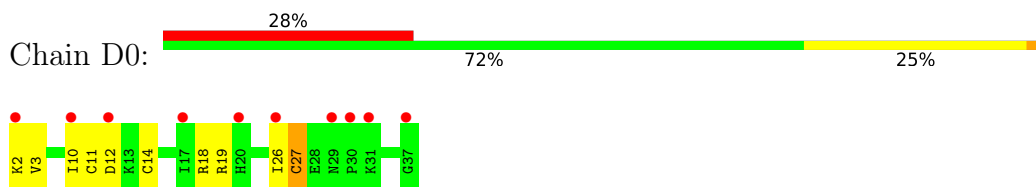
- Molecule 56: 50S ribosomal protein L35



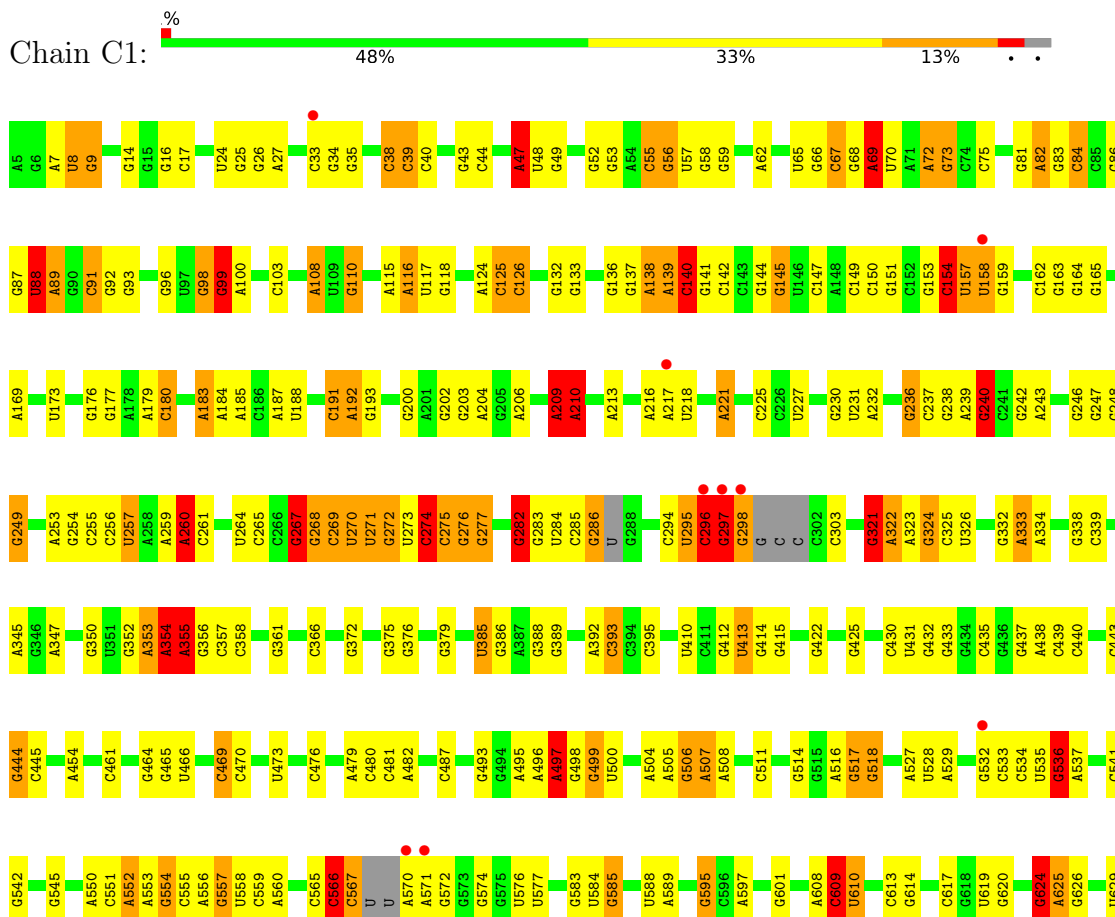
- Molecule 57: 50S ribosomal protein L36

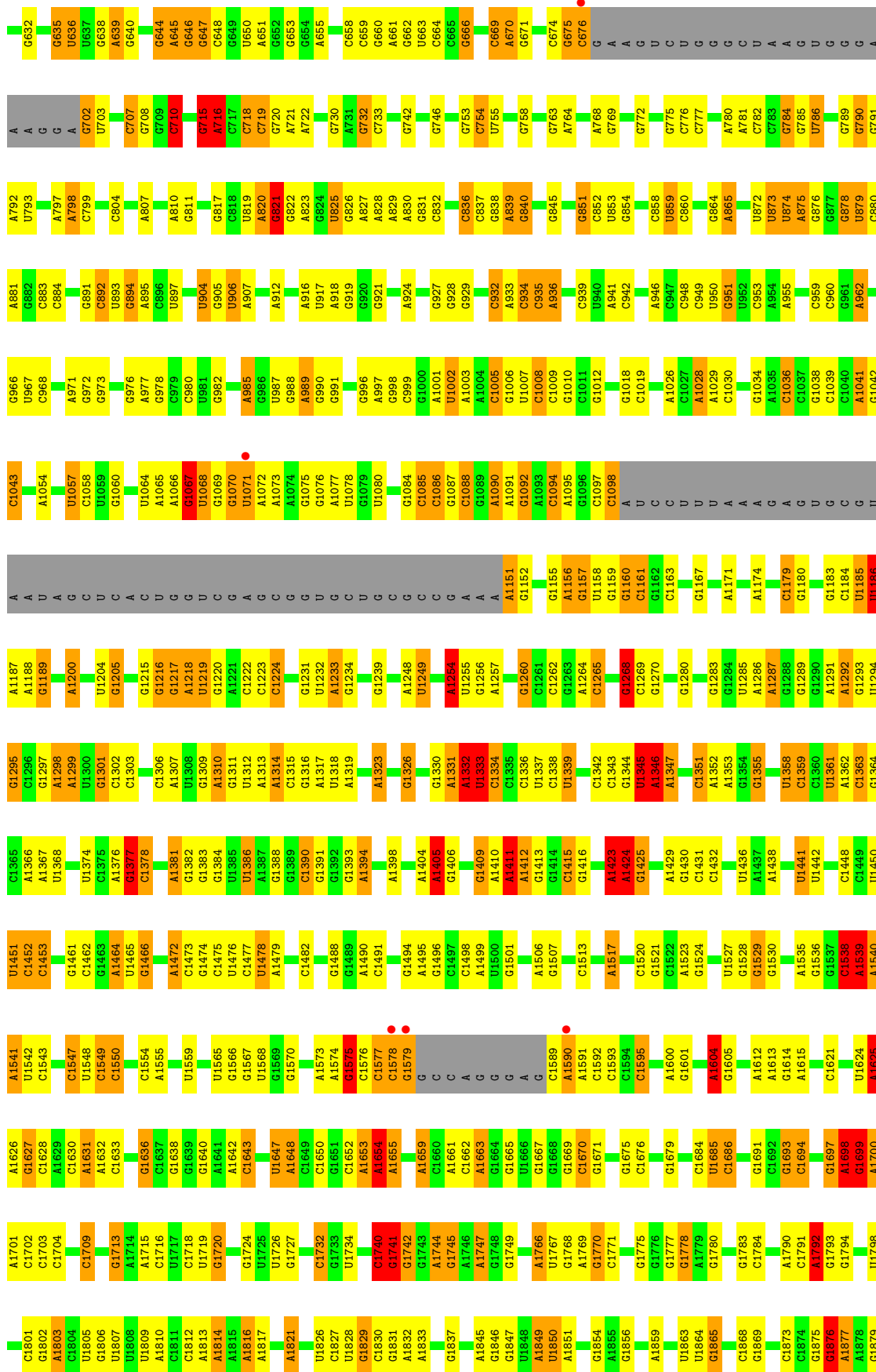


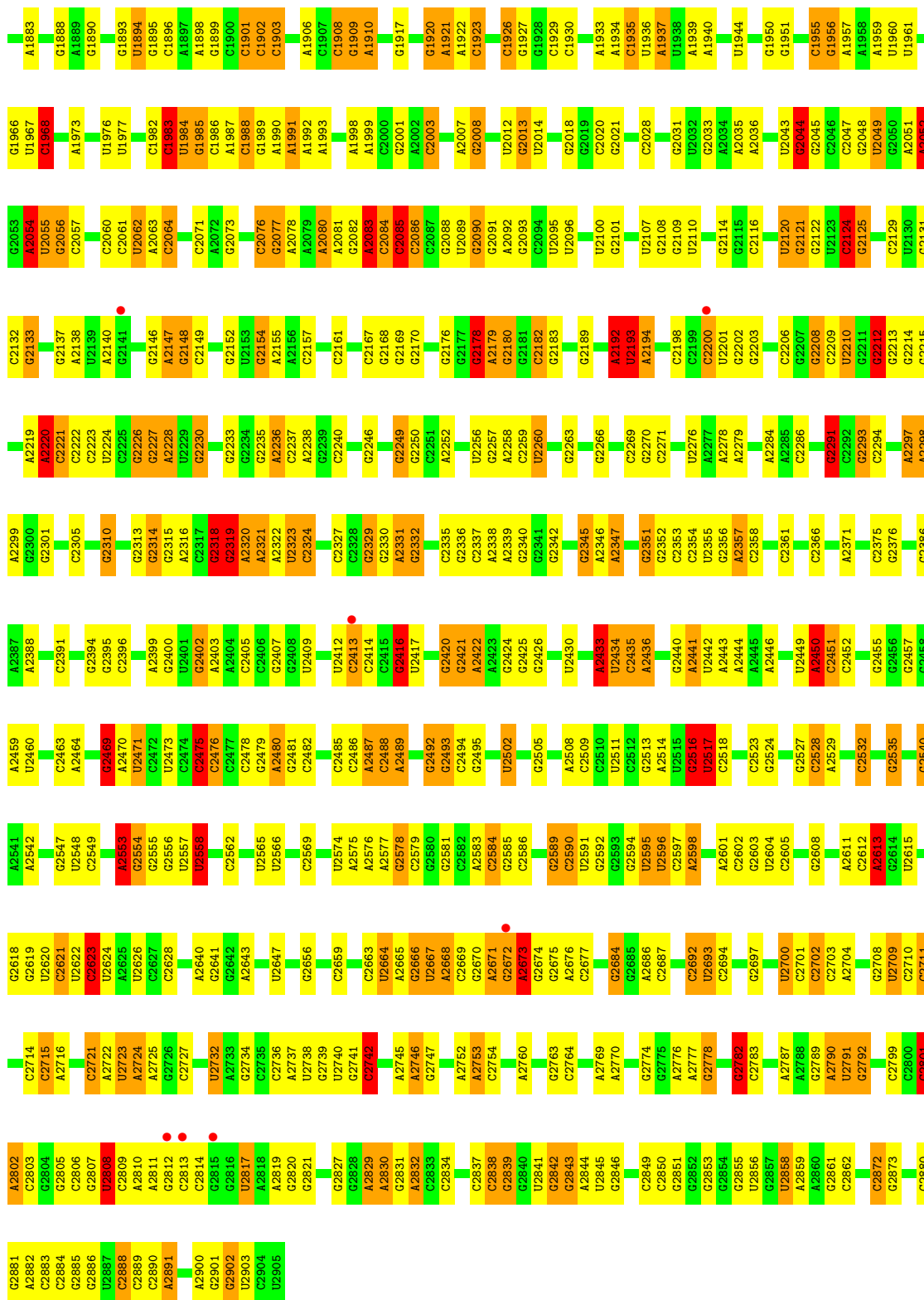
- Molecule 57: 50S ribosomal protein L36



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



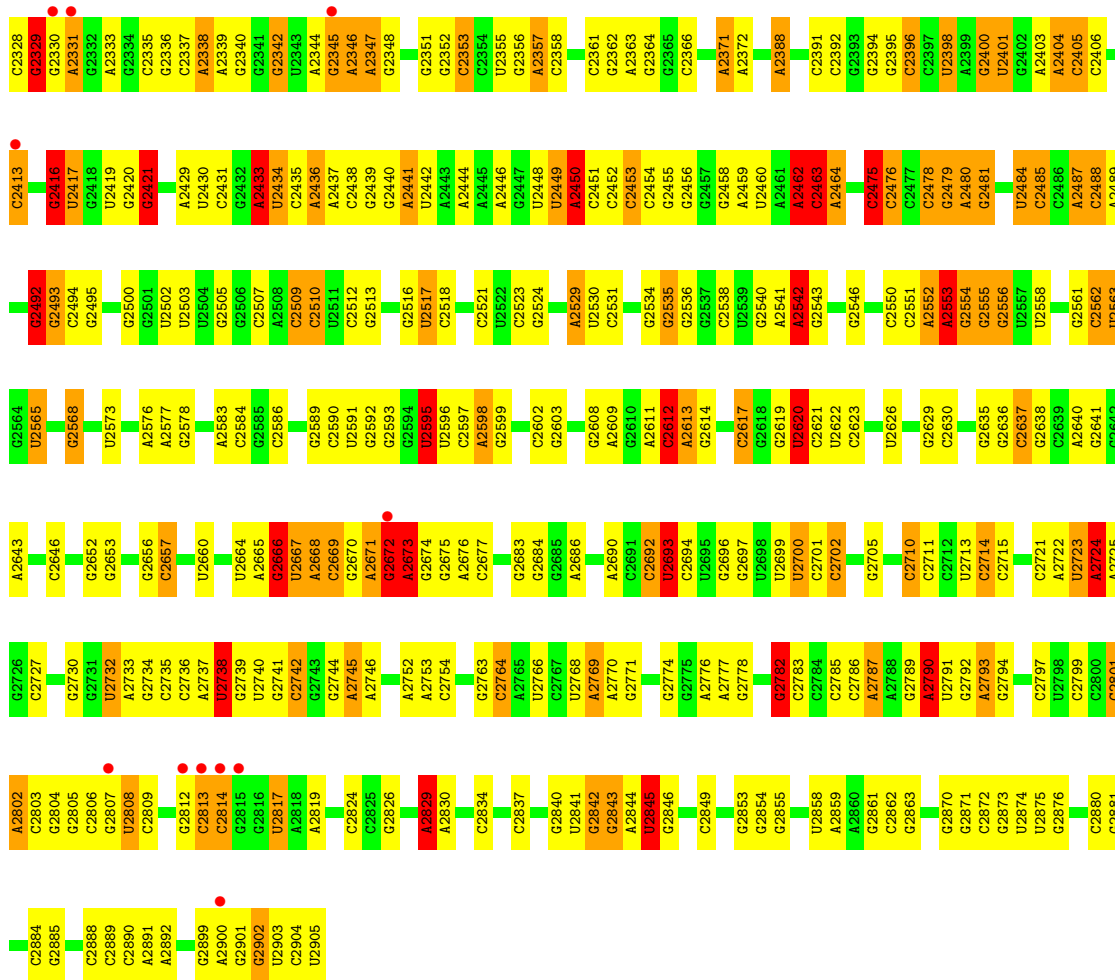




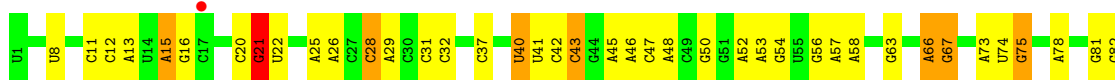
• Molecule 58: 23S rRNA (2899-MER)



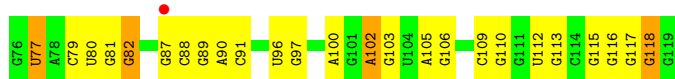
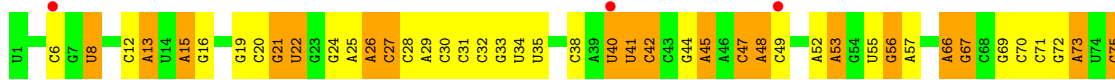
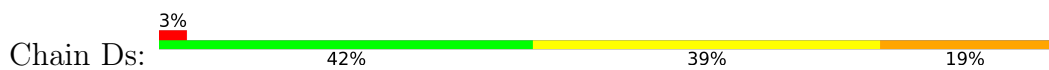
U2260	G2183	G2102	C2028	G1943	U1871	G1793	G1699	C1623	C1544	A1472	G1391	A1310	A1221
G2262	C2184	A2103	C2029	U1944	G1872	G1794	A1700	U1624	G1544	C1473	G1392	G1311	C1222
U2267	G2185	G2104	G2030	G1950	C1873	C1801	C1703	A1625	C1546	C1474	G1393	A1312	C1223
G2268	G2186	G2105	G2031	G1951	C1874	G1802	C1704	G1626	C1547	C1475	A1394	A1313	C1224
C2269	G2187	U2107	A2034	C1955	G1876	A1803	C1709	G1628	U1548	C1476	G1295	A1314	C1225
C2270	A2192	U2110	A2035	A1877	A1877	G1806	A1710	A1629	C1549	C1477	A1398	A1315	A1226
G2271	U2193	G2111	A2036	A1878	A1878	G1809	A1711	C1630	U1399	U1478	A1399	A1316	G1227
C2198	A2194	U2112	C2042	A1879	G1880	U1809	A1719	A1631	G1400	C1482	G1400	G1231	
C2199	C2198	U2113	U2043	A1958	U1881	A1810	U1719	C1632	G1403	G1486	A1403	U1232	
C2200	C2199	G2114	G2044	A1959	U1882	C1811	G1720	C1633	A1404	G1487	A1404	A1233	
U2201	C2200	G2115	G2045	A1963	A1883	C1812	A1723	U1635	A1405	G1488	A1405	G1234	
G2202	U2201	C2116	C2046	U1964	A1884	A1813	A1724	G1636	G1406	G1489	G1406	G1235	
G2203	G2202	U2120	C2047	U1965	G1886	A1814	G1724	C1637	C1407	U1490	C1407	G1239	
G2204	U2193	G2122	G2048	U1966	G1886	A1815	U1725	G1638	A1408	G1495	A1408	C1244	
G2205	A2194	U2123	U2049	C1968	G1887	A1816	U1726	G1639	G1409	G1496	G1409	C1245	
C2206	G2205	G2124	G2050	U1972	G1888	A1817	G1727	U1642	A1410	C1497	A1410	C1246	
G2207	A2063	C2125	A2062	U1973	U1889	C1820	G1728	C1643	G1413	C1498	G1413	G1247	
G2208	G2063	G2126	A2063	A1974	U1894	A1821	C1729	U1647	A1573	C1499	G1414	A1248	
C2209	A2064	C2127	U2055	G1975	G1895	U1828	C1731	A1648	A1574	A1499	G1414	U1249	
G2210	U2055	C2128	G2056	U1976	G1896	G1829	G1732	C1649	G1575	U1500	C1415	C1335	
G2211	C2057	G2131	G2057	G1980	A1897	C1830	G1733	C1650	C1577	G1501	C1336	G1250	
G2212	G2056	C2132	G2058	A1981	A1898	G1831	U1734	G1651	C1578	G1505	C1337	C1251	
G2213	G2059	G2133	C2060	C1982	U1899	A1832	A1735	C1652	G1579	A1506	C1338	C1252	
G2214	C2060	G2134	G2061	C1983	G1900	A1833	C1740	A1653	G1507	G1507	C1342	G1253	
A2219	A2063	G2137	A2063	U1984	A1901	A1834	G1741	A1655	C1510	C1510	G1343	A1254	
A2220	C2064	U2139	C2064	G1985	C1902	U1835	G1742	A1656	A1511	G1511	G1344	U1255	
C2221	C2065	G2140	C2065	C1986	C1903	C1836	G1743	A1657	A1512	G1512	G1345	G1256	
U2224	G2141	A2141	C2071	A1987	U1984	G1837	A1744	G1658	A1513	G1513	A1346	G1260	
G2225	G2142	U2142	A2072	C1988	A1905	U1837	A1745	C1659	A1514	G1514	A1347	C1261	
G2226	U2143	G2143	G2073	G1989	A1906	A1842	A1746	A1661	A1515	G1515	C1351	C1285	
G2227	G2144	G2144	G2074	A1990	C1907	G1843	A1747	C1662	A1516	G1516	C1352	G1268	
A2228	G2145	G2145	A2075	A1991	U1908	A1844	A1748	A1663	A1517	U1436	C1351	G1268	
U2229	G2146	C2146	A2075	A1992	G1909	A1845	G1763	A1663	A1590	U1439	C1352	G1268	
G2230	A2147	G2148	G2077	A1993	A1910	G1846	U1764	U1666	A1591	U1440	C1353	A1254	
A2236	G2148	G2148	C2077	A1999	G1911	U1849	G1765	G1667	A1592	G1521	C1354	U1255	
C2237	G2152	G2152	A2080	C2000	U1912	U1850	A1766	A1667	C1592	G1522	G1344	G1256	
A2238	U2153	U2153	A2081	G2001	C1913	U1851	U1767	G1671	C1593	G1523	G1345	G1256	
G2239	G2154	G2154	G2082	A2002	G1917	G1854	G1768	C1676	C1596	G1524	C1444	G1281	
C2240	A2155	A2155	A2083	C2003	G1920	A1855	A1770	A1677	C1597	U1527	C1448	G1365	
G2241	G2157	C2157	C2085	G2004	A1921	A1856	C1771	A1678	G1598	G1528	C1449	A1366	
G2242	C2157	C2157	C2086	G2005	A1922	C1857	C1772	G1679	A1599	G1530	U1450	A1367	
G2243	C2157	C2157	C2086	A2007	C1923	G1858	C1774	G1681	A1600	U1451	C1452	A1287	
G2244	C2161	C2161	C2087	G2008	G1924	A1859	G1775	G1682	A1604	G1531	C1453	A1291	
G2245	G2162	G2162	G2088	C2009	G1925	C1860	G1776	A1683	G1605	G1532	C1453	A1292	
G2246	C2163	C2163	G2010	G1926	C1926	G1861	G1777	A1684	G1606	G1533	G1459	G1293	
G2249	G2168	G2168	G2011	G1927	U1895	C1862	U1778	U1685	A1535	U1534	G1459	U1294	
G2250	U2012	U2012	U2012	U1927	U1863	C1862	A1779	C1686	A1612	A1535	U1460	G1295	
C2251	G2013	G2013	G2013	A1933	U1864	U1863	G1780	C1686	A1613	G1537	G1461	G1295	
G2252	U2014	U2014	U2014	A1934	G1865	U1864	G1780	C1686	A1613	G1537	G1462	A1298	
U2254	G2017	G2017	G2017	A1935	C1866	G1865	G1783	G1691	A1614	C1538	G1463	A1299	
U2255	G2018	G2018	G2018	U1936	C1867	C1866	C1784	G1692	A1615	A1539	G1464	A1299	
G2256	G2018	G2018	G2018	A1937	C1868	C1868	A1785	G1693	A1616	A1540	U1465	U1385	
G2257	G2018	G2018	G2018	U1938	C1870	C1870	A1792	C1694	A1621	U1541	G1468	G1390	
G2257	G2018	G2018	G2018	U1938	C1870	C1870	A1792	C1694	A1621	U1541	G1468	G1390	



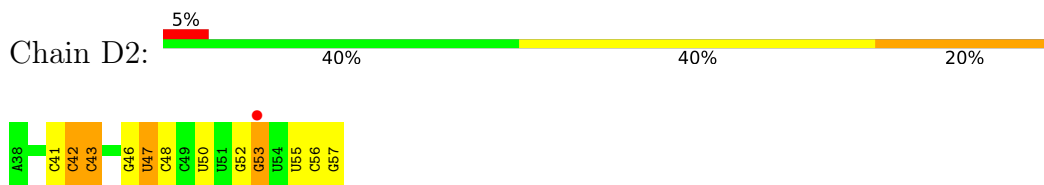
• Molecule 59: 5S rRNA (119-MER)



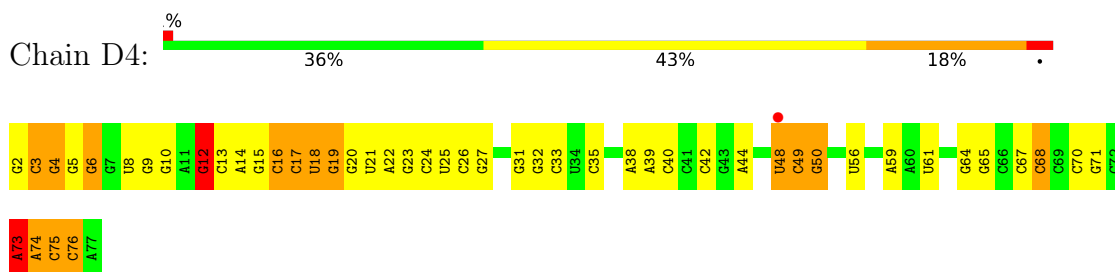
• Molecule 59: 5S rRNA (119-MER)



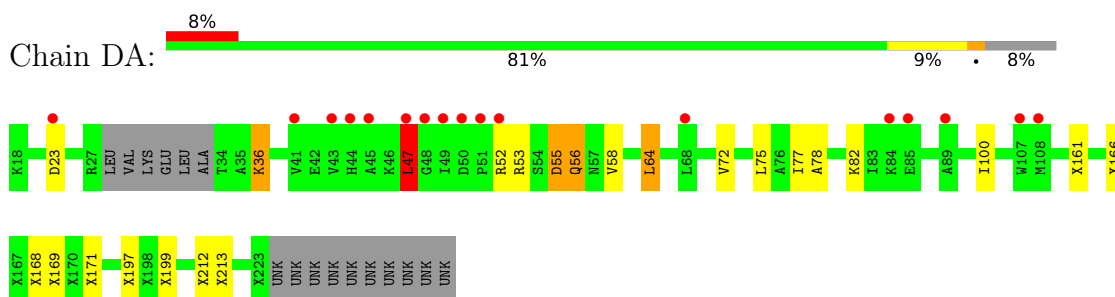
- Molecule 60: tRNA (5'-D(*AP*UP*CP*CP*CP*CP*GP*UP*GP*UP*CP*CP*UP*UP*GP*GP*UP*UP*CP*G)-3')



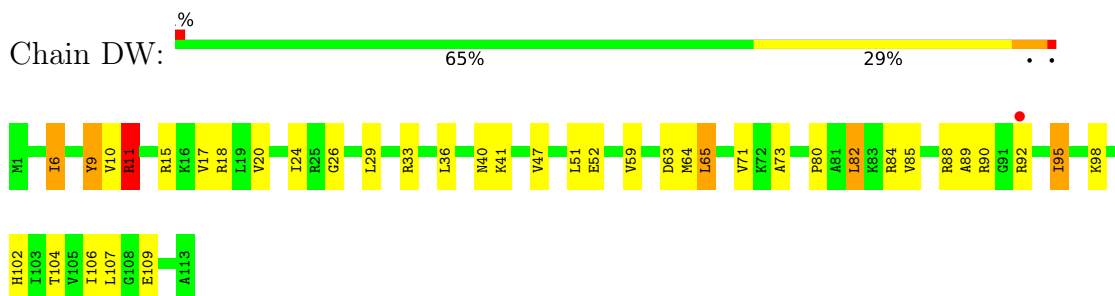
- Molecule 61: tRNA (76-MER)



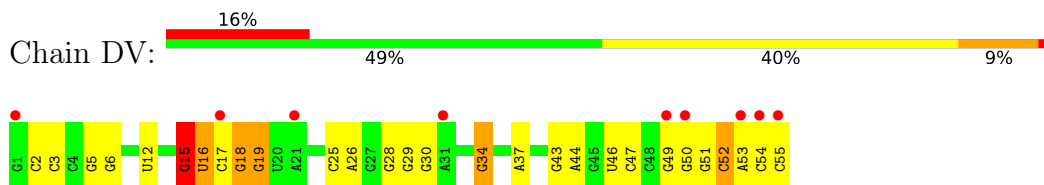
- Molecule 62: 50S ribosomal protein L1



- 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, α , β , γ	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) 98.5 (49.91-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.28	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 3.40Å)	Xtrriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.204 , 0.241 0.208 , 0.241	Depositor DCC
R_{free} test set	42005 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	74.2	Xtrriage
Anisotropy	0.256	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 68.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	295910	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtrriage'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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PAR, 3V6, 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	1.08	1/297 (0.3%)
2	AA	0.73	0/1936	0.99	7/2609 (0.3%)
2	BA	0.71	0/1936	0.92	0/2609
3	AC	0.89	0/1636	1.05	2/2205 (0.1%)
4	AD	0.90	4/1733 (0.2%)	1.12	13/2318 (0.6%)
4	BD	0.95	11/1733 (0.6%)	1.19	16/2318 (0.7%)
5	AE	0.80	0/1163	1.04	5/1564 (0.3%)
5	BE	0.73	0/1163	0.98	3/1564 (0.2%)
6	AF	0.73	0/856	0.97	2/1154 (0.2%)
6	BF	0.80	0/856	1.00	1/1154 (0.1%)
7	AG	0.71	0/1276	0.99	3/1709 (0.2%)
7	BG	0.78	0/1276	1.03	3/1709 (0.2%)
8	AH	0.74	0/1136	0.99	3/1527 (0.2%)
8	BH	0.72	0/1136	0.98	3/1527 (0.2%)
9	AI	0.80	0/1029	1.03	1/1378 (0.1%)
9	BI	0.78	0/1029	1.00	3/1378 (0.2%)
10	AJ	0.86	0/808	1.03	2/1085 (0.2%)
10	BJ	0.92	1/808 (0.1%)	1.00	0/1085
11	AK	0.83	0/900	1.12	5/1213 (0.4%)
11	BK	0.78	0/900	1.06	1/1213 (0.1%)
12	AL	0.90	0/987	1.17	7/1320 (0.5%)
12	BL	0.92	1/987 (0.1%)	1.13	4/1320 (0.3%)
13	AM	0.82	0/999	1.16	8/1336 (0.6%)
13	BM	0.87	0/999	1.13	5/1336 (0.4%)
14	AN	0.81	0/501	1.06	1/664 (0.2%)
14	BN	0.92	1/501 (0.2%)	1.10	1/664 (0.2%)
15	AO	0.71	0/745	0.90	0/992
15	BO	0.73	0/745	1.04	0/992
16	AP	0.79	0/717	1.01	3/963 (0.3%)
16	BP	0.79	0/717	1.01	1/963 (0.1%)
17	AR	0.75	0/837	1.03	0/1117
17	BR	0.67	0/837	0.94	0/1117

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
18	AS	0.74	0/579	0.92	1/768 (0.1%)
18	BS	0.76	0/579	1.01	0/768
19	AT	0.85	0/643	1.04	0/865
19	BT	0.81	0/643	1.01	0/865
20	AU	0.77	0/765	1.06	1/1007 (0.1%)
20	BU	0.71	0/765	1.06	3/1007 (0.3%)
21	AW	0.83	0/213	1.04	1/277 (0.4%)
21	BW	0.87	0/213	1.08	0/277
22	Ab	0.52	1/36190 (0.0%)	0.98	180/56486 (0.3%)
22	Bb	0.52	1/36190 (0.0%)	0.97	148/56486 (0.3%)
23	B2	0.44	0/216	1.03	1/334 (0.3%)
24	BC	0.79	0/1637	0.97	3/2205 (0.1%)
25	C2	0.44	0/1784	0.79	0/2780
25	C3	0.47	0/1809	0.92	4/2819 (0.1%)
25	D3	0.46	0/1809	0.88	2/2819 (0.1%)
26	C4	0.52	0/1832	1.05	15/2855 (0.5%)
27	CA	0.90	0/646	1.00	2/869 (0.2%)
28	CB	0.98	4/2155 (0.2%)	1.21	10/2905 (0.3%)
28	DB	1.09	4/2155 (0.2%)	1.32	16/2905 (0.6%)
29	CC	1.01	5/1597 (0.3%)	1.20	8/2153 (0.4%)
29	DC	1.03	3/1597 (0.2%)	1.24	9/2153 (0.4%)
30	CD	0.90	0/1659	1.19	8/2244 (0.4%)
30	DD	0.94	0/1659	1.25	9/2244 (0.4%)
31	CE	0.82	0/1499	1.08	7/2016 (0.3%)
31	DE	0.83	0/1499	1.03	3/2016 (0.1%)
32	CF	0.87	0/1246	1.12	8/1682 (0.5%)
32	DF	0.97	1/1246 (0.1%)	1.24	9/1682 (0.5%)
33	CI	0.88	0/1147	1.07	2/1551 (0.1%)
33	DI	0.87	2/1147 (0.2%)	1.04	2/1551 (0.1%)
35	CM	0.85	0/1132	1.09	5/1525 (0.3%)
35	DM	0.88	0/1132	1.12	4/1525 (0.3%)
36	CN	0.84	0/943	1.09	3/1269 (0.2%)
36	DN	0.90	0/943	1.15	3/1269 (0.2%)
37	CO	1.12	4/1131 (0.4%)	1.46	17/1504 (1.1%)
37	DO	1.22	8/1131 (0.7%)	1.52	16/1504 (1.1%)
38	CP	0.83	1/1143 (0.1%)	1.02	1/1527 (0.1%)
38	DP	0.89	0/1143	1.14	4/1527 (0.3%)
39	CQ	0.94	1/974 (0.1%)	1.18	2/1302 (0.2%)
39	DQ	1.07	2/974 (0.2%)	1.29	4/1302 (0.3%)
40	CR	0.92	0/779	1.10	3/1036 (0.3%)
40	DR	1.03	0/779	1.18	2/1036 (0.2%)
41	CS	0.94	0/1156	1.31	8/1542 (0.5%)
41	DS	1.03	1/1156 (0.1%)	1.40	15/1542 (1.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
42	CT	0.85	0/975	1.12	2/1297 (0.2%)
42	DT	1.00	0/975	1.23	4/1297 (0.3%)
43	CU	0.85	0/790	1.13	2/1057 (0.2%)
43	DU	0.91	1/790 (0.1%)	1.22	4/1057 (0.4%)
44	CW	0.96	1/907 (0.1%)	1.11	3/1216 (0.2%)
45	CX	0.88	0/740	1.12	1/993 (0.1%)
45	DX	0.90	0/740	1.21	3/993 (0.3%)
46	CY	1.14	0/789	1.38	10/1051 (1.0%)
46	DY	1.16	2/789 (0.3%)	1.44	12/1051 (1.1%)
47	CZ	0.74	1/1436 (0.1%)	1.02	3/1949 (0.2%)
47	DZ	0.77	0/1436	1.02	7/1949 (0.4%)
48	Ca	0.85	0/671	1.06	2/892 (0.2%)
48	Da	0.95	1/671 (0.1%)	1.18	3/892 (0.3%)
49	CH	0.91	0/741	1.22	2/984 (0.2%)
49	DH	0.85	0/741	1.10	3/984 (0.3%)
50	CK	0.74	0/600	1.03	1/793 (0.1%)
50	DK	0.79	0/600	1.10	1/793 (0.1%)
51	CL	0.74	0/473	1.08	0/634
51	DL	0.87	1/473 (0.2%)	1.10	0/634
52	C5	0.86	0/229	1.13	0/309
52	D5	0.90	0/229	1.17	3/309 (1.0%)
53	C6	0.99	1/473 (0.2%)	1.22	5/639 (0.8%)
53	D6	0.92	0/473	1.22	2/639 (0.3%)
54	C7	1.26	1/387 (0.3%)	1.26	2/515 (0.4%)
54	D7	1.10	0/387	1.22	4/515 (0.8%)
55	C8	0.96	0/427	1.20	0/561
55	D8	1.05	0/427	1.16	0/561
56	C9	1.02	1/516 (0.2%)	1.42	7/679 (1.0%)
56	D9	1.03	1/516 (0.2%)	1.30	3/679 (0.4%)
57	C0	0.86	0/302	0.88	0/397
57	D0	0.92	0/302	0.98	1/397 (0.3%)
58	C1	0.55	2/67709 (0.0%)	1.07	518/105690 (0.5%)
58	D1	0.58	6/67709 (0.0%)	1.11	628/105690 (0.6%)
59	Cs	0.50	0/2853	0.99	17/4451 (0.4%)
59	Ds	0.54	0/2853	1.04	20/4451 (0.4%)
60	D2	0.46	0/459	0.86	0/712
61	D4	0.52	0/1813	1.02	10/2825 (0.4%)
62	DA	0.90	0/645	1.00	1/867 (0.1%)
63	DW	0.94	0/907	1.11	1/1216 (0.1%)
64	DV	0.44	0/1269	0.80	1/1956 (0.1%)
All	All	0.66	75/318931 (0.0%)	1.07	1929/476973 (0.4%)

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
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 (75) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	DB	220	HIS	C-O	8.89	1.34	1.24
41	DS	79	HIS	CA-C	8.53	1.62	1.52
4	AD	12	CYS	CA-CB	8.31	1.67	1.53
29	DC	127	ASP	CA-C	7.92	1.63	1.52
37	DO	40	SER	N-CA	7.32	1.55	1.46
4	BD	12	CYS	CA-CB	7.22	1.65	1.53
12	BL	25	PRO	CA-C	7.21	1.59	1.52
29	DC	127	ASP	CG-OD2	7.12	1.38	1.25
37	DO	42	SER	CA-C	7.09	1.62	1.52
47	CZ	176	PRO	CA-C	6.97	1.58	1.52
39	DQ	5	LYS	CA-C	6.93	1.63	1.52
4	BD	26	CYS	CA-C	6.76	1.61	1.52
4	BD	9	CYS	N-CA	6.74	1.54	1.46
28	DB	237	GLU	CA-CB	6.71	1.61	1.52
58	C1	296	C	O3'-P	6.62	1.71	1.61
29	DC	127	ASP	CB-CG	6.60	1.68	1.52
39	DQ	87	TYR	CA-C	-6.58	1.48	1.52
4	BD	26	CYS	CA-CB	6.45	1.64	1.53
4	AD	26	CYS	CA-C	6.32	1.61	1.52
37	DO	39	LYS	CA-C	6.28	1.61	1.52
28	DB	43	ARG	N-CA	6.22	1.54	1.46
4	BD	12	CYS	CA-C	6.15	1.61	1.52
43	DU	79	VAL	CA-C	6.14	1.60	1.52
56	C9	50	LEU	N-CA	6.14	1.53	1.45
4	BD	13	ARG	N-CA	6.08	1.54	1.46
37	DO	23	PRO	CA-C	6.08	1.59	1.53
58	C1	589	A	P-OP1	6.08	1.61	1.49
4	AD	12	CYS	CA-C	6.07	1.60	1.52
14	BN	26	ARG	CA-C	6.00	1.58	1.53
44	CW	40	ASN	CA-C	5.96	1.59	1.53
58	D1	1346	A	O3'-P	5.95	1.70	1.61
33	DI	134	PRO	CA-C	5.95	1.59	1.52
10	BJ	59	SER	CA-C	5.92	1.60	1.52
46	DY	76	CYS	N-CA	5.86	1.52	1.46
37	DO	36	LYS	CA-C	5.83	1.60	1.52
29	CC	141	ILE	CA-C	5.80	1.58	1.52
33	DI	131	LYS	CA-C	5.79	1.57	1.52
37	CO	23	PRO	CA-C	5.79	1.60	1.52
4	BD	26	CYS	N-CA	5.78	1.53	1.46
58	D1	1429	A	O3'-P	-5.77	1.52	1.61
32	DF	167	GLU	C-N	5.69	1.40	1.33
28	DB	43	ARG	CA-C	5.56	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	BD	9	CYS	CA-CB	5.55	1.62	1.53
29	CC	127	ASP	CB-CG	5.53	1.65	1.52
58	D1	2027	C	P-OP1	5.49	1.59	1.49
46	DY	98	VAL	N-CA	5.49	1.53	1.46
37	DO	39	LYS	N-CA	5.46	1.53	1.46
29	CC	127	ASP	CA-CB	5.46	1.63	1.53
29	CC	127	ASP	CA-C	5.32	1.60	1.52
38	CP	133	ARG	CA-C	5.29	1.55	1.52
51	DL	29	ARG	CA-C	-5.28	1.48	1.52
4	BD	9	CYS	CA-C	5.27	1.59	1.52
4	AD	4	TYR	CA-C	5.27	1.59	1.52
53	C6	6	VAL	CA-C	5.26	1.58	1.52
58	D1	2254	U	P-OP1	5.25	1.59	1.49
29	CC	131	ALA	CA-C	-5.22	1.46	1.53
37	DO	27	HIS	CA-C	5.21	1.58	1.52
37	DO	38	GLN	CA-CB	5.20	1.62	1.53
28	CB	64	ILE	CA-CB	5.18	1.60	1.54
28	CB	24	ILE	CA-CB	5.16	1.61	1.54
4	BD	12	CYS	N-CA	5.16	1.52	1.46
28	CB	43	ARG	N-CA	5.11	1.53	1.46
58	D1	1858	G	P-OP1	5.09	1.59	1.49
48	Da	3	HIS	CA-C	5.08	1.58	1.52
37	CO	40	SER	N-CA	5.08	1.54	1.46
39	CQ	5	LYS	CA-C	5.07	1.59	1.52
4	BD	27	TYR	N-CA	5.06	1.52	1.45
28	CB	49	ILE	CA-CB	5.06	1.59	1.54
37	CO	39	LYS	N-CA	5.05	1.52	1.46
54	C7	13	CYS	N-CA	5.05	1.52	1.46
22	Ab	1482	G	O3'-P	5.03	1.68	1.61
56	D9	51	ALA	CA-C	5.02	1.59	1.52
58	D1	2603	G	P-OP1	5.02	1.58	1.49
22	Bb	349	A	O3'-P	5.01	1.68	1.61
37	CO	27	HIS	CA-C	5.00	1.58	1.52

All (1929) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	D1	2013	G	C2'-C3'-O3'	17.75	136.13	109.50
58	C1	1345	U	C2'-C3'-O3'	16.55	134.33	109.50
22	Bb	1476	U	C2'-C3'-O3'	16.34	134.01	109.50
58	C1	2013	G	C2'-C3'-O3'	15.74	133.11	109.50
58	D1	1740	C	C2'-C3'-O3'	15.50	136.95	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	C1	1529	G	C2'-C3'-O3'	15.31	136.67	113.70
58	D1	1699	G	C2'-C3'-O3'	15.26	132.38	109.50
58	C1	2236	A	C2'-C3'-O3'	14.60	131.40	109.50
58	C1	1829	G	C2'-C3'-O3'	14.59	131.39	109.50
58	D1	1955	C	C2'-C3'-O3'	14.54	135.51	113.70
37	DO	116	GLY	N-CA-C	14.15	124.69	111.67
58	D1	2236	A	C2'-C3'-O3'	13.73	130.09	109.50
58	C1	715	G	C2'-C3'-O3'	13.68	130.01	109.50
58	C1	715	G	C4'-C3'-O3'	13.54	129.72	109.40
58	C1	1955	C	C2'-C3'-O3'	13.35	133.73	113.70
58	D1	1698	A	C2'-C3'-O3'	13.17	133.46	113.70
22	Ab	1050	A	C2'-C3'-O3'	13.00	129.00	109.50
58	D1	715	G	C4'-C3'-O3'	12.67	128.40	109.40
22	Ab	1476	U	C2'-C3'-O3'	12.66	128.50	109.50
58	C1	1699	G	C2'-C3'-O3'	12.65	128.47	109.50
22	Bb	891	A	C2'-C3'-O3'	12.56	128.34	109.50
58	C1	1740	C	C2'-C3'-O3'	12.40	132.31	113.70
58	C1	1983	C	C2'-C3'-O3'	12.28	127.92	109.50
58	D1	1424	A	N9-C1'-C2'	12.27	130.40	112.00
22	Bb	109	G	C2'-C3'-O3'	11.84	127.26	109.50
32	CF	167	GLU	CA-C-N	11.75	134.52	119.84
32	CF	167	GLU	C-N-CA	11.75	134.52	119.84
58	D1	989	A	N9-C1'-C2'	11.55	129.32	112.00
58	D1	1067	G	C2'-C3'-O3'	11.44	126.66	109.50
58	D1	2808	U	N1-C1'-C2'	11.26	128.88	112.00
58	C1	2416	G	C2'-C3'-O3'	11.06	126.10	109.50
22	Bb	424	G	C2'-C3'-O3'	11.05	126.08	109.50
58	D1	497	A	C4'-C3'-O3'	11.04	129.56	113.00
22	Ab	891	A	C2'-C3'-O3'	10.93	125.90	109.50
58	C1	1850	U	C4'-C3'-O3'	10.90	125.75	109.40
58	D1	625	A	C2'-C3'-O3'	10.87	125.81	109.50
58	D1	1345	U	C2'-C3'-O3'	10.86	125.79	109.50
58	D1	552	A	C1'-C2'-O2'	10.85	128.08	111.80
22	Ab	1183	A	C2'-C3'-O3'	10.77	125.66	109.50
58	D1	1792	A	C2'-C3'-O3'	-10.71	97.63	113.70
58	C1	989	A	N9-C1'-C2'	10.61	127.91	112.00
58	D1	2054	A	C4'-C3'-O3'	10.60	125.30	109.40
58	C1	625	A	C2'-C3'-O3'	10.41	125.11	109.50
58	D1	72	A	C2'-C3'-O3'	10.26	124.89	109.50
58	C1	2293	G	C4'-C3'-O3'	10.26	124.79	109.40
58	D1	836	C	C2'-C3'-O3'	10.25	124.88	109.50
58	C1	2212	G	C2'-C3'-O3'	10.23	129.05	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	Ab	109	G	C2'-C3'-O3'	10.22	124.83	109.50
58	D1	1829	G	C2'-C3'-O3'	10.22	124.82	109.50
58	C1	497	A	C2'-C3'-O3'	10.20	129.00	113.70
58	C1	864	G	C2'-C3'-O3'	-10.20	98.41	113.70
22	Ab	1267	A	C2'-C3'-O3'	10.17	124.76	109.50
58	D1	2212	G	C4'-C3'-O3'	10.15	128.23	113.00
58	C1	354	A	C2'-C3'-O3'	10.09	124.64	109.50
58	D1	1604	A	C2'-C3'-O3'	10.09	124.63	109.50
58	C1	639	A	C4'-C3'-O3'	10.04	124.46	109.40
58	D1	1864	U	C2'-C3'-O3'	-10.04	98.65	113.70
58	D1	1849	A	C4'-C3'-O3'	10.03	124.45	109.40
58	D1	2212	G	C2'-C3'-O3'	10.00	128.70	113.70
58	D1	1345	U	C5'-C4'-C3'	9.98	130.17	115.20
22	Bb	408	A	N9-C1'-C2'	9.95	126.92	112.00
58	D1	639	A	C4'-C3'-O3'	9.94	124.31	109.40
58	C1	1792	A	C2'-C3'-O3'	-9.90	98.86	113.70
58	D1	1529	G	C2'-C3'-O3'	9.85	128.47	113.70
58	C1	499	G	C4'-C3'-O3'	9.84	124.15	109.40
58	D1	497	A	C2'-C3'-O3'	9.83	128.44	113.70
58	D1	1352	A	C1'-C2'-O2'	9.80	123.10	108.40
22	Bb	1267	A	C2'-C3'-O3'	9.79	124.18	109.50
58	C1	1654	A	C3'-C2'-O2'	-9.79	99.92	114.60
58	C1	1067	G	C2'-C3'-O3'	9.71	124.07	109.50
58	D1	1983	C	N1-C1'-C2'	9.66	128.49	114.00
58	C1	798	A	C2'-C3'-O3'	9.62	123.94	109.50
58	D1	2591	U	C4'-C3'-O3'	-9.60	98.61	113.00
31	CE	86	MET	CA-C-N	-9.57	107.88	119.84
31	CE	86	MET	C-N-CA	-9.57	107.88	119.84
22	Ab	61	A	C2'-C3'-O3'	9.55	123.83	109.50
58	C1	2297	A	N9-C1'-C2'	9.53	126.29	112.00
58	C1	413	U	C2'-C3'-O3'	9.52	123.78	109.50
58	D1	1590	A	N9-C1'-C2'	9.51	126.27	112.00
58	D1	1983	C	C2'-C3'-O3'	9.51	123.76	109.50
58	D1	1424	A	C4'-C3'-O3'	-9.49	98.76	113.00
39	DQ	38	VAL	CB-CA-C	-9.48	104.69	113.70
59	Cs	66	A	C2'-C3'-O3'	9.42	123.63	109.50
58	C1	2673	A	N9-C1'-C2'	9.36	126.04	112.00
58	C1	1604	A	C2'-C3'-O3'	9.36	123.53	109.50
58	D1	499	G	C4'-C3'-O3'	9.31	123.36	109.40
58	C1	506	G	C2'-C3'-O3'	9.29	123.43	109.50
22	Bb	324	C	C2'-C3'-O3'	9.26	123.38	109.50
58	C1	1983	C	N1-C1'-C2'	9.22	127.84	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	C1	2212	G	C4'-C3'-O3'	9.20	126.79	113.00
22	Ab	408	A	N9-C1'-C2'	9.17	125.76	112.00
32	CF	167	GLU	N-CA-C	9.17	118.89	108.25
13	AM	70	LEU	N-CA-C	-9.05	99.99	112.12
22	Bb	469	G	C2'-C3'-O3'	9.00	123.00	109.50
58	D1	1820	C	C2'-C3'-O3'	-8.96	100.25	113.70
22	Ab	671	A	C2'-C3'-O3'	8.94	122.90	109.50
58	C1	98	G	N9-C1'-C2'	8.89	127.34	114.00
58	D1	98	G	N9-C1'-C2'	8.87	125.30	112.00
22	Ab	78	G	C2'-C3'-O3'	8.86	122.79	109.50
58	C1	1424	A	N9-C1'-C2'	8.86	125.29	112.00
58	C1	817	G	C3'-C2'-O2'	8.86	123.99	110.70
37	CO	142	GLY	N-CA-C	8.86	122.54	110.58
58	C1	274	C	C4'-C3'-O3'	8.84	122.66	109.40
58	D1	2297	A	N9-C1'-C2'	8.83	125.25	112.00
25	C3	47	U	N1-C1'-C2'	8.82	125.23	112.00
58	D1	2464	A	C1'-C2'-O2'	8.81	121.61	108.40
28	DB	43	ARG	N-CA-C	8.78	124.05	113.16
28	DB	244	ARG	CA-C-N	8.78	129.42	120.38
28	DB	244	ARG	C-N-CA	8.78	129.42	120.38
58	D1	1520	C	C1'-C2'-O2'	8.74	121.51	108.40
41	DS	30	VAL	N-CA-C	8.70	127.43	109.34
37	DO	15	ARG	N-CA-C	8.66	122.54	108.34
22	Ab	559	G	C4'-C3'-O3'	8.65	122.37	109.40
58	D1	1345	U	C1'-C2'-O2'	-8.64	98.84	111.80
58	D1	413	U	C4'-C3'-O3'	8.63	122.34	109.40
22	Ab	262	G	C3'-C2'-O2'	8.62	123.64	110.70
58	C1	2054	A	C4'-C3'-O3'	8.59	122.28	109.40
58	D1	2530	U	C1'-C2'-O2'	-8.58	98.93	111.80
28	DB	229	VAL	CB-CA-C	-8.57	99.54	112.05
58	D1	354	A	C2'-C3'-O3'	8.55	122.33	109.50
22	Bb	1050	A	C2'-C3'-O3'	8.54	122.31	109.50
58	D1	1488	G	C2'-C3'-O3'	8.52	126.49	113.70
58	D1	1424	A	C2'-C3'-O3'	8.52	126.48	113.70
22	Ab	113	A	C2'-C3'-O3'	8.51	122.27	109.50
22	Ab	1215	G	C3'-C2'-O2'	8.51	123.47	110.70
58	C1	1849	A	C2'-C3'-O3'	8.50	122.25	109.50
58	C1	1345	U	N1-C1'-C2'	8.47	126.71	114.00
37	CO	59	LEU	N-CA-C	-8.45	101.42	112.41
32	DF	167	GLU	CA-C-N	8.40	128.34	120.03
32	DF	167	GLU	C-N-CA	8.40	128.34	120.03
58	D1	1345	U	C5'-C4'-O4'	8.39	121.68	109.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	CY	76	CYS	CA-C-N	8.38	130.31	119.84
46	CY	76	CYS	C-N-CA	8.38	130.31	119.84
58	C1	1654	A	C4'-C3'-O3'	8.36	121.95	109.40
58	D1	47	A	C2'-C3'-O3'	8.36	122.04	109.50
58	D1	2608	G	C2'-C3'-O3'	-8.35	101.18	113.70
29	CC	203	LYS	N-CA-C	8.32	123.37	112.72
58	C1	108	A	C3'-C2'-O2'	8.32	123.17	110.70
58	C1	836	C	C4'-C3'-O3'	8.30	121.86	109.40
58	C1	1590	A	N9-C1'-C2'	8.30	124.44	112.00
22	Ab	1048	U	C2'-C3'-O3'	8.29	121.94	109.50
58	D1	495	A	C2'-C3'-O3'	-8.29	101.26	113.70
22	Bb	1215	G	C3'-C2'-O2'	8.27	123.10	110.70
58	C1	980	C	C3'-C2'-O2'	8.26	123.08	110.70
58	D1	69	A	C4'-C3'-O3'	8.25	121.78	109.40
58	D1	1814	A	C2'-C3'-O3'	-8.24	97.14	109.50
22	Bb	495	C	C2'-C3'-O3'	8.23	121.84	109.50
58	D1	2742	C	C1'-C2'-O2'	8.20	120.69	108.40
58	D1	899	G	C3'-C2'-O2'	8.19	122.99	110.70
58	D1	1423	A	C4'-C3'-O3'	8.19	121.68	109.40
41	DS	29	ARG	N-CA-C	8.16	120.78	108.46
58	C1	1472	A	C2'-C3'-O3'	8.13	121.70	109.50
58	D1	2700	U	C2'-C3'-O3'	8.13	121.70	109.50
22	Bb	1381	A	C1'-C2'-O2'	8.13	120.59	108.40
22	Bb	1183	A	C2'-C3'-O3'	8.12	121.68	109.50
58	D1	817	G	C3'-C2'-O2'	8.12	122.87	110.70
58	D1	851	G	C4'-C3'-O3'	8.10	121.55	109.40
58	D1	2724	A	C2'-C3'-O3'	-8.10	101.55	113.70
22	Bb	239	A	C2'-C3'-O3'	8.07	121.61	109.50
22	Bb	753	G	C1'-C2'-O2'	-8.07	96.29	108.40
22	Bb	1048	U	C2'-C3'-O3'	8.07	121.61	109.50
4	BD	38	TYR	CA-C-N	8.07	125.55	119.66
4	BD	38	TYR	C-N-CA	8.07	125.55	119.66
22	Bb	559	G	C4'-C3'-O3'	8.05	121.47	109.40
58	D1	2007	A	C1'-C2'-O2'	8.05	120.47	108.40
22	Ab	732	C	C2'-C3'-O3'	8.04	121.55	109.50
47	CZ	176	PRO	N-CA-C	8.03	120.49	110.70
46	DY	76	CYS	CA-C-N	8.03	129.87	119.84
46	DY	76	CYS	C-N-CA	8.03	129.87	119.84
58	C1	435	C	C3'-C2'-O2'	8.00	122.70	110.70
58	D1	2670	G	C2'-C3'-O3'	8.00	125.69	113.70
58	D1	1987	A	C2'-C3'-O3'	7.99	121.48	109.50
37	DO	59	LEU	N-CA-C	-7.97	103.63	112.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	D1	2293	G	C4'-C3'-O3'	7.96	121.34	109.40
22	Ab	424	G	C2'-C3'-O3'	7.95	121.43	109.50
58	D1	2071	C	C4'-C3'-O3'	-7.93	101.10	113.00
22	Bb	671	A	C2'-C3'-O3'	7.91	121.36	109.50
58	D1	1295	G	C3'-C2'-O2'	-7.89	102.77	114.60
58	D1	2553	A	C3'-C2'-O2'	7.86	126.40	114.60
58	C1	1298	A	C2'-C3'-O3'	7.86	121.28	109.50
58	C1	1988	C	C3'-C2'-O2'	7.85	122.47	110.70
58	D1	2666	G	C2'-C3'-O3'	7.84	121.26	109.50
22	Bb	246	A	C2'-C3'-O3'	7.84	121.26	109.50
22	Bb	517	A	C2'-C3'-O3'	7.84	121.25	109.50
58	D1	2283	U	C3'-C2'-O2'	7.83	122.44	110.70
58	D1	1451	U	C4'-C3'-O3'	-7.82	101.28	113.00
22	Ab	846	C	C1'-C2'-O2'	7.81	120.11	108.40
58	C1	566	C	C2'-C3'-O3'	7.80	125.40	113.70
58	D1	286	G	C2'-C3'-O3'	7.80	121.20	109.50
22	Ab	880	G	C3'-C2'-O2'	7.80	122.40	110.70
22	Bb	31	U	C2'-C3'-O3'	7.80	121.19	109.50
22	Bb	716	C	C2'-C3'-O3'	-7.79	102.02	113.70
46	DY	65	ALA	CA-C-N	7.78	129.57	119.84
46	DY	65	ALA	C-N-CA	7.78	129.57	119.84
58	D1	2635	G	C3'-C2'-O2'	7.77	122.36	110.70
58	C1	47	A	C2'-C3'-O3'	7.77	121.15	109.50
58	C1	517	G	C4'-C3'-O3'	-7.76	101.35	113.00
58	D1	1741	G	C2'-C3'-O3'	-7.76	102.06	113.70
37	CO	46	LYS	N-CA-C	7.75	120.41	111.11
58	D1	1450	U	C3'-C2'-O2'	7.74	122.31	110.70
13	AM	118	ALA	N-CA-C	7.73	120.61	108.79
22	Ab	707	U	C2'-C3'-O3'	-7.72	102.12	113.70
58	C1	2700	U	C4'-C3'-O3'	7.71	120.96	109.40
58	D1	1850	U	C4'-C3'-O3'	7.70	120.95	109.40
58	C1	1698	A	C4'-C3'-O3'	7.70	124.55	113.00
58	C1	1740	C	C4'-C3'-O3'	7.68	124.53	113.00
20	BU	96	GLY	N-CA-C	7.68	121.94	112.64
58	C1	88	U	C3'-C2'-O2'	7.68	122.22	110.70
22	Bb	262	G	C2'-C3'-O3'	7.67	125.20	113.70
46	CY	55	TYR	CA-C-N	7.67	129.42	119.84
46	CY	55	TYR	C-N-CA	7.67	129.42	119.84
4	BD	9	CYS	CA-CB-SG	7.66	132.02	114.40
58	D1	2437	A	C3'-C2'-O2'	-7.65	103.12	114.60
32	DF	19	VAL	N-CA-C	7.65	118.75	108.27
58	D1	1920	G	C3'-C2'-O2'	7.64	122.16	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	D1	653	G	C1'-C2'-O2'	7.63	119.84	108.40
58	D1	1377	G	C2'-C3'-O3'	7.62	120.94	109.50
59	Ds	56	G	C2'-C3'-O3'	7.62	120.94	109.50
58	C1	533	C	C2'-C3'-O3'	-7.61	102.29	113.70
58	D1	609	C	C2'-C3'-O3'	7.59	120.88	109.50
58	D1	787	G	C1'-C2'-O2'	7.59	119.78	108.40
58	D1	33	C	C2'-C3'-O3'	-7.58	102.33	113.70
41	CS	23	ARG	CA-C-N	7.57	129.30	119.84
41	CS	23	ARG	C-N-CA	7.57	129.30	119.84
37	DO	46	LYS	N-CA-C	7.56	120.59	111.82
58	C1	1345	U	C4'-C3'-O3'	7.56	120.74	109.40
58	C1	1538	C	C2'-C3'-O3'	7.55	120.82	109.50
58	C1	710	C	C3'-C2'-O2'	7.54	122.01	110.70
58	D1	1871	U	C3'-C2'-O2'	7.53	122.00	110.70
22	Ab	91	G	C4'-C3'-O3'	7.53	120.70	109.40
58	C1	2558	U	C1'-C2'-O2'	7.53	119.69	108.40
22	Bb	753	G	C3'-C2'-O2'	7.53	121.99	110.70
58	C1	988	G	C4'-C3'-O3'	-7.53	101.71	113.00
58	D1	2084	C	C4'-C3'-O3'	-7.53	101.71	113.00
58	D1	2082	G	C2'-C3'-O3'	7.51	120.77	109.50
58	D1	2673	A	N9-C1'-C2'	7.51	123.26	112.00
58	C1	1955	C	C4'-C3'-O3'	7.50	124.24	113.00
58	C1	820	A	C2'-C3'-O3'	-7.48	98.28	109.50
13	BM	70	LEU	N-CA-C	-7.48	102.10	112.12
58	C1	125	C	C4'-C3'-O3'	7.48	124.21	113.00
22	Ab	816	C	C4'-C3'-O3'	7.47	120.60	109.40
22	Ab	517	A	C4'-C3'-O3'	7.47	120.60	109.40
58	C1	2319	G	C4'-C3'-O3'	7.46	124.19	113.00
58	C1	2489	A	C3'-C2'-O2'	7.46	121.89	110.70
58	D1	1472	A	C2'-C3'-O3'	7.45	120.68	109.50
58	D1	1869	G	C2'-C3'-O3'	-7.44	102.54	113.70
58	C1	1291	A	C1'-C2'-O2'	7.44	119.56	108.40
58	C1	1346	A	C4'-C3'-O3'	7.43	120.55	109.40
58	D1	435	C	C3'-C2'-O2'	7.43	121.85	110.70
22	Ab	1032	U	C4'-C3'-O3'	7.43	120.54	109.40
58	D1	2771	G	C1'-C2'-O2'	7.43	119.54	108.40
22	Ab	324	C	C2'-C3'-O3'	7.42	120.63	109.50
58	C1	1423	A	C4'-C3'-O3'	7.42	120.53	109.40
58	D1	841	C	C4'-C3'-O3'	-7.41	101.88	113.00
58	D1	1451	U	C1'-C2'-O2'	7.41	119.51	108.40
58	D1	288	G	C3'-C2'-O2'	7.41	121.81	110.70
28	DB	118	VAL	N-CA-C	7.41	116.73	107.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	D1	603	C	C1'-C2'-O2'	7.40	119.50	108.40
2	AA	95	GLN	N-CA-C	7.39	114.84	108.78
22	Ab	970	U	C2'-C3'-O3'	7.39	120.58	109.50
58	D1	1367	A	C1'-C2'-O2'	7.38	119.47	108.40
22	Ab	224	A	C3'-C2'-O2'	7.38	121.77	110.70
58	D1	2083	A	C2'-C3'-O3'	-7.38	102.63	113.70
2	AA	23	ARG	N-CA-C	-7.38	102.82	112.41
13	AM	112	GLY	CA-C-N	7.38	129.06	119.84
13	AM	112	GLY	C-N-CA	7.38	129.06	119.84
14	BN	40	CYS	CA-CB-SG	7.37	131.34	114.40
58	C1	1339	U	C1'-C2'-O2'	7.37	119.45	108.40
58	C1	1345	U	C1'-C2'-O2'	-7.35	100.77	111.80
58	D1	1616	A	C3'-C2'-O2'	7.33	121.69	110.70
29	DC	128	SER	N-CA-C	7.33	117.68	108.45
58	D1	1933	A	C2'-C3'-O3'	-7.31	102.73	113.70
58	D1	1855	A	C3'-C2'-O2'	7.31	121.66	110.70
58	C1	259	A	C2'-C3'-O3'	7.31	124.66	113.70
41	DS	29	ARG	CA-C-N	7.30	135.12	121.97
41	DS	29	ARG	C-N-CA	7.30	135.12	121.97
58	C1	1345	U	C5'-C4'-C3'	7.30	126.15	115.20
58	C1	1073	A	C3'-C2'-O2'	7.29	121.63	110.70
30	DD	59	TYR	N-CA-C	7.28	119.97	110.43
22	Bb	923	G	C2'-C3'-O3'	-7.28	102.78	113.70
58	C1	2329	G	C2'-C3'-O3'	7.27	124.61	113.70
58	C1	715	G	N9-C1'-C2'	7.26	124.90	114.00
46	DY	55	TYR	CA-C-N	7.26	128.92	119.84
46	DY	55	TYR	C-N-CA	7.26	128.92	119.84
47	DZ	176	PRO	CA-C-N	7.26	128.92	119.84
47	DZ	176	PRO	C-N-CA	7.26	128.92	119.84
59	Ds	66	A	C2'-C3'-O3'	7.26	124.60	113.70
58	D1	2669	C	C4'-C3'-O3'	-7.26	102.11	113.00
58	C1	2656	G	C2'-C3'-O3'	7.26	120.39	109.50
58	C1	1301	G	C2'-C3'-O3'	-7.26	102.82	113.70
58	C1	2061	C	C3'-C2'-O2'	7.26	121.58	110.70
58	D1	138	A	C2'-C3'-O3'	7.26	124.58	113.70
58	D1	2329	G	C2'-C3'-O3'	7.25	124.58	113.70
22	Bb	493	A	C3'-C2'-O2'	7.25	121.58	110.70
37	CO	41	ARG	N-CA-C	-7.24	94.61	107.28
41	DS	57	PHE	N-CA-C	-7.24	101.22	110.19
58	C1	2318	G	C3'-C2'-O2'	7.24	121.55	110.70
59	Cs	116	G	C3'-C2'-O2'	7.23	121.55	110.70
58	C1	2601	A	C3'-C2'-O2'	7.23	121.54	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	D1	1658	G	C1'-C2'-O2'	7.22	119.22	108.40
46	CY	6	HIS	N-CA-C	7.21	119.82	108.79
58	C1	276	G	C2'-C3'-O3'	-7.21	102.89	113.70
58	C1	439	C	C4'-C3'-O3'	-7.20	102.20	113.00
58	C1	267	G	C4'-C3'-O3'	7.20	123.80	113.00
58	C1	789	G	C1'-C2'-O2'	7.19	119.19	108.40
58	C1	83	G	C3'-C2'-O2'	7.19	121.48	110.70
22	Bb	923	G	C1'-C2'-O2'	7.18	119.17	108.40
58	D1	2561	G	C2'-C3'-O3'	-7.18	102.93	113.70
58	C1	545	G	C1'-C2'-O2'	7.15	119.13	108.40
58	C1	2450	A	C2'-C3'-O3'	-7.13	98.80	109.50
58	C1	959	C	C1'-C2'-O2'	7.13	119.10	108.40
22	Ab	517	A	C2'-C3'-O3'	7.13	120.20	109.50
28	DB	233	HIS	N-CA-C	7.13	120.09	111.82
58	D1	1310	A	C1'-C2'-O2'	7.13	122.49	111.80
22	Bb	1259	C	C4'-C3'-O3'	7.12	123.68	113.00
58	C1	2085	C	C4'-C3'-O3'	-7.12	102.32	113.00
58	C1	666	G	C1'-C2'-O2'	7.11	119.07	108.40
58	D1	2553	A	C1'-C2'-O2'	-7.11	101.14	111.80
58	D1	1244	C	C1'-C2'-O2'	7.10	119.05	108.40
58	C1	445	C	C3'-C2'-O2'	7.09	121.34	110.70
58	D1	1698	A	C4'-C3'-O3'	7.09	123.64	113.00
58	C1	1849	A	C4'-C3'-O3'	7.08	120.02	109.40
58	D1	1424	A	C3'-C2'-O2'	7.08	121.31	110.70
58	D1	2444	A	C3'-C2'-O2'	7.07	121.31	110.70
58	D1	1393	G	C3'-C2'-O2'	7.07	121.30	110.70
58	D1	1783	G	C1'-C2'-O2'	7.07	119.00	108.40
58	D1	1315	C	C2'-C3'-O3'	-7.06	103.10	113.70
58	D1	517	G	C1'-C2'-O2'	7.06	118.99	108.40
58	C1	2623	C	C2'-C3'-O3'	-7.06	103.11	113.70
25	D3	47	U	N1-C1'-C2'	7.06	122.59	112.00
22	Bb	414	C	C3'-C2'-O2'	7.05	121.28	110.70
58	D1	2555	G	C3'-C2'-O2'	7.05	121.28	110.70
4	BD	8	VAL	CA-C-O	-7.04	114.72	120.70
10	AJ	60	ARG	N-CA-C	7.04	117.78	108.07
22	Ab	432	C	C4'-C3'-O3'	7.04	119.95	109.40
58	C1	609	C	C2'-C3'-O3'	7.03	120.04	109.50
58	D1	2612	C	C1'-C2'-O2'	7.02	118.94	108.40
58	D1	2637	C	C3'-C2'-O2'	7.02	121.23	110.70
33	DI	135	GLU	N-CA-C	7.02	120.46	110.14
58	D1	2289	A	C1'-C2'-O2'	7.02	118.93	108.40
58	D1	1984	U	O4'-C1'-C2'	-7.02	98.78	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	BD	26	CYS	CA-CB-SG	7.01	130.53	114.40
58	D1	355	A	C2'-C3'-O3'	7.01	120.02	109.50
58	D1	2782	G	C1'-C2'-O2'	7.01	118.92	108.40
58	D1	1373	G	C2'-C3'-O3'	7.00	124.21	113.70
58	C1	2220	A	C2'-C3'-O3'	7.00	124.20	113.70
22	Ab	1224	C	C3'-C2'-O2'	7.00	121.19	110.70
58	D1	533	C	C2'-C3'-O3'	-6.98	103.22	113.70
58	C1	2076	C	C3'-C2'-O2'	6.98	121.17	110.70
58	D1	715	G	N9-C1'-C2'	6.98	124.47	114.00
58	D1	504	A	C4'-C3'-O3'	6.97	119.86	109.40
12	AL	119	LYS	N-CA-C	-6.97	101.33	110.53
58	D1	2193	U	C2'-C3'-O3'	6.97	119.96	109.50
48	Da	6	GLY	N-CA-C	6.97	119.95	111.93
4	BD	12	CYS	CA-CB-SG	6.97	130.43	114.40
58	D1	169	A	C3'-C2'-O2'	6.96	121.15	110.70
58	D1	2620	U	C2'-C3'-O3'	-6.96	99.06	109.50
58	C1	1982	C	C3'-C2'-O2'	6.95	121.13	110.70
58	D1	110	G	C4'-C3'-O3'	-6.95	102.57	113.00
58	C1	1987	A	C2'-C3'-O3'	6.95	119.92	109.50
61	D4	38	A	C1'-C2'-O2'	6.94	118.81	108.40
22	Bb	1496	A	C1'-C2'-O2'	6.93	118.80	108.40
58	C1	2083	A	C1'-C2'-O2'	-6.93	101.40	111.80
29	CC	128	SER	N-CA-C	6.93	117.64	108.07
58	C1	27	A	C1'-C2'-O2'	6.93	118.80	108.40
22	Bb	900	G	C3'-C2'-O2'	6.93	121.09	110.70
58	C1	1798	U	C3'-C2'-O2'	6.92	121.09	110.70
58	D1	1171	A	C1'-C2'-O2'	-6.91	101.43	111.80
58	D1	2546	G	C1'-C2'-O2'	6.91	118.77	108.40
58	C1	1698	A	C2'-C3'-O3'	6.91	124.06	113.70
22	Ab	776	A	C2'-C3'-O3'	-6.90	99.15	109.50
58	C1	1665	G	C2'-C3'-O3'	-6.90	103.36	113.70
58	D1	2475	C	C4'-C3'-O3'	6.89	123.34	113.00
22	Bb	838	A	C3'-C2'-O2'	6.88	121.03	110.70
22	Bb	1437	C	C3'-C2'-O2'	6.88	121.02	110.70
58	D1	710	C	C3'-C2'-O2'	6.88	121.02	110.70
59	Ds	66	A	C4'-C3'-O3'	-6.88	102.68	113.00
58	D1	1549	C	C4'-C3'-O3'	6.88	123.31	113.00
58	C1	1411	A	C1'-C2'-O2'	6.87	118.71	108.40
58	C1	614	G	C1'-C2'-O2'	6.87	118.71	108.40
58	D1	2433	A	C4'-C3'-O3'	6.87	123.31	113.00
58	D1	1923	C	C3'-C2'-O2'	6.87	121.00	110.70
58	C1	821	G	C4'-C3'-O3'	6.87	119.70	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	D1	2505	G	C1'-C2'-O2'	6.86	118.69	108.40
58	D1	2215	G	C4'-C3'-O3'	-6.86	102.72	113.00
58	C1	1685	U	C3'-C2'-O2'	6.85	120.97	110.70
42	DT	74	LEU	N-CA-C	6.85	119.37	110.53
58	D1	589	A	C4'-C3'-O3'	-6.84	102.73	113.00
58	D1	2250	G	C2'-C3'-O3'	-6.84	103.43	113.70
58	D1	1846	G	C2'-C3'-O3'	-6.84	103.44	113.70
58	D1	413	U	C2'-C3'-O3'	6.82	119.73	109.50
58	C1	24	U	C3'-C2'-O2'	6.82	120.92	110.70
58	C1	2829	A	C4'-C3'-O3'	-6.82	99.17	109.40
58	C1	746	G	C1'-C2'-O2'	6.81	118.62	108.40
58	D1	498	G	C3'-C2'-O2'	6.81	120.92	110.70
58	C1	240	G	C3'-C2'-O2'	6.81	120.91	110.70
5	AE	67	VAL	N-CA-C	6.80	117.27	107.88
58	C1	2220	A	C4'-C3'-O3'	-6.80	102.81	113.00
58	C1	1254	A	C2'-C3'-O3'	6.79	119.68	109.50
58	C1	2742	C	C1'-C2'-O2'	6.79	118.58	108.40
58	C1	2872	C	C4'-C3'-O3'	-6.79	102.82	113.00
58	C1	2071	C	C4'-C3'-O3'	-6.78	102.83	113.00
58	C1	2855	G	C1'-C2'-O2'	6.78	118.57	108.40
22	Bb	493	A	C2'-C3'-O3'	6.78	123.86	113.70
58	C1	820	A	C4'-C3'-O3'	6.77	119.56	109.40
48	Ca	12	ASN	N-CA-C	6.77	125.23	110.80
58	D1	27	A	C4'-C3'-O3'	-6.77	102.84	113.00
58	D1	2613	A	N9-C1'-C2'	6.77	124.16	114.00
58	C1	839	A	C2'-C3'-O3'	6.77	119.65	109.50
61	D4	76	C	P-O5'-C5'	-6.77	110.75	120.90
58	D1	585	G	C2'-C3'-O3'	-6.76	103.55	113.70
58	D1	791	G	C1'-C2'-O2'	6.76	118.54	108.40
58	C1	851	G	C4'-C3'-O3'	6.75	119.53	109.40
22	Ab	898	U	C1'-C2'-O2'	6.75	118.53	108.40
58	D1	1999	A	C1'-C2'-O2'	6.75	118.53	108.40
22	Ab	239	A	C2'-C3'-O3'	6.75	119.63	109.50
58	C1	1999	A	C1'-C2'-O2'	6.75	118.53	108.40
58	D1	84	C	C3'-C2'-O2'	6.75	120.82	110.70
22	Ab	262	G	C2'-C3'-O3'	6.75	123.82	113.70
11	AK	38	ASN	CA-C-N	6.74	127.14	119.93
11	AK	38	ASN	C-N-CA	6.74	127.14	119.93
58	D1	2048	G	C1'-C2'-O2'	6.73	118.50	108.40
58	C1	536	G	C2'-C3'-O3'	6.72	119.59	109.50
22	Bb	732	C	C2'-C3'-O3'	6.72	119.58	109.50
58	C1	2433	A	C4'-C3'-O3'	6.72	123.08	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	D1	2262	G	C3'-C2'-O2'	6.71	120.77	110.70
58	C1	2753	A	C3'-C2'-O2'	6.71	120.77	110.70
58	D1	2693	U	C2'-C3'-O3'	-6.71	103.64	113.70
59	Cs	75	G	C1'-C2'-O2'	6.70	118.45	108.40
58	D1	647	G	C4'-C3'-O3'	-6.70	102.94	113.00
22	Ab	787	G	C1'-C2'-O2'	6.70	118.45	108.40
22	Bb	517	A	C4'-C3'-O3'	6.70	119.45	109.40
58	C1	1923	C	C2'-C3'-O3'	-6.69	103.66	113.70
58	D1	1392	G	C1'-C2'-O2'	6.69	118.43	108.40
58	D1	2683	G	C4'-C3'-O3'	-6.69	102.97	113.00
29	DC	132	HIS	CA-C-N	-6.68	113.21	123.17
29	DC	132	HIS	C-N-CA	-6.68	113.21	123.17
58	D1	138	A	C3'-C2'-O2'	6.68	120.73	110.70
58	D1	1654	A	C2'-C3'-O3'	-6.68	99.47	109.50
58	C1	1295	G	C3'-C2'-O2'	-6.68	104.58	114.60
58	D1	1810	A	C2'-C3'-O3'	6.68	119.52	109.50
30	DD	52	LYS	N-CA-C	6.68	119.81	107.99
58	C1	236	G	C1'-C2'-O2'	6.67	118.41	108.40
58	D1	1188	A	C2'-C3'-O3'	6.67	119.50	109.50
22	Ab	1275	G	C4'-C3'-O3'	6.67	119.40	109.40
46	DY	8	LYS	N-CA-C	6.67	119.29	109.69
30	CD	65	TRP	CA-C-N	6.66	128.17	119.84
30	CD	65	TRP	C-N-CA	6.66	128.17	119.84
22	Bb	61	A	C2'-C3'-O3'	6.66	119.49	109.50
58	D1	1647	U	C1'-C2'-O2'	6.66	121.79	111.80
58	D1	1651	G	C2'-C3'-O3'	-6.66	103.71	113.70
4	AD	38	TYR	CA-C-N	6.65	124.52	119.66
4	AD	38	TYR	C-N-CA	6.65	124.52	119.66
58	D1	2034	A	C1'-C2'-O2'	-6.65	98.43	108.40
30	DD	154	VAL	N-CA-C	6.64	117.69	108.12
12	AL	26	ALA	N-CA-C	-6.64	105.25	113.15
43	DU	28	GLU	CA-C-N	6.63	128.13	119.84
43	DU	28	GLU	C-N-CA	6.63	128.13	119.84
58	D1	1294	U	C2'-C3'-O3'	-6.62	103.76	113.70
58	D1	2438	C	C2'-C3'-O3'	-6.62	103.76	113.70
21	AW	13	ILE	CB-CA-C	-6.62	103.40	111.88
22	Ab	144	A	C4'-C3'-O3'	6.62	119.33	109.40
58	C1	1988	C	C4'-C3'-O3'	-6.62	103.07	113.00
58	C1	2085	C	C3'-C2'-O2'	6.62	120.63	110.70
22	Ab	889	U	C3'-C2'-O2'	6.62	120.63	110.70
32	DF	140	LYS	N-CA-C	6.62	118.15	111.07
58	C1	1716	C	C3'-C2'-O2'	6.61	120.62	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	C1	585	G	C2'-C3'-O3'	-6.61	103.78	113.70
58	C1	2553	A	C3'-C2'-O2'	6.60	124.50	114.60
22	Bb	649	A	C2'-C3'-O3'	-6.60	103.81	113.70
22	Ab	116	G	C2'-C3'-O3'	-6.59	103.81	113.70
58	C1	2045	G	C3'-C2'-O2'	6.59	120.59	110.70
58	C1	2193	U	C2'-C3'-O3'	6.59	119.38	109.50
58	C1	2470	A	C2'-C3'-O3'	-6.59	103.82	113.70
58	D1	122	G	C3'-C2'-O2'	-6.58	104.73	114.60
58	D1	1376	A	C3'-C2'-O2'	6.58	120.56	110.70
22	Bb	113	A	C2'-C3'-O3'	6.57	119.36	109.50
59	Ds	100	A	C4'-C3'-O3'	-6.57	103.15	113.00
36	DN	63	VAL	CB-CA-C	-6.57	103.53	110.62
58	D1	715	G	C3'-C2'-O2'	-6.57	104.75	114.60
22	Bb	42	G	C3'-C2'-O2'	6.56	120.54	110.70
58	D1	2766	U	C3'-C2'-O2'	6.56	120.54	110.70
58	C1	2891	A	C3'-C2'-O2'	6.56	120.53	110.70
58	C1	2276	U	C1'-C2'-O2'	6.56	118.23	108.40
58	D1	150	C	C3'-C2'-O2'	6.55	120.53	110.70
58	C1	786	U	C2'-C3'-O3'	-6.55	103.88	113.70
22	Ab	52	A	C2'-C3'-O3'	6.55	119.32	109.50
58	C1	2475	C	C2'-C3'-O3'	-6.55	103.88	113.70
30	DD	86	GLY	N-CA-C	6.55	122.65	111.98
58	D1	1414	G	C1'-C2'-O2'	6.55	118.22	108.40
58	D1	1801	C	C1'-C2'-O2'	6.55	118.22	108.40
47	DZ	176	PRO	N-CA-C	6.54	118.68	110.70
58	D1	798	A	C4'-C3'-O3'	6.54	119.21	109.40
22	Ab	1285	C	C3'-C2'-O2'	6.54	120.50	110.70
58	D1	1346	A	C4'-C3'-O3'	6.53	119.20	109.40
58	D1	2388	A	C3'-C2'-O2'	6.53	120.50	110.70
58	C1	1726	U	C2'-C3'-O3'	6.53	123.49	113.70
32	DF	43	VAL	N-CA-C	6.52	116.11	106.85
58	D1	1732	C	C3'-C2'-O2'	6.52	120.49	110.70
1	A2	14	A	C3'-C2'-O2'	6.52	120.48	110.70
58	C1	209	A	C2'-C3'-O3'	6.52	119.28	109.50
22	Ab	1508	G	C2'-C3'-O3'	-6.52	103.92	113.70
4	BD	12	CYS	N-CA-C	-6.52	96.91	110.80
58	D1	2396	C	C3'-C2'-O2'	6.51	120.47	110.70
58	C1	246	G	C3'-C2'-O2'	6.51	120.47	110.70
58	C1	1883	A	C1'-C2'-O2'	6.51	118.17	108.40
58	D1	654	G	C1'-C2'-O2'	6.51	118.17	108.40
58	D1	1959	A	C4'-C3'-O3'	6.51	119.16	109.40
22	Ab	31	U	C4'-C3'-O3'	6.51	119.16	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	C1	2464	A	C1'-C2'-O2'	6.51	118.16	108.40
22	Ab	1471	A	C3'-C2'-O2'	6.50	120.45	110.70
22	Bb	598	A	C1'-C2'-O2'	6.50	118.15	108.40
58	D1	1205	G	C3'-C2'-O2'	6.50	120.45	110.70
58	D1	1740	C	N1-C1'-C2'	6.50	121.75	112.00
29	CC	44	TYR	N-CA-C	6.49	124.63	110.80
58	D1	1984	U	C4'-C3'-O3'	-6.49	99.66	109.40
58	C1	647	G	C4'-C3'-O3'	-6.49	103.27	113.00
58	C1	1697	G	C1'-C2'-O2'	6.49	118.13	108.40
58	D1	1092	G	C2'-C3'-O3'	-6.48	103.98	113.70
25	C3	75	C	C3'-C2'-O2'	6.48	120.42	110.70
58	C1	2031	G	C1'-C2'-O2'	6.48	118.12	108.40
58	C1	2221	C	C2'-C3'-O3'	6.48	123.41	113.70
58	D1	2595	U	C1'-C2'-O2'	6.48	118.11	108.40
22	Bb	909	C	C4'-C3'-O3'	6.47	122.71	113.00
58	C1	2856	U	C1'-C2'-O2'	6.47	118.11	108.40
22	Ab	1286	G	C4'-C3'-O3'	-6.47	103.30	113.00
58	D1	2550	C	C3'-C2'-O2'	6.46	120.39	110.70
58	C1	1234	G	C1'-C2'-O2'	6.46	118.09	108.40
58	D1	53	G	C2'-C3'-O3'	-6.46	104.01	113.70
39	CQ	10	LEU	N-CA-C	6.45	118.71	107.49
58	D1	935	C	C2'-C3'-O3'	6.45	119.17	109.50
22	Ab	379	A	C1'-C2'-O2'	6.44	118.07	108.40
46	CY	7	VAL	N-CA-C	6.44	122.74	109.34
58	D1	1345	U	N1-C1'-C2'	6.44	123.67	114.00
58	D1	2617	C	C4'-C3'-O3'	6.44	122.67	113.00
22	Ab	770	G	C1'-C2'-O2'	6.44	118.06	108.40
18	AS	44	LEU	N-CA-C	6.44	118.17	110.44
58	D1	827	A	C4'-C3'-O3'	-6.43	103.36	113.00
58	D1	720	G	C1'-C2'-O2'	6.43	118.04	108.40
58	D1	2272	C	C1'-C2'-O2'	6.43	118.04	108.40
58	D1	2700	U	C4'-C3'-O3'	6.42	119.03	109.40
12	BL	119	LYS	N-CA-C	-6.42	100.78	110.28
59	Ds	27	C	C3'-C2'-O2'	6.42	120.33	110.70
22	Ab	798	A	C3'-C2'-O2'	6.42	120.33	110.70
36	CN	50	GLY	N-CA-C	-6.42	101.50	111.00
58	D1	2829	A	C4'-C3'-O3'	-6.42	99.78	109.40
49	CH	36	GLY	N-CA-C	6.41	119.86	110.38
58	D1	2192	A	C4'-C3'-O3'	6.41	119.01	109.40
13	AM	65	LYS	CA-C-N	6.40	133.23	121.70
13	AM	65	LYS	C-N-CA	6.40	133.23	121.70
58	C1	1985	G	C3'-C2'-O2'	-6.40	105.00	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	Bb	1206	G	C4'-C3'-O3'	6.40	119.00	109.40
58	C1	601	G	C4'-C3'-O3'	-6.40	103.40	113.00
36	CN	94	ARG	N-CA-C	-6.40	105.11	113.17
58	D1	1625	A	C4'-C3'-O3'	-6.40	103.40	113.00
43	CU	45	THR	N-CA-C	6.39	118.04	111.14
22	Ab	1036	G	C2'-C3'-O3'	-6.38	99.92	109.50
58	D1	1595	C	C4'-C3'-O3'	-6.38	103.42	113.00
58	D1	1613	A	C2'-C3'-O3'	6.38	119.08	109.50
58	C1	1987	A	C4'-C3'-O3'	-6.38	99.83	109.40
22	Bb	970	U	C2'-C3'-O3'	6.38	119.07	109.50
58	D1	282	G	C4'-C3'-O3'	-6.38	103.43	113.00
58	D1	2841	U	C3'-C2'-O2'	6.38	124.17	114.60
58	D1	1647	U	C4'-C3'-O3'	6.38	118.97	109.40
58	C1	257	U	C2'-C3'-O3'	-6.38	104.13	113.70
58	C1	2235	G	C4'-C3'-O3'	-6.38	103.44	113.00
58	D1	1837	G	C1'-C2'-O2'	6.38	117.96	108.40
58	C1	227	U	C3'-C2'-O2'	6.37	120.26	110.70
58	C1	1625	A	C3'-C2'-O2'	6.37	120.26	110.70
58	C1	124	A	C1'-C2'-O2'	6.37	117.95	108.40
48	Da	14	ARG	N-CA-C	6.37	119.50	110.14
28	CB	244	ARG	CA-C-N	6.37	126.94	120.38
28	CB	244	ARG	C-N-CA	6.37	126.94	120.38
59	Ds	28	C	C3'-C2'-O2'	6.37	120.25	110.70
37	CO	40	SER	CA-C-N	6.36	130.74	121.26
37	CO	40	SER	C-N-CA	6.36	130.74	121.26
58	D1	1345	U	C4'-C3'-O3'	6.36	118.95	109.40
58	C1	972	G	C1'-C2'-O2'	6.36	117.94	108.40
58	C1	1803	A	C3'-C2'-O2'	6.36	120.24	110.70
61	D4	3	C	C3'-C2'-O2'	6.36	120.24	110.70
58	D1	1635	U	C1'-C2'-O2'	6.36	117.94	108.40
22	Bb	468	C	C1'-C2'-O2'	6.35	117.93	108.40
58	C1	2516	G	C1'-C2'-O2'	6.35	117.93	108.40
22	Bb	1488	U	C3'-C2'-O2'	6.35	120.22	110.70
58	C1	2110	U	C1'-C2'-O2'	6.35	117.92	108.40
58	C1	1080	U	C1'-C2'-O2'	6.35	117.92	108.40
58	C1	2340	G	C3'-C2'-O2'	6.35	120.22	110.70
30	DD	75	HIS	N-CA-C	6.35	118.42	108.96
38	DP	132	VAL	N-CA-C	6.35	119.44	108.90
58	C1	2482	C	C2'-C3'-O3'	6.34	123.22	113.70
56	C9	32	LEU	N-CA-C	-6.34	104.37	111.28
59	Cs	91	C	C3'-C2'-O2'	6.34	120.20	110.70
22	Ab	511	G	C2'-C3'-O3'	-6.33	104.20	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	C1	295	U	C4'-C3'-O3'	6.33	122.50	113.00
22	Bb	144	A	C4'-C3'-O3'	6.33	118.89	109.40
58	C1	69	A	C4'-C3'-O3'	6.33	118.89	109.40
29	DC	44	TYR	N-CA-C	6.32	124.27	110.80
28	DB	118	VAL	CB-CA-C	-6.32	105.80	111.74
58	D1	2250	G	C4'-C3'-O3'	-6.31	103.53	113.00
22	Ab	706	A	C4'-C3'-O3'	-6.31	103.54	113.00
58	D1	259	A	C4'-C3'-O3'	-6.31	103.53	113.00
58	D1	1991	A	C5'-C4'-C3'	6.31	124.66	115.20
58	D1	2562	C	C4'-C3'-O3'	-6.31	103.54	113.00
58	D1	1649	C	C2'-C3'-O3'	-6.31	104.24	113.70
22	Bb	1477	A	C3'-C2'-O2'	6.30	120.16	110.70
58	C1	2586	C	C2'-C3'-O3'	-6.30	104.24	113.70
58	D1	1408	C	C1'-C2'-O2'	6.30	117.85	108.40
2	AA	172	ILE	CB-CA-C	-6.29	103.64	112.14
22	Bb	1032	U	C4'-C3'-O3'	6.29	118.84	109.40
58	C1	1179	C	C2'-C3'-O3'	-6.29	104.26	113.70
58	C1	617	C	C3'-C2'-O2'	6.29	120.13	110.70
58	D1	1213	G	C3'-C2'-O2'	6.29	120.13	110.70
22	Bb	671	A	C4'-C3'-O3'	6.29	118.83	109.40
58	C1	133	G	C3'-C2'-O2'	6.28	120.12	110.70
58	D1	1284	G	C2'-C3'-O3'	-6.28	104.27	113.70
22	Ab	874	C	C3'-C2'-O2'	6.28	120.11	110.70
58	D1	576	U	C3'-C2'-O2'	6.28	120.12	110.70
58	D1	715	G	C2'-C3'-O3'	6.28	118.92	109.50
58	D1	795	C	C1'-C2'-O2'	6.28	117.81	108.40
58	D1	531	A	C4'-C3'-O3'	-6.27	103.59	113.00
58	D1	1723	A	C1'-C2'-O2'	6.27	117.81	108.40
22	Ab	105	G	C1'-C2'-O2'	6.27	117.81	108.40
58	C1	2049	U	N1-C1'-C2'	6.27	121.41	112.00
58	D1	1378	C	C1'-C2'-O2'	6.27	117.80	108.40
58	C1	249	G	C3'-C2'-O2'	6.26	120.10	110.70
58	C1	1186	U	C4'-C3'-O3'	-6.26	103.61	113.00
58	C1	1983	C	C5'-C4'-O4'	6.26	118.49	109.10
58	D1	779	G	C1'-C2'-O2'	6.26	117.79	108.40
3	AC	59	ARG	N-CA-C	6.26	118.03	108.52
58	D1	2614	G	C1'-C2'-O2'	6.26	117.79	108.40
22	Bb	732	C	C4'-C3'-O3'	6.26	118.79	109.40
59	Ds	6	C	C3'-C2'-O2'	6.26	120.08	110.70
58	D1	1654	A	C3'-C2'-O2'	-6.26	105.22	114.60
26	C4	43	G	C3'-C2'-O2'	6.25	120.08	110.70
58	C1	702	G	C4'-C3'-O3'	-6.25	103.62	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	Ab	804	U	C4'-C3'-O3'	6.25	118.78	109.40
58	D1	2576	A	C3'-C2'-O2'	6.25	120.08	110.70
58	C1	1718	C	C2'-C3'-O3'	-6.25	104.33	113.70
58	C1	2553	A	C1'-C2'-O2'	-6.25	102.43	111.80
58	C1	1265	C	C1'-C2'-O2'	6.25	117.77	108.40
31	DE	86	MET	CA-C-N	6.25	127.65	119.84
31	DE	86	MET	C-N-CA	6.25	127.65	119.84
58	D1	412	G	C1'-C2'-O2'	6.25	121.17	111.80
41	DS	23	ARG	CA-C-N	6.24	127.64	119.84
41	DS	23	ARG	C-N-CA	6.24	127.64	119.84
22	Bb	1476	U	C4'-C3'-O3'	-6.24	100.04	109.40
58	C1	1956	G	C3'-C2'-O2'	6.24	120.06	110.70
22	Ab	434	G	C4'-C3'-O3'	6.24	118.75	109.40
58	D1	2436	A	C1'-C2'-O2'	6.23	121.15	111.80
5	AE	32	VAL	N-CA-C	6.23	117.67	108.45
13	BM	65	LYS	CA-C-N	6.23	132.91	121.70
13	BM	65	LYS	C-N-CA	6.23	132.91	121.70
53	C6	33	CYS	CA-C-N	-6.23	114.21	120.31
53	C6	33	CYS	C-N-CA	-6.23	114.21	120.31
58	C1	1821	A	C1'-C2'-O2'	6.22	117.73	108.40
58	C1	1895	G	C1'-C2'-O2'	6.22	117.73	108.40
58	C1	2124	C	C3'-C2'-O2'	6.22	120.03	110.70
32	DF	13	LYS	N-CA-C	6.22	124.06	110.80
58	D1	1042	G	C3'-C2'-O2'	6.22	120.03	110.70
22	Bb	713	A	C3'-C2'-O2'	6.22	120.03	110.70
58	C1	1071	U	C2'-C3'-O3'	-6.22	104.37	113.70
30	CD	95	ARG	N-CA-C	6.22	118.52	109.07
58	C1	2792	G	C2'-C3'-O3'	6.21	118.82	109.50
59	Ds	116	G	C2'-C3'-O3'	6.21	123.02	113.70
22	Ab	586	A	C1'-C2'-O2'	6.21	117.71	108.40
58	D1	2103	A	C3'-C2'-O2'	6.21	120.01	110.70
56	C9	24	ALA	N-CA-C	6.21	117.30	108.74
58	D1	895	A	C3'-C2'-O2'	6.21	120.01	110.70
37	CO	27	HIS	N-CA-C	6.20	119.67	108.69
58	C1	2221	C	C4'-C3'-O3'	-6.20	103.69	113.00
58	D1	63	C	C1'-C2'-O2'	6.20	117.71	108.40
22	Ab	239	A	C4'-C3'-O3'	6.20	118.70	109.40
22	Bb	262	G	C3'-C2'-O2'	6.20	120.00	110.70
58	C1	2400	G	C2'-C3'-O3'	-6.20	104.40	113.70
41	DS	59	THR	N-CA-C	-6.20	100.41	110.20
28	CB	43	ARG	N-CA-C	6.19	120.52	113.15
58	D1	1643	C	C2'-C3'-O3'	6.19	122.99	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	DO	9	ASN	CA-C-N	-6.19	112.18	119.05
37	DO	9	ASN	C-N-CA	-6.19	112.18	119.05
26	C4	20	G	C2'-C3'-O3'	6.19	118.78	109.50
58	C1	1901	C	C3'-C2'-O2'	6.19	119.98	110.70
58	D1	2542	A	C1'-C2'-O2'	6.19	117.68	108.40
58	C1	47	A	C4'-C3'-O3'	6.18	118.68	109.40
58	C1	259	A	C4'-C3'-O3'	-6.18	103.72	113.00
58	C1	1864	U	C2'-C3'-O3'	-6.18	104.43	113.70
58	D1	518	G	C3'-C2'-O2'	6.18	119.97	110.70
22	Ab	41	C	C3'-C2'-O2'	6.18	119.96	110.70
58	C1	276	G	C4'-C3'-O3'	6.18	122.27	113.00
58	C1	62	A	C3'-C2'-O2'	6.17	119.96	110.70
58	D1	2621	C	C4'-C3'-O3'	-6.17	100.14	109.40
58	C1	2850	C	C3'-C2'-O2'	6.17	119.95	110.70
59	Cs	21	G	C3'-C2'-O2'	6.17	119.95	110.70
58	D1	246	G	C3'-C2'-O2'	6.17	119.95	110.70
58	C1	845	G	C1'-C2'-O2'	-6.16	99.15	108.40
58	C1	1333	U	C2'-C3'-O3'	6.16	118.73	109.50
58	C1	1816	A	N9-C1'-C2'	6.16	123.23	114.00
58	C1	2540	G	C4'-C3'-O3'	-6.15	103.77	113.00
58	D1	2310	G	C3'-C2'-O2'	6.15	119.93	110.70
22	Bb	432	C	C4'-C3'-O3'	6.15	118.63	109.40
58	C1	140	C	C3'-C2'-O2'	6.15	119.93	110.70
58	C1	269	C	C1'-C2'-O2'	6.15	117.63	108.40
58	C1	2686	A	C1'-C2'-O2'	6.15	117.63	108.40
58	D1	1024	G	C1'-C2'-O2'	6.15	117.63	108.40
58	D1	2541	A	C2'-C3'-O3'	-6.15	104.48	113.70
22	Bb	1032	U	C2'-C3'-O3'	6.15	118.72	109.50
58	D1	990	G	C3'-C2'-O2'	6.14	119.92	110.70
58	C1	183	A	C4'-C3'-O3'	-6.14	103.79	113.00
58	C1	881	A	C1'-C2'-O2'	6.14	117.61	108.40
58	D1	1435	U	C4'-C3'-O3'	-6.14	103.79	113.00
59	Ds	82	G	C2'-C3'-O3'	-6.14	104.49	113.70
58	C1	2249	G	C2'-C3'-O3'	6.14	118.71	109.50
54	D7	32	ASN	N-CA-C	6.14	119.25	108.75
4	BD	31	CYS	CA-CB-SG	-6.13	100.30	114.40
58	C1	1249	U	C4'-C3'-O3'	6.13	118.59	109.40
61	D4	12	G	C1'-C2'-O2'	6.13	117.59	108.40
58	D1	1816	A	N9-C1'-C2'	6.13	123.19	114.00
11	BK	126	ARG	N-CA-C	-6.13	104.44	112.41
58	C1	557	G	C2'-C3'-O3'	-6.13	104.51	113.70
58	C1	1283	G	C3'-C2'-O2'	6.12	119.88	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	Bb	969	U	C4'-C3'-O3'	-6.12	103.83	113.00
41	CS	29	ARG	N-CA-C	6.11	123.82	110.80
58	D1	715	G	C5'-C4'-C3'	6.11	124.37	115.20
54	C7	13	CYS	N-CA-C	6.11	118.71	108.02
58	C1	55	C	C3'-C2'-O2'	6.11	119.86	110.70
58	C1	2007	A	C3'-C2'-O2'	6.11	119.87	110.70
58	D1	2686	A	C1'-C2'-O2'	6.11	117.57	108.40
58	D1	2730	G	C4'-C3'-O3'	-6.11	103.83	113.00
58	D1	2008	G	C2'-C3'-O3'	6.11	122.86	113.70
22	Bb	1263	U	C2'-C3'-O3'	6.11	118.66	109.50
58	C1	1409	G	C3'-C2'-O2'	6.11	119.86	110.70
58	C1	497	A	C4'-C3'-O3'	6.10	122.15	113.00
58	D1	1591	A	C4'-C3'-O3'	-6.10	103.85	113.00
58	D1	2085	C	C4'-C3'-O3'	-6.10	103.84	113.00
58	D1	602	C	C3'-C2'-O2'	6.10	119.85	110.70
43	CU	22	VAL	N-CA-C	6.09	122.02	109.34
58	C1	742	G	C1'-C2'-O2'	6.09	117.54	108.40
58	C1	1559	U	C4'-C3'-O3'	-6.09	103.86	113.00
58	C1	647	G	C2'-C3'-O3'	6.09	122.83	113.70
28	CB	233	HIS	N-CA-C	6.09	117.92	111.28
58	C1	1642	A	C2'-C3'-O3'	-6.08	104.57	113.70
58	C1	2584	C	C3'-C2'-O2'	6.08	119.82	110.70
22	Ab	692	C	C1'-C2'-O2'	6.07	117.50	108.40
58	D1	2276	U	C1'-C2'-O2'	6.07	117.50	108.40
37	DO	54	GLY	N-CA-C	-6.06	106.79	115.64
58	C1	777	C	C2'-C3'-O3'	-6.06	104.61	113.70
58	C1	2305	C	C1'-C2'-O2'	6.06	117.50	108.40
58	D1	476	C	C3'-C2'-O2'	6.06	119.79	110.70
58	D1	1381	A	C1'-C2'-O2'	6.06	117.49	108.40
58	D1	1856	G	C1'-C2'-O2'	6.06	117.49	108.40
22	Ab	884	G	C3'-C2'-O2'	6.06	119.79	110.70
31	CE	125	PHE	N-CA-C	-6.06	104.63	112.68
58	C1	2044	G	C2'-C3'-O3'	-6.05	104.62	113.70
59	Cs	105	A	C1'-C2'-O2'	6.05	117.48	108.40
58	D1	1606	G	C1'-C2'-O2'	6.05	117.48	108.40
58	D1	1642	A	C2'-C3'-O3'	-6.05	104.62	113.70
58	D1	2790	A	C2'-C3'-O3'	6.05	118.58	109.50
58	C1	2132	C	C2'-C3'-O3'	-6.05	104.62	113.70
22	Ab	812	A	C4'-C3'-O3'	6.05	122.07	113.00
58	C1	715	G	O4'-C4'-C3'	-6.05	100.05	106.10
22	Ab	60	A	C4'-C3'-O3'	-6.05	103.93	113.00
22	Ab	1482	G	C4'-C3'-O3'	6.05	118.47	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	Bb	819	U	C3'-C2'-O2'	6.05	119.77	110.70
58	D1	1247	G	C4'-C3'-O3'	-6.05	103.93	113.00
26	C4	36	A	O5'-P-OP2	-6.04	89.87	108.00
26	C4	73	A	C3'-C2'-O2'	6.04	119.76	110.70
58	D1	2059	G	C1'-C2'-O2'	6.04	117.46	108.40
58	D1	2219	A	C4'-C3'-O3'	6.04	118.46	109.40
29	DC	125	GLY	CA-C-N	6.04	125.80	119.76
29	DC	125	GLY	C-N-CA	6.04	125.80	119.76
58	C1	1339	U	C4'-C3'-O3'	-6.04	103.94	113.00
22	Ab	223	G	C3'-C2'-O2'	6.03	119.75	110.70
58	D1	625	A	C4'-C3'-O3'	6.03	118.44	109.40
58	D1	829	A	C4'-C3'-O3'	6.03	122.05	113.00
58	D1	1987	A	C4'-C3'-O3'	-6.03	100.36	109.40
58	D1	2227	G	C3'-C2'-O2'	6.03	119.74	110.70
27	CA	35	ALA	N-CA-C	6.03	116.19	108.24
58	D1	2046	C	C4'-C3'-O3'	-6.03	103.96	113.00
22	Ab	246	A	C4'-C3'-O3'	6.02	118.43	109.40
58	D1	1633	C	C1'-C2'-O2'	6.02	117.43	108.40
58	D1	1298	A	C1'-C2'-O2'	-6.02	102.77	111.80
22	Ab	414	C	C3'-C2'-O2'	6.02	119.73	110.70
49	DH	29	GLY	N-CA-C	6.02	117.64	111.56
59	Ds	47	C	C1'-C2'-O2'	6.02	117.43	108.40
58	D1	1498	C	C2'-C3'-O3'	6.02	118.52	109.50
22	Ab	493	A	C2'-C3'-O3'	6.01	122.72	113.70
58	C1	2594	G	C3'-C2'-O2'	6.01	119.72	110.70
58	D1	789	G	C1'-C2'-O2'	6.01	117.42	108.40
12	BL	93	LEU	CA-C-N	-6.01	113.57	119.76
12	BL	93	LEU	C-N-CA	-6.01	113.57	119.76
58	C1	2693	U	C2'-C3'-O3'	-6.01	104.69	113.70
41	DS	110	ILE	CB-CA-C	-6.01	104.28	111.97
58	D1	899	G	C2'-C3'-O3'	6.01	122.71	113.70
61	D4	76	C	C3'-C2'-O2'	6.00	119.70	110.70
58	D1	1070	G	C2'-C3'-O3'	6.00	118.50	109.50
58	C1	827	A	C4'-C3'-O3'	-6.00	104.00	113.00
58	D1	1385	U	C3'-C2'-O2'	6.00	123.60	114.60
3	AC	149	ALA	N-CA-C	6.00	117.51	108.46
22	Ab	1035	U	C1'-C2'-O2'	6.00	117.39	108.40
58	C1	2482	C	C4'-C3'-O3'	-6.00	104.01	113.00
58	C1	2721	C	C3'-C2'-O2'	5.99	119.69	110.70
58	D1	317	A	C1'-C2'-O2'	5.99	117.39	108.40
37	CO	71	VAL	CA-C-N	-5.99	113.51	119.56
37	CO	71	VAL	C-N-CA	-5.99	113.51	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	Bb	669	G	C3'-C2'-O2'	5.99	119.68	110.70
58	D1	1858	G	C3'-C2'-O2'	-5.99	105.62	114.60
22	Ab	328	G	C4'-C3'-O3'	-5.99	104.02	113.00
58	D1	1373	G	C4'-C3'-O3'	-5.99	104.02	113.00
58	D1	1203	C	C3'-C2'-O2'	5.98	119.67	110.70
58	D1	2092	A	C2'-C3'-O3'	-5.98	104.73	113.70
58	D1	1312	U	C4'-C3'-O3'	-5.98	104.03	113.00
22	Bb	202	A	C2'-C3'-O3'	-5.98	104.74	113.70
58	D1	2045	G	C3'-C2'-O2'	5.98	119.67	110.70
22	Ab	83	U	C3'-C2'-O2'	5.97	119.65	110.70
22	Bb	1467	G	C3'-C2'-O2'	5.97	119.65	110.70
58	D1	2740	U	C3'-C2'-O2'	5.97	119.66	110.70
58	C1	1805	U	C1'-C2'-O2'	5.96	117.35	108.40
58	D1	2586	C	C2'-C3'-O3'	-5.96	104.75	113.70
58	D1	1472	A	C4'-C3'-O3'	5.96	118.34	109.40
58	D1	166	G	C1'-C2'-O2'	5.96	117.34	108.40
58	D1	2362	G	C4'-C3'-O3'	-5.96	104.06	113.00
22	Ab	495	C	C2'-C3'-O3'	5.96	118.44	109.50
58	C1	1659	A	C2'-C3'-O3'	-5.96	104.77	113.70
58	C1	1956	G	C2'-C3'-O3'	5.96	122.64	113.70
58	D1	798	A	C2'-C3'-O3'	5.95	118.43	109.50
58	D1	1385	U	C1'-C2'-O2'	-5.95	102.87	111.80
4	AD	6	GLY	CA-C-N	5.95	127.28	119.84
4	AD	6	GLY	C-N-CA	5.95	127.28	119.84
58	D1	2666	G	N9-C1'-C2'	5.95	122.93	114.00
58	D1	1972	U	C1'-C2'-O2'	5.95	117.33	108.40
58	D1	2291	G	C1'-C2'-O2'	5.95	117.33	108.40
22	Bb	1462	C	C1'-C2'-O2'	5.95	117.32	108.40
58	C1	1973	A	C3'-C2'-O2'	5.95	119.62	110.70
58	D1	2007	A	C4'-C3'-O3'	-5.95	104.08	113.00
58	D1	2086	C	C4'-C3'-O3'	-5.95	104.08	113.00
58	C1	1028	A	C3'-C2'-O2'	5.94	119.61	110.70
58	D1	1816	A	O4'-C1'-C2'	-5.94	99.86	105.80
22	Bb	1442	G	C3'-C2'-O2'	5.94	119.61	110.70
39	DQ	58	GLY	N-CA-C	5.94	127.26	113.18
22	Bb	812	A	C2'-C3'-O3'	-5.94	104.79	113.70
58	C1	1312	U	C1'-C2'-O2'	-5.94	99.49	108.40
58	D1	2353	C	C4'-C3'-O3'	-5.94	104.09	113.00
58	D1	2629	G	C2'-C3'-O3'	-5.94	104.80	113.70
58	D1	837	C	C4'-C3'-O3'	5.93	118.30	109.40
22	Ab	784	G	C1'-C2'-O2'	5.93	117.30	108.40
22	Bb	1038	A	C2'-C3'-O3'	-5.93	104.80	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	C1	1285	U	C4'-C3'-O3'	-5.93	104.10	113.00
58	D1	1659	A	C2'-C3'-O3'	-5.93	104.80	113.70
58	D1	1709	C	C2'-C3'-O3'	5.93	122.60	113.70
58	D1	1811	C	C2'-C3'-O3'	5.93	118.40	109.50
46	DY	29	GLU	CA-C-N	5.93	129.40	120.75
46	DY	29	GLU	C-N-CA	5.93	129.40	120.75
58	D1	1806	G	C2'-C3'-O3'	-5.93	104.81	113.70
58	C1	1289	G	C3'-C2'-O2'	5.93	119.59	110.70
4	BD	31	CYS	N-CA-CB	5.92	122.99	110.67
58	D1	1231	G	C3'-C2'-O2'	5.92	119.58	110.70
58	C1	2395	G	C3'-C2'-O2'	-5.92	105.72	114.60
29	DC	168	MET	N-CA-C	5.92	119.36	109.95
22	Ab	1470	A	C3'-C2'-O2'	5.92	119.58	110.70
58	C1	639	A	C3'-C2'-O2'	-5.92	105.73	114.60
22	Ab	923	G	C1'-C2'-O2'	5.91	117.27	108.40
58	D1	407	G	C1'-C2'-O2'	5.91	117.27	108.40
58	D1	1598	G	C1'-C2'-O2'	5.91	117.27	108.40
22	Ab	805	G	C3'-C2'-O2'	5.91	119.57	110.70
58	D1	268	G	C3'-C2'-O2'	5.91	119.57	110.70
58	D1	900	G	C1'-C2'-O2'	5.91	117.26	108.40
59	Cs	87	G	C3'-C2'-O2'	5.91	119.56	110.70
58	D1	1654	A	C1'-C2'-O2'	-5.91	102.94	111.80
58	D1	838	G	C2'-C3'-O3'	5.90	118.36	109.50
58	C1	2590	C	C3'-C2'-O2'	5.90	119.55	110.70
58	D1	1801	C	C2'-C3'-O3'	-5.90	104.85	113.70
11	AK	40	ILE	CB-CA-C	-5.90	104.84	111.80
59	Ds	15	A	C1'-C2'-O2'	-5.90	102.95	111.80
58	C1	1719	U	C1'-C2'-O2'	5.90	117.24	108.40
58	C1	2471	U	C2'-C3'-O3'	-5.89	104.86	113.70
37	DO	10	PRO	N-CA-C	-5.89	105.34	113.53
58	D1	1156	A	C1'-C2'-O2'	-5.89	102.96	111.80
58	D1	1028	A	C3'-C2'-O2'	5.89	119.53	110.70
58	D1	1444	C	C1'-C2'-O2'	5.89	117.23	108.40
22	Ab	908	C	C3'-C2'-O2'	5.89	119.53	110.70
22	Bb	970	U	C4'-C3'-O3'	5.89	118.23	109.40
58	C1	355	A	C4'-C3'-O3'	5.89	118.23	109.40
58	D1	1638	G	C4'-C3'-O3'	-5.88	104.17	113.00
58	C1	259	A	C3'-C2'-O2'	5.88	119.53	110.70
58	C1	1438	A	C2'-C3'-O3'	-5.88	104.88	113.70
58	C1	2608	G	C4'-C3'-O3'	-5.88	104.18	113.00
32	DF	136	ILE	CB-CA-C	-5.88	104.11	112.22
58	D1	985	A	C3'-C2'-O2'	5.88	119.52	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	D1	1983	C	C5'-C4'-C3'	5.88	124.02	115.20
22	Bb	1298	G	C2'-C3'-O3'	-5.88	104.89	113.70
58	C1	1529	G	C4'-C3'-O3'	5.88	121.81	113.00
58	C1	1922	A	C2'-C3'-O3'	-5.88	104.89	113.70
22	Ab	400	U	C3'-C2'-O2'	5.87	119.51	110.70
58	D1	2696	G	C1'-C2'-O2'	5.87	117.21	108.40
58	C1	1294	U	C2'-C3'-O3'	-5.87	104.89	113.70
58	C1	2576	A	C1'-C2'-O2'	5.87	117.21	108.40
58	C1	2687	C	C3'-C2'-O2'	5.87	119.51	110.70
58	D1	2340	G	C3'-C2'-O2'	5.87	119.51	110.70
58	D1	2442	U	C1'-C2'-O2'	5.87	117.21	108.40
58	C1	507	A	C4'-C3'-O3'	-5.87	104.20	113.00
58	D1	1539	A	C3'-C2'-O2'	5.87	119.50	110.70
58	D1	468	A	C2'-C3'-O3'	-5.87	104.90	113.70
22	Ab	893	A	C3'-C2'-O2'	5.86	119.50	110.70
43	DU	34	GLU	N-CA-C	-5.86	99.68	109.24
58	D1	2475	C	C2'-C3'-O3'	-5.86	104.91	113.70
58	C1	660	G	C4'-C3'-O3'	-5.86	104.21	113.00
22	Bb	571	G	C4'-C3'-O3'	5.86	118.18	109.40
58	D1	744	C	C4'-C3'-O3'	-5.85	104.22	113.00
58	D1	2314	G	C3'-C2'-O2'	5.85	119.48	110.70
26	C4	5	G	C3'-C2'-O2'	5.85	119.48	110.70
22	Bb	784	G	C1'-C2'-O2'	5.85	117.18	108.40
58	C1	916	A	C4'-C3'-O3'	-5.85	104.22	113.00
46	DY	75	ILE	N-CA-C	5.85	117.10	108.45
22	Bb	405	G	C3'-C2'-O2'	5.85	119.47	110.70
58	D1	1389	G	C1'-C2'-O2'	5.85	120.57	111.80
58	D1	2584	C	C3'-C2'-O2'	5.85	119.47	110.70
22	Ab	1108	U	C3'-C2'-O2'	5.84	119.47	110.70
58	C1	879	U	C3'-C2'-O2'	5.84	119.47	110.70
26	C4	13	C	C1'-C2'-O2'	5.84	117.16	108.40
36	CN	91	LEU	N-CA-C	5.84	120.21	113.38
58	C1	2791	U	C1'-O4'-C4'	-5.84	103.86	109.70
58	C1	1343	C	C2'-C3'-O3'	-5.84	104.94	113.70
58	D1	2313	G	C2'-C3'-O3'	5.84	122.46	113.70
58	D1	1968	C	C2'-C3'-O3'	5.83	122.45	113.70
2	AA	233	SER	CA-C-N	-5.83	113.93	119.76
2	AA	233	SER	C-N-CA	-5.83	113.93	119.76
28	DB	210	GLY	N-CA-C	-5.83	99.36	113.18
58	D1	2660	U	C3'-C2'-O2'	5.83	119.45	110.70
58	D1	2280	A	C4'-C3'-O3'	-5.83	104.25	113.00
58	C1	2523	C	C3'-C2'-O2'	5.83	119.44	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	C1	147	C	C1'-C2'-O2'	5.83	117.14	108.40
4	AD	28	SER	CA-C-N	-5.83	112.75	120.96
4	AD	28	SER	C-N-CA	-5.83	112.75	120.96
58	C1	892	C	C4'-C3'-O3'	5.83	118.14	109.40
58	C1	1268	G	C1'-C2'-O2'	5.82	117.13	108.40
58	C1	1863	U	C1'-C2'-O2'	5.82	117.13	108.40
13	AM	9	ILE	CB-CA-C	-5.82	100.77	111.36
58	C1	2562	C	C4'-C3'-O3'	-5.82	104.27	113.00
59	Ds	77	U	C2'-C3'-O3'	5.82	122.43	113.70
30	CD	58	ALA	N-CA-C	5.82	117.62	111.28
58	C1	1876	G	C2'-C3'-O3'	-5.82	104.97	113.70
58	D1	73	G	C1'-C2'-O2'	5.82	117.13	108.40
13	BM	112	GLY	CA-C-N	5.81	127.11	119.84
13	BM	112	GLY	C-N-CA	5.81	127.11	119.84
58	D1	1268	G	C1'-C2'-O2'	5.81	117.12	108.40
22	Bb	547	A	C1'-C2'-O2'	5.81	117.12	108.40
58	C1	732	G	C4'-C3'-O3'	5.81	118.12	109.40
58	C1	2621	C	C4'-C3'-O3'	-5.81	100.69	109.40
58	C1	2838	C	C3'-C2'-O2'	5.81	119.42	110.70
58	D1	574	G	C3'-C2'-O2'	5.81	119.42	110.70
58	D1	588	U	C3'-C2'-O2'	5.81	119.41	110.70
58	C1	98	G	O4'-C1'-C2'	5.81	111.61	105.80
58	C1	1845	A	C3'-C2'-O2'	-5.80	105.89	114.60
46	DY	30	VAL	CB-CA-C	-5.80	103.27	111.28
58	D1	910	G	C1'-C2'-O2'	5.80	117.11	108.40
58	C1	1030	C	C2'-C3'-O3'	-5.80	105.00	113.70
58	D1	535	U	C4'-C3'-O3'	-5.80	104.30	113.00
58	C1	1378	C	C2'-C3'-O3'	-5.80	105.00	113.70
58	D1	1772	C	C2'-C3'-O3'	5.80	122.40	113.70
22	Ab	7	G	C4'-C3'-O3'	-5.80	104.30	113.00
58	D1	411	C	C4'-C3'-O3'	-5.79	104.31	113.00
22	Ab	800	A	C1'-C2'-O2'	5.79	117.09	108.40
58	C1	715	G	C5'-C4'-C3'	5.79	123.89	115.20
58	D1	1983	C	C5'-C4'-O4'	5.79	117.79	109.10
41	DS	30	VAL	CB-CA-C	-5.79	101.79	111.29
58	D1	2834	C	C1'-C2'-O2'	5.79	117.08	108.40
58	C1	1043	C	C1'-C2'-O2'	5.79	117.08	108.40
58	C1	1715	A	C1'-C2'-O2'	5.78	117.07	108.40
58	C1	1894	U	C4'-C3'-O3'	-5.78	104.32	113.00
58	D1	839	A	C4'-C3'-O3'	-5.78	100.73	109.40
22	Ab	1064	G	C3'-C2'-O2'	5.78	119.37	110.70
58	D1	50	A	C4'-C3'-O3'	-5.78	104.33	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	C1	2700	U	C2'-C3'-O3'	5.78	118.16	109.50
22	Ab	1462	C	C3'-C2'-O2'	5.77	119.36	110.70
58	C1	784	G	C1'-C2'-O2'	5.77	117.06	108.40
31	DE	70	VAL	CB-CA-C	-5.77	105.68	111.80
58	C1	1299	A	C4'-C3'-O3'	-5.77	104.34	113.00
22	Bb	1107	G	C4'-C3'-O3'	-5.77	104.35	113.00
58	C1	832	C	C3'-C2'-O2'	5.77	119.35	110.70
22	Ab	557	A	C4'-C3'-O3'	-5.77	104.35	113.00
58	D1	609	C	C4'-C3'-O3'	5.77	118.05	109.40
58	C1	2807	G	C2'-C3'-O3'	-5.77	105.05	113.70
58	D1	2228	A	C2'-C3'-O3'	-5.76	105.05	113.70
38	DP	41	TRP	N-CA-C	-5.76	99.89	109.46
22	Ab	493	A	C3'-C2'-O2'	5.76	119.34	110.70
37	CO	58	THR	CA-C-N	5.76	131.54	122.49
37	CO	58	THR	C-N-CA	5.76	131.54	122.49
58	C1	840	G	C2'-C3'-O3'	-5.76	105.06	113.70
22	Ab	359	A	C4'-C3'-O3'	-5.76	104.36	113.00
6	BF	63	TYR	CB-CA-C	-5.76	104.29	111.43
22	Ab	910	C	C1'-C2'-O2'	5.76	117.03	108.40
22	Bb	1292	G	C3'-C2'-O2'	5.75	119.33	110.70
31	CE	54	GLU	N-CA-C	-5.75	106.24	113.72
22	Ab	1323	U	C4'-C3'-O3'	5.75	121.63	113.00
59	Ds	100	A	C3'-C2'-O2'	5.75	119.33	110.70
12	AL	44	THR	CA-C-N	5.75	126.07	119.92
12	AL	44	THR	C-N-CA	5.75	126.07	119.92
58	C1	1432	C	C1'-C2'-O2'	5.75	117.03	108.40
58	D1	2702	C	C1'-C2'-O2'	5.75	117.03	108.40
58	C1	542	G	C3'-C2'-O2'	5.75	119.33	110.70
22	Bb	520	C	C3'-C2'-O2'	5.75	119.32	110.70
58	C1	297	G	C4'-C3'-O3'	5.75	118.02	109.40
58	C1	1412	A	C1'-C2'-O2'	5.75	117.02	108.40
22	Bb	1486	G	C3'-C2'-O2'	5.75	119.32	110.70
58	C1	827	A	C2'-C3'-O3'	5.75	122.32	113.70
58	C1	1077	A	C3'-C2'-O2'	5.75	119.32	110.70
58	D1	1691	G	C4'-C3'-O3'	-5.75	104.38	113.00
8	BH	112	LEU	N-CA-C	5.74	117.74	108.32
26	C4	77	A	C1'-C2'-O2'	-5.74	103.19	111.80
53	C6	4	HIS	CA-C-N	-5.74	114.02	119.76
53	C6	4	HIS	C-N-CA	-5.74	114.02	119.76
7	BG	73	MET	N-CA-C	5.74	117.79	109.07
58	C1	154	C	C3'-C2'-O2'	5.74	119.31	110.70
58	D1	1021	C	C1'-C2'-O2'	5.74	117.00	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	C1	2514	A	C2'-C3'-O3'	5.74	118.10	109.50
58	C1	2569	C	C1'-C2'-O2'	5.74	117.00	108.40
58	C1	2595	U	C1'-C2'-O2'	5.74	117.00	108.40
61	D4	73	A	O4'-C4'-C3'	-5.74	98.27	104.00
58	D1	1333	U	C3'-C2'-O2'	-5.74	106.00	114.60
58	D1	1832	A	C4'-C3'-O3'	-5.73	104.40	113.00
22	Ab	346	G	C3'-C2'-O2'	5.73	119.30	110.70
58	C1	180	C	C2'-C3'-O3'	-5.73	105.10	113.70
49	DH	90	ILE	CB-CA-C	-5.73	104.64	111.97
37	CO	52	GLU	N-CA-C	5.73	123.00	110.80
41	DS	64	ARG	N-CA-C	5.73	117.86	108.52
58	D1	1681	G	C1'-C2'-O2'	5.73	116.99	108.40
58	C1	2013	G	C3'-C2'-O2'	5.73	123.19	114.60
58	D1	179	A	C1'-C2'-O2'	5.73	116.99	108.40
58	D1	2421	G	C3'-C2'-O2'	5.73	119.29	110.70
58	C1	2337	C	C2'-C3'-O3'	-5.72	105.11	113.70
58	D1	1679	G	C4'-C3'-O3'	-5.72	104.41	113.00
58	D1	2055	U	C2'-C3'-O3'	-5.72	105.11	113.70
58	D1	858	C	C3'-C2'-O2'	5.72	119.28	110.70
22	Ab	538	C	C1'-C2'-O2'	5.72	116.98	108.40
22	Bb	1251	A	C3'-C2'-O2'	5.72	119.28	110.70
29	CC	74	PRO	N-CA-C	5.72	120.06	111.14
58	D1	423	G	C3'-C2'-O2'	5.72	119.28	110.70
22	Bb	754	C	C2'-C3'-O3'	-5.72	105.12	113.70
22	Bb	534	G	C3'-C2'-O2'	5.71	119.27	110.70
58	C1	221	A	C3'-C2'-O2'	5.71	119.27	110.70
58	D1	504	A	C2'-C3'-O3'	-5.71	100.93	109.50
58	C1	176	G	C3'-C2'-O2'	5.71	119.27	110.70
58	D1	1398	A	C3'-C2'-O2'	5.71	119.27	110.70
58	C1	2233	G	C1'-C2'-O2'	5.71	116.97	108.40
30	DD	86	GLY	O-C-N	5.71	127.17	122.71
58	D1	469	C	C2'-C3'-O3'	-5.71	105.13	113.70
58	D1	1719	U	C1'-C2'-O2'	5.71	116.97	108.40
58	D1	585	G	C1'-C2'-O2'	5.71	116.96	108.40
58	C1	2313	G	C3'-C2'-O2'	5.71	119.26	110.70
46	DY	76	CYS	N-CA-C	5.71	115.47	108.11
58	C1	321	G	C1'-C2'-O2'	5.71	116.96	108.40
58	C1	1740	C	C1'-C2'-O2'	-5.71	99.84	108.40
41	DS	29	ARG	O-C-N	5.70	129.79	123.52
22	Ab	362	C	C2'-C3'-O3'	5.70	118.05	109.50
58	D1	1009	C	C1'-C2'-O2'	5.70	116.95	108.40
56	C9	49	VAL	N-CA-C	-5.70	99.58	108.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	D1	2697	G	C1'-C2'-O2'	5.70	116.95	108.40
48	Ca	3	HIS	N-CA-C	5.70	118.07	107.99
22	Bb	758	G	C2'-C3'-O3'	-5.69	105.16	113.70
58	C1	758	G	C3'-C2'-O2'	5.69	119.24	110.70
40	DR	103	GLU	N-CA-C	5.69	116.42	108.00
58	D1	966	G	C1'-C2'-O2'	5.69	116.94	108.40
58	D1	1452	C	C4'-C3'-O3'	-5.69	104.46	113.00
58	D1	1488	G	C4'-C3'-O3'	-5.69	104.46	113.00
58	C1	2109	G	C4'-C3'-O3'	-5.69	104.47	113.00
61	D4	40	C	C2'-C3'-O3'	-5.69	105.17	113.70
28	CB	229	VAL	CB-CA-C	-5.69	103.34	112.16
58	C1	2517	U	C1'-C2'-O2'	-5.69	103.27	111.80
56	D9	26	LYS	N-CA-C	5.69	118.57	110.10
58	D1	1545	G	C4'-C3'-O3'	-5.69	104.47	113.00
4	BD	12	CYS	CB-CA-C	5.68	121.73	110.42
58	D1	1256	G	C2'-C3'-O3'	5.68	118.03	109.50
41	CS	47	GLY	N-CA-C	5.68	118.89	110.42
58	C1	1740	C	C5'-C4'-C3'	5.68	124.52	116.00
58	D1	191	C	C4'-C3'-O3'	-5.68	104.48	113.00
58	C1	410	U	C4'-C3'-O3'	-5.68	104.48	113.00
58	D1	1170	G	C3'-C2'-O2'	5.68	119.22	110.70
58	D1	2553	A	O5'-C5'-C4'	-5.68	103.18	111.70
58	D1	44	C	C1'-C2'-O2'	5.68	116.92	108.40
58	D1	2065	C	C3'-C2'-O2'	5.67	119.21	110.70
16	AP	20	VAL	N-CA-C	5.67	115.71	107.88
45	DX	80	ILE	CB-CA-C	5.67	117.48	110.73
58	D1	2028	C	O5'-P-OP2	-5.67	90.99	108.00
58	D1	2672	G	N9-C1'-C2'	5.67	122.50	114.00
54	D7	37	ARG	N-CA-C	5.67	117.62	108.32
22	Ab	110	A	C1'-C2'-O2'	5.67	116.90	108.40
22	Ab	1485	A	C3'-C2'-O2'	5.67	119.20	110.70
58	D1	1333	U	C4'-C3'-O3'	5.67	117.90	109.40
22	Bb	131	C	C3'-C2'-O2'	5.67	119.20	110.70
58	C1	2837	C	C3'-C2'-O2'	5.66	119.19	110.70
7	AG	145	ALA	N-CA-C	-5.66	103.45	110.41
58	D1	2398	U	C1'-C2'-O2'	5.66	116.89	108.40
58	D1	2007	A	C3'-C2'-O2'	-5.66	102.21	110.70
49	CH	90	ILE	CB-CA-C	-5.65	104.64	111.88
58	D1	2260	U	C1'-C2'-O2'	-5.65	103.32	111.80
58	C1	1398	A	C2'-C3'-O3'	-5.65	105.22	113.70
58	D1	2257	G	C3'-C2'-O2'	5.65	119.18	110.70
56	C9	38	GLY	N-CA-C	-5.65	105.75	113.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	C1	286	G	C2'-C3'-O3'	5.65	117.97	109.50
58	D1	1653	A	C1'-C2'-O2'	-5.65	103.32	111.80
58	D1	192	A	C2'-C3'-O3'	5.65	117.97	109.50
58	D1	2309	A	C3'-C2'-O2'	5.65	119.17	110.70
58	C1	126	C	C1'-C2'-O2'	5.65	116.87	108.40
58	C1	461	C	C1'-C2'-O2'	5.64	116.86	108.40
29	CC	60	ASN	N-CA-C	5.64	122.81	110.80
33	DI	134	PRO	N-CA-C	5.64	119.72	111.03
58	D1	1043	C	C1'-C2'-O2'	5.64	116.86	108.40
58	D1	1049	C	C4'-C3'-O3'	-5.64	104.54	113.00
58	D1	2337	C	C2'-C3'-O3'	-5.64	105.24	113.70
58	C1	1817	A	C2'-C3'-O3'	-5.64	105.24	113.70
32	CF	113	VAL	N-CA-C	5.64	115.98	107.75
58	D1	2492	G	C2'-C3'-O3'	5.63	117.95	109.50
26	C4	23	G	C1'-C2'-O2'	5.63	116.85	108.40
58	D1	826	G	C1'-C2'-O2'	5.63	116.85	108.40
22	Ab	469	G	C2'-C3'-O3'	5.63	117.95	109.50
58	C1	2841	U	C2'-C3'-O3'	5.63	117.95	109.50
58	C1	2457	G	C3'-C2'-O2'	5.63	119.15	110.70
22	Bb	773	U	C2'-C3'-O3'	-5.63	105.26	113.70
58	C1	675	G	C2'-C3'-O3'	5.63	122.14	113.70
58	C1	2335	C	C3'-C2'-O2'	5.63	119.14	110.70
58	C1	2486	C	C2'-C3'-O3'	-5.63	105.26	113.70
58	D1	2395	G	C1'-C2'-O2'	5.63	120.24	111.80
37	CO	9	ASN	CA-C-N	-5.62	112.81	119.84
37	CO	9	ASN	C-N-CA	-5.62	112.81	119.84
58	D1	2400	G	C1'-C2'-O2'	5.62	116.84	108.40
4	BD	31	CYS	N-CA-C	-5.62	105.61	113.37
58	C1	797	A	C4'-C3'-O3'	-5.62	104.57	113.00
58	D1	448	A	C2'-C3'-O3'	-5.62	105.26	113.70
58	D1	652	G	C4'-C3'-O3'	-5.62	104.56	113.00
58	D1	2478	C	C3'-C2'-O2'	5.62	119.13	110.70
22	Bb	561	G	C3'-C2'-O2'	5.62	119.12	110.70
58	D1	2845	U	C1'-C2'-O2'	5.62	116.83	108.40
58	D1	1615	A	C3'-C2'-O2'	5.62	119.12	110.70
58	D1	1936	U	C4'-C3'-O3'	-5.62	104.58	113.00
58	D1	2603	G	O5'-P-OP2	-5.62	91.15	108.00
58	D1	183	A	C4'-C3'-O3'	-5.61	104.58	113.00
58	D1	2261	G	C2'-C3'-O3'	5.61	117.92	109.50
58	D1	1885	G	C1'-C2'-O2'	5.61	116.82	108.40
22	Bb	509	C	C1'-C2'-O2'	5.61	116.81	108.40
58	D1	2880	C	C2'-C3'-O3'	-5.61	105.29	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AA	98	LEU	N-CA-C	5.61	117.56	110.33
35	CM	46	VAL	N-CA-C	5.61	121.00	109.34
58	C1	2470	A	C1'-C2'-O2'	5.61	116.81	108.40
59	Ds	87	G	C3'-C2'-O2'	5.61	119.11	110.70
58	D1	882	G	C1'-C2'-O2'	5.61	116.81	108.40
22	Ab	472	A	C1'-C2'-O2'	5.60	116.81	108.40
58	C1	1837	G	C1'-C2'-O2'	5.60	116.80	108.40
58	C1	2647	U	C3'-C2'-O2'	5.60	119.10	110.70
58	D1	111	U	C4'-C3'-O3'	-5.60	104.60	113.00
5	BE	80	ILE	N-CA-C	5.60	118.19	108.95
58	C1	99	G	C4'-C3'-O3'	-5.60	104.60	113.00
58	D1	2080	A	C1'-C2'-O2'	5.60	116.80	108.40
58	D1	2314	G	C4'-C3'-O3'	-5.60	104.60	113.00
22	Ab	1225	C	C3'-C2'-O2'	5.60	119.10	110.70
58	C1	239	A	C1'-C2'-O2'	5.60	116.80	108.40
47	DZ	24	LEU	CA-C-N	5.60	125.60	119.89
47	DZ	24	LEU	C-N-CA	5.60	125.60	119.89
58	D1	1254	A	C2'-C3'-O3'	5.60	117.89	109.50
58	D1	2317	C	C2'-C3'-O3'	5.60	122.09	113.70
58	D1	2826	G	C1'-C2'-O2'	-5.60	100.00	108.40
58	D1	250	A	C3'-C2'-O2'	5.59	119.09	110.70
58	C1	1741	G	C2'-C3'-O3'	-5.59	105.31	113.70
58	D1	291	G	C3'-C2'-O2'	5.59	119.09	110.70
4	AD	12	CYS	N-CA-C	-5.59	98.90	110.80
58	C1	443	C	C1'-C2'-O2'	5.59	116.78	108.40
61	D4	6	G	C3'-C2'-O2'	5.59	119.08	110.70
37	DO	52	GLU	N-CA-C	5.59	122.70	110.80
59	Ds	34	U	C4'-C3'-O3'	5.59	117.78	109.40
22	Bb	105	G	C1'-C2'-O2'	5.58	116.78	108.40
58	C1	2310	G	C4'-C3'-O3'	-5.58	104.63	113.00
58	C1	2391	C	C3'-C2'-O2'	5.58	119.08	110.70
29	DC	130	GLY	N-CA-C	5.58	119.34	112.14
37	DO	8	PRO	N-CA-C	5.58	119.95	111.19
58	D1	1054	A	C3'-C2'-O2'	5.58	119.07	110.70
58	C1	2347	A	C2'-C3'-O3'	5.58	117.87	109.50
22	Ab	1038	A	C2'-C3'-O3'	-5.58	105.33	113.70
58	C1	1523	A	C3'-C2'-O2'	5.58	119.06	110.70
13	AM	47	ASP	N-CA-C	5.58	117.44	107.80
22	Bb	385	A	C2'-C3'-O3'	-5.58	105.34	113.70
58	D1	485	A	C2'-C3'-O3'	-5.58	105.34	113.70
11	AK	80	VAL	N-CA-C	5.57	115.91	108.27
58	D1	1894	U	C4'-C3'-O3'	-5.57	104.64	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	C1	469	C	C2'-C3'-O3'	-5.57	105.34	113.70
58	C1	2310	G	C2'-C3'-O3'	5.57	122.05	113.70
58	C1	2834	C	C3'-C2'-O2'	5.57	119.06	110.70
44	CW	85	VAL	N-CA-C	5.57	117.33	108.87
58	C1	202	G	O4'-C4'-C3'	-5.57	98.43	104.00
63	DW	20	VAL	CB-CA-C	-5.57	103.08	112.16
58	D1	1984	U	C1'-C2'-O2'	5.57	120.15	111.80
58	C1	39	C	C3'-C2'-O2'	5.57	119.05	110.70
28	DB	237	GLU	CB-CG-CD	5.57	122.06	112.60
58	D1	2521	C	C1'-C2'-O2'	5.57	116.75	108.40
58	D1	2620	U	C4'-C3'-O3'	5.57	117.75	109.40
22	Ab	294	A	C3'-C2'-O2'	5.56	119.05	110.70
58	D1	2503	U	C1'-C2'-O2'	5.56	116.74	108.40
58	C1	1386	U	C3'-C2'-O2'	-5.56	106.26	114.60
41	DS	80	SER	N-CA-C	5.56	122.10	109.81
58	D1	766	C	C3'-C2'-O2'	5.56	119.04	110.70
7	BG	145	ALA	N-CA-C	-5.56	103.36	110.53
4	AD	39	PRO	N-CA-C	5.56	115.80	110.47
45	DX	52	VAL	CB-CA-C	-5.56	106.17	111.06
22	Bb	379	A	C1'-C2'-O2'	5.55	116.73	108.40
22	Bb	937	A	C1'-C2'-O2'	5.55	116.73	108.40
22	Bb	939	U	C3'-C2'-O2'	5.55	119.03	110.70
61	D4	40	C	C1'-C2'-O2'	5.55	116.73	108.40
58	D1	650	U	C3'-C2'-O2'	5.55	119.03	110.70
22	Ab	1060	G	C1'-C2'-O2'	5.55	116.72	108.40
22	Bb	362	C	C4'-C3'-O3'	5.55	117.72	109.40
22	Ab	682	G	C3'-C2'-O2'	5.55	119.02	110.70
22	Bb	1463	U	C3'-C2'-O2'	5.55	119.02	110.70
58	D1	1625	A	C3'-C2'-O2'	5.55	119.02	110.70
22	Ab	739	G	C3'-C2'-O2'	5.54	119.01	110.70
22	Ab	947	A	C3'-C2'-O2'	5.54	119.01	110.70
58	C1	2133	G	C3'-C2'-O2'	5.54	119.01	110.70
58	D1	1984	U	N1-C1'-C2'	5.54	122.31	114.00
58	D1	1666	U	C2'-C3'-O3'	-5.54	105.39	113.70
58	D1	1968	C	C4'-C3'-O3'	-5.54	104.69	113.00
22	Bb	207	G	C4'-C3'-O3'	-5.54	104.69	113.00
22	Ab	508	G	C1'-C2'-O2'	5.54	116.70	108.40
58	C1	59	G	C3'-C2'-O2'	5.54	119.00	110.70
58	D1	2274	C	C1'-C2'-O2'	5.54	116.70	108.40
22	Ab	1283	U	C4'-C3'-O3'	5.53	117.70	109.40
22	Ab	408	A	O4'-C1'-C2'	5.53	113.13	107.60
58	C1	2524	G	C1'-C2'-O2'	5.53	116.70	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	D1	1539	A	C4'-C3'-O3'	5.53	121.29	113.00
58	C1	493	G	C1'-C2'-O2'	5.53	116.69	108.40
58	D1	566	C	C2'-C3'-O3'	5.53	121.99	113.70
58	C1	883	C	C1'-C2'-O2'	5.53	116.69	108.40
56	D9	49	VAL	CA-C-O	-5.53	116.22	121.64
58	D1	733	C	C2'-C3'-O3'	-5.53	105.41	113.70
58	D1	2797	C	C3'-C2'-O2'	5.53	118.99	110.70
58	D1	1625	A	C2'-C3'-O3'	5.52	121.99	113.70
58	D1	1860	C	C2'-C3'-O3'	-5.52	105.42	113.70
58	D1	1488	G	C3'-C2'-O2'	5.52	118.98	110.70
58	D1	2036	A	C1'-C2'-O2'	5.52	116.68	108.40
39	CQ	5	LYS	N-CA-C	-5.52	104.79	112.30
58	C1	1937	A	C1'-C2'-O2'	5.52	116.68	108.40
24	BC	72	LYS	CA-C-N	5.52	125.17	119.05
24	BC	72	LYS	C-N-CA	5.52	125.17	119.05
58	C1	444	G	C3'-C2'-O2'	5.51	118.97	110.70
35	DM	122	VAL	N-CA-C	5.51	116.68	108.46
22	Bb	44	C	C3'-C2'-O2'	5.51	118.97	110.70
22	Bb	331	C	C3'-C2'-O2'	5.51	118.97	110.70
58	C1	1438	A	C3'-C2'-O2'	5.51	118.97	110.70
58	C1	2400	G	C1'-C2'-O2'	5.51	116.66	108.40
53	D6	4	HIS	CA-C-N	-5.51	114.30	120.14
53	D6	4	HIS	C-N-CA	-5.51	114.30	120.14
58	C1	2851	G	C1'-C2'-O2'	5.51	116.66	108.40
58	D1	1043	C	C3'-C2'-O2'	5.51	118.96	110.70
58	C1	270	U	C2'-C3'-O3'	5.50	117.76	109.50
22	Bb	309	A	C3'-C2'-O2'	5.50	118.96	110.70
50	CK	57	ILE	CB-CA-C	-5.50	104.71	112.14
56	D9	24	ALA	N-CA-C	5.50	117.55	109.24
22	Ab	645	G	C3'-C2'-O2'	5.50	118.95	110.70
58	C1	991	G	C3'-C2'-O2'	5.50	118.95	110.70
37	DO	39	LYS	CB-CG-CD	5.50	123.95	111.30
58	D1	80	G	C1'-C2'-O2'	5.50	116.65	108.40
58	D1	1284	G	C1'-C2'-O2'	5.50	116.65	108.40
58	D1	1710	A	C4'-C3'-O3'	-5.50	104.75	113.00
28	CB	120	GLY	CA-C-N	5.49	124.84	118.85
28	CB	120	GLY	C-N-CA	5.49	124.84	118.85
36	DN	115	VAL	CB-CA-C	-5.49	104.94	111.97
58	D1	2721	C	C4'-C3'-O3'	-5.49	104.76	113.00
59	Cs	101	G	C3'-C2'-O2'	5.49	118.94	110.70
22	Bb	570	C	C3'-C2'-O2'	5.49	118.94	110.70
58	C1	1595	C	C3'-C2'-O2'	5.49	118.94	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	Ds	55	U	C3'-C2'-O2'	5.49	118.94	110.70
54	D7	13	CYS	N-CA-C	5.49	117.79	108.02
58	D1	2699	U	C2'-C3'-O3'	-5.49	105.47	113.70
22	Ab	919	G	C1'-C2'-O2'	5.49	116.63	108.40
22	Ab	920	G	C2'-C3'-O3'	-5.48	105.47	113.70
58	D1	2221	C	C2'-C3'-O3'	5.48	121.93	113.70
22	Bb	742	G	C4'-C3'-O3'	-5.48	104.78	113.00
58	C1	2727	C	C1'-C2'-O2'	5.48	116.62	108.40
58	D1	99	G	N9-C1'-C2'	5.48	120.22	112.00
58	D1	190	U	C4'-C3'-O3'	-5.48	104.78	113.00
58	D1	2267	G	C1'-C2'-O2'	5.48	116.62	108.40
22	Bb	895	G	C1'-C2'-O2'	5.48	116.62	108.40
58	D1	1811	C	C4'-C3'-O3'	-5.48	101.18	109.40
22	Ab	904	G	C1'-C2'-O2'	5.48	116.62	108.40
59	Cs	46	A	C3'-C2'-O2'	5.48	118.92	110.70
52	D5	54	LYS	CA-C-N	5.48	126.69	119.84
52	D5	54	LYS	C-N-CA	5.48	126.69	119.84
58	D1	2591	U	N1-C1'-C2'	5.47	120.21	112.00
23	B2	16	A	C3'-C2'-O2'	5.47	118.91	110.70
9	BI	104	ARG	N-CA-C	5.47	118.42	111.69
58	C1	1351	C	C1'-C2'-O2'	5.47	116.60	108.40
25	D3	73	A	C3'-C2'-O2'	5.47	118.90	110.70
58	C1	1358	U	N1-C1'-C2'	5.47	120.20	112.00
22	Ab	602	C	C1'-C2'-O2'	5.47	116.60	108.40
22	Ab	1289	U	C1'-C2'-O2'	5.47	116.60	108.40
28	DB	224	ALA	N-CA-C	-5.47	101.81	109.96
58	D1	2670	G	C4'-C3'-O3'	-5.47	104.80	113.00
41	DS	47	GLY	N-CA-C	5.46	119.51	110.55
58	D1	2841	U	C2'-C3'-O3'	5.46	117.70	109.50
42	CT	13	LYS	N-CA-C	-5.46	105.48	111.82
4	AD	9	CYS	CA-C-N	5.46	130.80	122.23
4	AD	9	CYS	C-N-CA	5.46	130.80	122.23
6	AF	60	PHE	N-CA-C	5.46	118.30	109.40
59	Ds	115	G	C3'-C2'-O2'	5.46	118.89	110.70
58	D1	158	U	N1-C1'-C2'	5.46	120.19	112.00
58	C1	2734	G	C4'-C3'-O3'	-5.46	104.81	113.00
58	D1	1815	A	C1'-C2'-O2'	5.46	116.59	108.40
22	Ab	1461	A	C3'-C2'-O2'	5.46	118.88	110.70
28	CB	210	GLY	N-CA-C	-5.46	100.25	113.18
58	C1	935	C	C2'-C3'-O3'	5.46	117.69	109.50
58	C1	1816	A	O4'-C1'-C2'	-5.46	100.34	105.80
58	C1	2880	C	C1'-C2'-O2'	5.46	116.59	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	D1	2653	G	C1'-C2'-O2'	5.46	116.59	108.40
22	Ab	1491	A	C3'-C2'-O2'	5.46	118.88	110.70
58	C1	295	U	C2'-C3'-O3'	-5.45	105.52	113.70
58	C1	566	C	C3'-C2'-O2'	5.45	118.88	110.70
58	C1	807	A	C1'-C2'-O2'	5.45	116.58	108.40
61	D4	65	G	C3'-C2'-O2'	5.45	118.88	110.70
58	D1	601	G	C3'-C2'-O2'	5.45	118.88	110.70
22	Ab	1325	G	C1'-C2'-O2'	5.45	116.58	108.40
58	D1	84	C	C2'-C3'-O3'	5.45	121.88	113.70
58	D1	755	U	C3'-C2'-O2'	5.45	118.88	110.70
58	C1	2110	U	C2'-C3'-O3'	5.45	121.87	113.70
58	D1	1060	G	C2'-C3'-O3'	-5.45	105.53	113.70
58	D1	1167	G	C2'-C3'-O3'	-5.45	105.53	113.70
22	Ab	175	U	C1'-C2'-O2'	5.45	116.57	108.40
58	C1	43	G	C1'-C2'-O2'	5.44	116.57	108.40
58	C1	2266	G	C1'-C2'-O2'	5.44	116.56	108.40
22	Ab	970	U	O4'-C4'-C3'	-5.44	100.66	106.10
26	C4	38	A	C3'-C2'-O2'	5.44	118.86	110.70
41	CS	30	VAL	CB-CA-C	-5.44	102.37	111.29
58	C1	2092	A	C2'-C3'-O3'	-5.44	105.54	113.70
58	C1	2673	A	C4'-C3'-O3'	-5.44	104.84	113.00
58	D1	594	A	C3'-C2'-O2'	5.44	118.86	110.70
58	D1	837	C	C3'-C2'-O2'	5.44	122.76	114.60
41	CS	80	SER	CA-C-N	-5.44	113.04	119.84
41	CS	80	SER	C-N-CA	-5.44	113.04	119.84
45	CX	39	ILE	CB-CA-C	-5.44	105.01	111.97
58	D1	2538	C	C2'-C3'-O3'	5.44	121.86	113.70
32	CF	115	VAL	N-CA-C	5.44	115.88	107.78
58	C1	72	A	C4'-C3'-O3'	5.44	117.55	109.40
58	C1	1693	G	C1'-C2'-O2'	-5.44	103.65	111.80
22	Bb	396	C	C3'-C2'-O2'	5.43	118.85	110.70
58	C1	73	G	C1'-C2'-O2'	5.43	116.55	108.40
48	Da	84	LEU	N-CA-C	-5.43	102.24	110.28
22	Ab	273	C	C1'-C2'-O2'	5.43	116.55	108.40
58	C1	1790	A	C1'-C2'-O2'	5.43	116.55	108.40
58	D1	2064	C	C3'-C2'-O2'	5.43	118.85	110.70
58	D1	2329	G	O4'-C4'-C3'	-5.43	98.57	104.00
58	D1	1575	G	N9-C1'-C2'	5.43	120.15	112.00
58	C1	2192	A	C4'-C3'-O3'	5.43	117.55	109.40
58	D1	2013	G	C1'-C2'-O2'	-5.43	103.66	111.80
22	Ab	44	C	C3'-C2'-O2'	5.43	118.84	110.70
22	Bb	530	G	C4'-C3'-O3'	-5.43	104.86	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	C1	2888	C	C2'-C3'-O3'	-5.43	101.36	109.50
37	DO	25	SER	CA-C-N	5.42	126.97	120.13
37	DO	25	SER	C-N-CA	5.42	126.97	120.13
58	C1	84	C	C1'-C2'-O2'	5.42	116.53	108.40
58	D1	213	A	C1'-C2'-O2'	5.42	116.53	108.40
22	Ab	929	G	C2'-C3'-O3'	-5.42	105.57	113.70
42	DT	40	PHE	N-CA-C	-5.42	105.28	111.14
22	Ab	671	A	C4'-C3'-O3'	5.42	117.53	109.40
22	Ab	674	G	C3'-C2'-O2'	5.42	118.83	110.70
22	Ab	1301	A	C2'-C3'-O3'	5.42	117.63	109.50
24	BC	75	VAL	CB-CA-C	-5.42	104.14	112.05
22	Bb	223	G	C3'-C2'-O2'	5.42	118.83	110.70
58	D1	227	U	C4'-C3'-O3'	-5.42	104.88	113.00
58	D1	988	G	C1'-C2'-O2'	-5.42	100.28	108.40
22	Ab	779	C	C2'-C3'-O3'	-5.41	105.58	113.70
58	C1	1716	C	C4'-C3'-O3'	-5.41	104.88	113.00
58	C1	2436	A	C1'-C2'-O2'	5.41	119.92	111.80
58	D1	1006	G	C3'-C2'-O2'	5.41	118.82	110.70
58	C1	2663	C	C3'-C2'-O2'	5.41	118.82	110.70
35	DM	5	VAL	N-CA-C	5.41	120.57	108.88
58	D1	820	A	C2'-C3'-O3'	-5.41	105.58	113.70
58	C1	1807	U	C2'-C3'-O3'	-5.41	105.59	113.70
58	D1	1643	C	C4'-C3'-O3'	-5.41	104.89	113.00
58	C1	210	A	C2'-C3'-O3'	-5.41	101.39	109.50
22	Bb	1047	G	C2'-C3'-O3'	-5.40	101.40	109.50
58	C1	1303	C	C2'-C3'-O3'	-5.40	105.60	113.70
58	D1	715	G	C5'-C4'-O4'	5.40	117.20	109.10
58	C1	707	C	C1'-C2'-O2'	5.40	116.50	108.40
58	D1	729	C	C2'-C3'-O3'	-5.40	105.60	113.70
58	D1	1589	C	C3'-C2'-O2'	5.40	118.80	110.70
11	AK	127	LYS	N-CA-C	-5.40	104.80	111.33
30	CD	24	LEU	CA-C-N	-5.40	113.09	119.84
30	CD	24	LEU	C-N-CA	-5.40	113.09	119.84
58	C1	324	G	C2'-C3'-O3'	5.40	117.59	109.50
58	C1	1224	C	C4'-C3'-O3'	-5.40	104.90	113.00
58	D1	321	G	C1'-C2'-O2'	5.40	116.50	108.40
58	D1	2406	C	C4'-C3'-O3'	-5.40	104.90	113.00
58	C1	225	C	C1'-C2'-O2'	5.40	116.49	108.40
58	C1	1478	U	C4'-C3'-O3'	-5.40	104.91	113.00
58	C1	790	G	C4'-C3'-O3'	-5.39	104.91	113.00
58	D1	2741	G	C2'-C3'-O3'	5.39	121.79	113.70
22	Ab	1109	U	C3'-C2'-O2'	5.39	118.79	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	Ab	1235	G	C3'-C2'-O2'	5.39	118.79	110.70
26	C4	36	A	O5'-P-OP1	5.39	124.18	108.00
22	Ab	1252	C	C3'-C2'-O2'	5.39	118.78	110.70
22	Bb	956	A	C4'-C3'-O3'	-5.39	104.92	113.00
58	C1	2008	G	C2'-C3'-O3'	5.39	121.78	113.70
58	D1	2589	G	C3'-C2'-O2'	5.39	118.78	110.70
58	C1	2035	A	C3'-C2'-O2'	5.39	118.78	110.70
58	C1	798	A	C4'-C3'-O3'	5.39	117.48	109.40
28	DB	44	ASN	N-CA-C	5.39	116.45	108.86
58	D1	547	C	C3'-C2'-O2'	5.39	118.78	110.70
58	D1	1980	G	C1'-C2'-O2'	-5.39	100.32	108.40
58	C1	177	G	C1'-C2'-O2'	5.38	116.48	108.40
58	C1	1893	G	C4'-C3'-O3'	-5.38	104.92	113.00
58	C1	2263	G	C3'-C2'-O2'	5.38	118.78	110.70
58	D1	2705	G	C2'-C3'-O3'	-5.38	105.62	113.70
37	DO	7	ARG	CA-C-N	5.38	125.14	119.76
37	DO	7	ARG	C-N-CA	5.38	125.14	119.76
58	D1	1323	A	C3'-C2'-O2'	5.38	118.77	110.70
22	Bb	456	C	C4'-C3'-O3'	5.38	117.47	109.40
35	CM	67	LEU	N-CA-C	-5.38	100.13	108.90
28	DB	240	ALA	CA-C-N	-5.38	113.12	119.84
28	DB	240	ALA	C-N-CA	-5.38	113.12	119.84
58	D1	526	A	C1'-C2'-O2'	5.38	116.47	108.40
58	D1	1424	A	O4'-C1'-C2'	5.38	112.98	107.60
58	C1	829	A	C4'-C3'-O3'	5.38	121.07	113.00
22	Ab	1337	G	C2'-C3'-O3'	-5.38	105.64	113.70
7	BG	68	ASN	N-CA-C	5.38	118.63	111.75
58	D1	449	A	C1'-C2'-O2'	5.37	116.46	108.40
58	C1	1968	C	C1'-C2'-O2'	5.37	116.46	108.40
58	C1	2791	U	C5'-C4'-O4'	5.37	117.16	109.10
9	AI	104	ARG	N-CA-C	5.37	119.91	112.45
22	Ab	483	A	C4'-C3'-O3'	5.37	117.45	109.40
37	CO	41	ARG	NE-CZ-NH2	5.37	124.03	119.20
5	BE	32	VAL	N-CA-C	5.37	116.39	108.45
58	C1	1452	C	C4'-C3'-O3'	-5.37	104.95	113.00
58	C1	2013	G	C1'-C2'-O2'	-5.37	103.75	111.80
47	DZ	124	ILE	N-CA-C	5.37	116.64	108.80
50	DK	11	GLU	N-CA-C	5.37	117.13	111.28
58	D1	140	C	C3'-C2'-O2'	5.37	118.75	110.70
58	D1	621	G	C3'-C2'-O2'	5.37	118.75	110.70
22	Ab	1167	G	C3'-C2'-O2'	5.36	118.75	110.70
58	C1	2388	A	C3'-C2'-O2'	5.36	118.75	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	Cs	116	G	C2'-C3'-O3'	5.36	121.74	113.70
58	D1	967	U	C1'-C2'-O2'	5.36	116.44	108.40
22	Bb	31	U	C4'-C3'-O3'	5.36	117.44	109.40
58	C1	1908	C	C1'-C2'-O2'	5.36	116.44	108.40
22	Ab	854	G	C3'-C2'-O2'	5.36	118.73	110.70
58	C1	1377	G	C2'-C3'-O3'	5.36	117.54	109.50
58	C1	1802	G	C1'-C2'-O2'	5.36	116.44	108.40
58	D1	610	U	C4'-C3'-O3'	-5.36	104.96	113.00
22	Ab	337	C	C3'-C2'-O2'	5.36	118.73	110.70
58	C1	2318	G	C2'-C3'-O3'	5.36	121.73	113.70
58	D1	1844	G	C4'-C3'-O3'	-5.36	104.97	113.00
58	D1	2060	C	C2'-C3'-O3'	-5.36	105.67	113.70
8	BH	93	VAL	N-CA-C	5.35	115.83	108.12
58	D1	611	C	C3'-C2'-O2'	5.35	118.73	110.70
22	Ab	489	G	C1'-C2'-O2'	5.35	116.42	108.40
58	C1	118	G	C4'-C3'-O3'	-5.35	104.98	113.00
58	C1	1332	A	C2'-C3'-O3'	-5.35	105.68	113.70
58	D1	2500	G	C3'-C2'-O2'	5.35	118.72	110.70
22	Ab	214	C	C3'-C2'-O2'	5.34	118.72	110.70
22	Ab	989	G	C3'-C2'-O2'	5.34	118.72	110.70
26	C4	36	A	O5'-C5'-C4'	5.34	119.52	111.50
31	CE	180	PHE	N-CA-C	5.34	117.68	109.07
58	D1	906	U	C3'-C2'-O2'	5.34	118.72	110.70
58	D1	2595	U	C2'-C3'-O3'	-5.34	105.69	113.70
58	C1	1956	G	C4'-C3'-O3'	-5.34	104.98	113.00
58	C1	372	G	C2'-C3'-O3'	5.34	121.71	113.70
58	D1	47	A	C1'-C2'-O2'	-5.34	103.79	111.80
22	Bb	536	U	C1'-C2'-O2'	5.34	116.41	108.40
58	C1	1382	G	C1'-C2'-O2'	5.34	116.41	108.40
58	D1	1076	G	C3'-C2'-O2'	5.34	118.71	110.70
58	C1	191	C	C3'-C2'-O2'	-5.34	102.69	110.70
12	BL	18	VAL	N-CA-C	5.34	120.44	109.34
31	CE	88	ILE	CA-C-N	5.34	127.89	121.38
31	CE	88	ILE	C-N-CA	5.34	127.89	121.38
58	C1	715	G	C3'-C2'-O2'	-5.34	106.60	114.60
58	C1	1549	C	C4'-C3'-O3'	5.34	117.41	109.40
58	C1	2594	G	C1'-C2'-O2'	-5.34	100.39	108.40
58	D1	347	A	C1'-C2'-O2'	5.34	116.41	108.40
22	Bb	1031	G	C3'-C2'-O2'	5.33	118.70	110.70
58	C1	769	G	C3'-C2'-O2'	5.33	118.70	110.70
58	D1	2035	A	C1'-C2'-O2'	5.33	116.40	108.40
22	Bb	52	A	C2'-C3'-O3'	5.33	117.50	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	C1	2709	U	C4'-C3'-O3'	-5.33	105.00	113.00
27	CA	49	ILE	CB-CA-C	-5.33	105.00	111.88
58	D1	1164	C	C3'-C2'-O2'	5.33	118.69	110.70
22	Bb	388	G	C1'-C2'-O2'	5.33	116.39	108.40
26	C4	3	C	O4'-C1'-C2'	-5.33	102.27	107.60
58	D1	1975	G	C2'-C3'-O3'	5.33	117.49	109.50
58	D1	1197	C	C3'-C2'-O2'	5.33	118.69	110.70
58	D1	2599	G	C1'-C2'-O2'	5.33	116.39	108.40
22	Bb	721	A	C1'-C2'-O2'	5.32	116.39	108.40
38	DP	77	LYS	CA-C-N	5.32	126.49	119.84
38	DP	77	LYS	C-N-CA	5.32	126.49	119.84
22	Bb	600	G	C1'-C2'-O2'	5.32	116.38	108.40
58	C1	282	G	C4'-C3'-O3'	-5.32	105.02	113.00
58	C1	780	A	C3'-C2'-O2'	5.32	118.68	110.70
58	C1	1575	G	N9-C1'-C2'	5.32	119.97	112.00
58	C1	1998	A	C1'-C2'-O2'	5.32	116.38	108.40
59	Cs	66	A	C4'-C3'-O3'	-5.32	101.43	109.40
58	C1	415	G	C3'-C2'-O2'	5.31	118.67	110.70
58	D1	705	C	C1'-C2'-O2'	5.31	116.37	108.40
22	Bb	1217	U	C2'-C3'-O3'	-5.31	105.73	113.70
58	C1	1233	A	C4'-C3'-O3'	-5.31	105.03	113.00
22	Bb	1412	C	C3'-C2'-O2'	5.31	118.66	110.70
30	CD	83	PHE	N-CA-C	5.31	119.52	112.30
58	D1	2609	A	C2'-C3'-O3'	5.31	121.66	113.70
58	D1	2241	G	C1'-C2'-O2'	5.31	116.36	108.40
58	C1	609	C	C4'-C3'-O3'	5.30	117.36	109.40
58	C1	1650	C	C3'-C2'-O2'	5.30	118.66	110.70
59	Ds	19	G	C3'-C2'-O2'	5.30	118.66	110.70
22	Ab	537	A	C1'-C2'-O2'	5.30	116.36	108.40
58	C1	1926	C	C3'-C2'-O2'	5.30	118.65	110.70
58	D1	2453	C	C1'-C2'-O2'	5.30	116.35	108.40
22	Bb	776	A	O4'-C1'-C2'	-5.30	100.50	105.80
22	Bb	1491	A	C1'-C2'-O2'	5.30	116.35	108.40
58	D1	2590	C	C3'-C2'-O2'	5.30	118.65	110.70
58	C1	2252	A	C1'-C2'-O2'	5.30	116.35	108.40
22	Ab	1336	C	C3'-C2'-O2'	5.30	118.64	110.70
4	AD	87	GLY	N-CA-C	-5.29	106.36	112.29
58	C1	2420	G	C1'-C2'-O2'	5.29	116.34	108.40
58	C1	2801	C	C3'-C2'-O2'	5.29	118.64	110.70
22	Ab	699	A	C3'-C2'-O2'	5.29	118.63	110.70
58	C1	1538	C	N1-C1'-C2'	5.29	121.93	114.00
58	D1	521	A	C1'-C2'-O2'	5.29	116.33	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	AH	112	LEU	N-CA-C	5.29	117.11	108.76
58	D1	1683	A	C1'-C2'-O2'	-5.29	100.47	108.40
58	D1	2463	C	C4'-C3'-O3'	-5.29	105.07	113.00
58	C1	1451	U	C4'-C3'-O3'	-5.28	105.08	113.00
58	D1	2088	G	C4'-C3'-O3'	5.28	117.33	109.40
43	DU	41	GLY	N-CA-C	-5.28	103.25	111.12
58	D1	2111	G	C3'-C2'-O2'	5.28	118.62	110.70
58	D1	1917	G	C2'-C3'-O3'	-5.28	105.78	113.70
37	CO	15	ARG	N-CA-C	5.28	118.30	107.37
58	D1	2416	G	C2'-C3'-O3'	5.28	121.62	113.70
58	D1	1223	C	C4'-C3'-O3'	-5.28	105.08	113.00
54	C7	45	LYS	N-CA-C	5.28	117.88	110.23
56	C9	49	VAL	CA-C-O	-5.28	115.69	121.28
58	C1	2080	A	C1'-C2'-O2'	5.28	116.31	108.40
58	C1	662	G	C2'-C3'-O3'	-5.27	105.79	113.70
58	C1	2215	G	C4'-C3'-O3'	-5.27	105.09	113.00
4	BD	26	CYS	N-CA-CB	5.27	119.39	110.49
58	C1	1709	C	C2'-C3'-O3'	5.27	121.60	113.70
22	Ab	760	G	C3'-C2'-O2'	5.27	118.60	110.70
58	C1	884	C	C1'-C2'-O2'	5.27	116.30	108.40
58	D1	1397	U	C2'-C3'-O3'	-5.26	105.80	113.70
58	D1	2568	G	C1'-C2'-O2'	5.26	116.30	108.40
58	C1	2613	A	C1'-C2'-O2'	5.26	119.69	111.80
58	D1	1163	C	C3'-C2'-O2'	5.26	118.59	110.70
58	D1	983	G	C1'-C2'-O2'	5.26	116.29	108.40
59	Cs	63	G	C3'-C2'-O2'	5.26	118.59	110.70
47	DZ	98	MET	N-CA-C	5.26	115.48	108.38
58	D1	493	G	C2'-C3'-O3'	-5.26	105.81	113.70
22	Bb	1465	G	C3'-C2'-O2'	5.26	118.58	110.70
58	C1	267	G	C2'-C3'-O3'	-5.26	105.81	113.70
58	C1	2808	U	C1'-C2'-O2'	5.26	116.28	108.40
59	Cs	11	C	C2'-C3'-O3'	-5.26	105.81	113.70
22	Ab	635	C	C4'-C3'-O3'	-5.25	105.12	113.00
22	Bb	552	G	C2'-C3'-O3'	-5.25	105.82	113.70
22	Bb	1056	U	C1'-C2'-O2'	5.25	116.28	108.40
58	D1	2031	G	C1'-C2'-O2'	5.25	116.28	108.40
58	C1	2591	U	N1-C1'-C2'	5.25	119.87	112.00
22	Ab	1077	G	C2'-C3'-O3'	5.25	117.37	109.50
22	Ab	1475	G	C3'-C2'-O2'	5.25	118.57	110.70
58	D1	518	G	C1'-C2'-O2'	5.25	116.27	108.40
58	D1	776	C	C1'-C2'-O2'	5.25	116.27	108.40
7	AG	75	VAL	N-CA-C	5.25	115.51	108.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	D1	1348	G	C3'-C2'-O2'	5.25	118.57	110.70
58	C1	584	U	C3'-C2'-O2'	-5.24	106.73	114.60
41	DS	2	ASN	N-CA-C	5.24	119.16	112.34
58	D1	832	C	C1'-C2'-O2'	5.24	116.26	108.40
22	Ab	547	A	C4'-C3'-O3'	-5.24	105.14	113.00
58	C1	2319	G	C2'-C3'-O3'	-5.24	105.84	113.70
22	Ab	1414	C	C3'-C2'-O2'	5.24	118.56	110.70
58	C1	1405	A	C2'-C3'-O3'	5.24	121.56	113.70
59	Ds	118	G	C3'-C2'-O2'	5.24	118.56	110.70
58	D1	2727	C	C3'-C2'-O2'	5.24	118.56	110.70
47	CZ	38	TYR	N-CA-C	5.24	118.21	107.37
22	Bb	1508	G	C3'-C2'-O2'	5.24	118.55	110.70
56	C9	56	GLU	CB-CA-C	-5.23	102.05	110.74
58	C1	1720	G	C2'-C3'-O3'	5.23	117.35	109.50
58	D1	537	A	C4'-C3'-O3'	-5.23	105.15	113.00
58	D1	1155	G	C2'-C3'-O3'	5.23	117.35	109.50
33	CI	138	ILE	CB-CA-C	-5.23	105.84	111.59
58	D1	2335	C	C4'-C3'-O3'	-5.23	105.16	113.00
58	D1	2669	C	C1'-C2'-O2'	5.23	116.24	108.40
52	D5	57	ILE	N-CA-C	5.23	115.50	107.77
58	C1	784	G	C2'-C3'-O3'	-5.22	105.86	113.70
58	D1	632	G	C3'-C2'-O2'	5.22	118.54	110.70
58	D1	2029	C	C1'-C2'-O2'	5.22	116.24	108.40
58	D1	2288	G	C1'-C2'-O2'	5.22	116.24	108.40
58	D1	366	C	C3'-C2'-O2'	5.22	118.53	110.70
58	D1	721	A	C4'-C3'-O3'	-5.22	105.17	113.00
22	Ab	719	C	C3'-C2'-O2'	5.22	118.53	110.70
30	DD	13	SER	CA-C-N	5.22	126.37	119.84
30	DD	13	SER	C-N-CA	5.22	126.37	119.84
58	D1	1590	A	C1'-C2'-O2'	5.22	116.23	108.40
16	AP	33	ILE	CB-CA-C	-5.22	105.20	112.04
22	Ab	285	G	C2'-C3'-O3'	-5.22	105.87	113.70
8	AH	73	ASP	CA-C-N	5.22	126.36	119.84
8	AH	73	ASP	C-N-CA	5.22	126.36	119.84
4	BD	11	LEU	N-CA-C	-5.22	106.60	113.12
58	C1	1988	C	C1'-C2'-O2'	-5.22	100.57	108.40
58	D1	1064	U	C1'-C2'-O2'	-5.22	100.57	108.40
22	Bb	113	A	C4'-C3'-O3'	5.22	117.22	109.40
58	C1	536	G	C3'-C2'-O2'	-5.22	106.78	114.60
36	DN	89	ASN	N-CA-C	5.22	117.71	111.71
22	Ab	1395	C	C3'-C2'-O2'	5.21	118.52	110.70
58	D1	2052	A	C2'-C3'-O3'	5.21	117.32	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	C1	1075	G	C3'-C2'-O2'	5.21	118.52	110.70
39	DQ	5	LYS	N-CA-C	-5.21	104.73	111.71
58	D1	562	G	C1'-C2'-O2'	5.21	116.22	108.40
64	DV	15	G	C4'-C3'-O3'	5.21	117.22	109.40
58	C1	1991	A	C2'-C3'-O3'	-5.21	101.69	109.50
58	C1	58	G	C3'-C2'-O2'	-5.21	106.79	114.60
58	C1	2547	G	C3'-C2'-O2'	5.21	118.51	110.70
58	D1	1836	C	C1'-C2'-O2'	5.21	116.21	108.40
58	C1	1260	G	C2'-C3'-O3'	-5.21	105.89	113.70
58	D1	1533	G	C4'-C3'-O3'	-5.21	105.19	113.00
58	C1	653	G	C2'-C3'-O3'	5.20	121.50	113.70
22	Ab	744	G	C1'-C2'-O2'	5.20	116.20	108.40
9	BI	25	LYS	N-CA-C	5.20	117.63	110.35
46	CY	11	ASP	N-CA-C	5.20	115.40	108.38
58	C1	2618	G	C1'-C2'-O2'	5.20	116.20	108.40
26	C4	44	A	C2'-C3'-O3'	-5.20	105.90	113.70
6	AF	6	VAL	CB-CA-C	-5.20	104.65	111.25
49	DH	4	VAL	N-CA-C	5.19	116.14	108.45
58	D1	864	G	C2'-C3'-O3'	-5.19	105.91	113.70
58	D1	1727	G	C1'-C2'-O2'	-5.19	104.01	111.80
58	D1	1783	G	C3'-C2'-O2'	-5.19	102.91	110.70
12	AL	24	VAL	CA-C-N	5.19	126.33	119.84
12	AL	24	VAL	C-N-CA	5.19	126.33	119.84
58	C1	878	G	C2'-C3'-O3'	-5.19	105.91	113.70
58	D1	824	G	C4'-C3'-O3'	-5.19	105.22	113.00
22	Ab	1303	C	C3'-C2'-O2'	5.19	118.48	110.70
22	Ab	1361	C	C4'-C3'-O3'	-5.19	105.22	113.00
4	BD	25	ARG	CA-C-O	-5.19	115.55	121.00
58	C1	1791	C	C2'-C3'-O3'	-5.19	105.92	113.70
58	C1	2386	G	C3'-C2'-O2'	5.19	118.48	110.70
58	D1	1008	C	C3'-C2'-O2'	-5.19	102.92	110.70
22	Ab	1309	C	C3'-C2'-O2'	5.18	118.48	110.70
53	C6	49	CYS	CA-CB-SG	5.18	126.33	114.40
37	DO	15	ARG	CA-C-O	5.18	125.74	120.24
58	D1	395	C	C1'-C2'-O2'	5.18	116.17	108.40
22	Bb	1236	C	C2'-C3'-O3'	5.18	121.47	113.70
12	AL	105	TYR	CB-CA-C	-5.18	110.18	117.23
20	AU	96	GLY	N-CA-C	5.18	125.46	113.18
22	Bb	1025	G	C3'-C2'-O2'	5.18	118.47	110.70
22	Bb	1334	C	C4'-C3'-O3'	-5.18	105.23	113.00
4	BD	145	GLU	N-CA-C	5.18	116.92	108.63
4	AD	31	CYS	N-CA-CB	5.18	119.24	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	Ab	701	C	C2'-C3'-O3'	5.18	117.26	109.50
20	BU	12	ALA	N-CA-C	-5.18	106.65	113.17
44	CW	100	THR	N-CA-C	5.18	116.94	108.76
58	C1	624	G	C3'-C2'-O2'	5.18	118.47	110.70
58	C1	2557	U	C4'-C3'-O3'	-5.18	105.23	113.00
58	D1	1532	G	C3'-C2'-O2'	5.18	118.46	110.70
58	D1	1540	A	C1'-C2'-O2'	5.18	116.16	108.40
22	Ab	444	C	C1'-C2'-O2'	5.17	116.16	108.40
58	D1	474	A	C2'-C3'-O3'	-5.17	105.94	113.70
58	C1	2435	C	C3'-C2'-O2'	5.17	118.46	110.70
22	Bb	955	A	C1'-C2'-O2'	5.17	116.16	108.40
58	C1	2178	G	C4'-C3'-O3'	-5.17	105.24	113.00
58	D1	106	G	C1'-C2'-O2'	5.17	116.16	108.40
58	D1	843	C	C2'-C3'-O3'	-5.17	105.94	113.70
58	D1	2065	C	C1'-C2'-O2'	-5.17	100.64	108.40
58	D1	378	G	C1'-C2'-O2'	5.17	116.16	108.40
22	Ab	1277	G	C3'-C2'-O2'	5.17	118.45	110.70
22	Bb	940	C	C3'-C2'-O2'	5.17	118.45	110.70
29	CC	102	VAL	N-CA-C	5.17	116.16	108.46
58	C1	2677	C	C1'-C2'-O2'	5.17	116.15	108.40
62	DA	47	LEU	N-CA-C	5.17	114.43	108.49
58	C1	1416	G	C4'-C3'-O3'	-5.16	105.25	113.00
58	D1	1817	A	C1'-C2'-O2'	5.16	116.15	108.40
58	D1	2091	G	C3'-C2'-O2'	5.16	118.44	110.70
22	Bb	544	U	C2'-C3'-O3'	5.16	121.44	113.70
22	Bb	1211	A	C1'-C2'-O2'	5.16	116.14	108.40
58	C1	1381	A	C1'-C2'-O2'	5.16	116.14	108.40
58	C1	1415	C	C4'-C3'-O3'	-5.16	105.26	113.00
58	C1	2446	A	C1'-C2'-O2'	5.16	116.14	108.40
58	C1	2589	G	C1'-C2'-O2'	5.16	116.14	108.40
58	C1	2839	G	C2'-C3'-O3'	5.16	121.44	113.70
58	C1	1361	U	C3'-C2'-O2'	5.16	118.44	110.70
22	Ab	1380	C	C3'-C2'-O2'	5.16	118.44	110.70
28	CB	75	ILE	N-CA-C	-5.16	104.19	108.63
29	DC	59	VAL	N-CA-C	5.16	118.10	113.10
58	D1	2090	G	C3'-C2'-O2'	5.16	118.44	110.70
22	Ab	673	C	C3'-C2'-O2'	5.16	118.43	110.70
30	CD	21	ALA	N-CA-C	5.16	121.78	110.80
56	C9	47	LYS	N-CA-C	5.16	116.64	108.96
58	C1	487	C	C1'-C2'-O2'	5.16	116.13	108.40
28	DB	235	GLY	N-CA-C	5.16	118.27	111.52
58	D1	231	U	C2'-C3'-O3'	-5.16	105.97	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	Ab	1418	G	C3'-C2'-O2'	5.15	118.43	110.70
35	CM	122	VAL	N-CA-C	5.15	115.27	107.75
42	DT	15	LYS	N-CA-CB	5.15	119.07	110.41
58	D1	2342	G	C3'-C2'-O2'	5.15	118.43	110.70
58	D1	2462	A	C3'-C2'-O2'	5.15	118.43	110.70
22	Ab	1286	G	C1'-C2'-O2'	-5.15	100.67	108.40
25	C3	1	G	C5'-C4'-C3'	5.15	123.72	116.00
58	C1	1323	A	C3'-C2'-O2'	5.15	118.43	110.70
58	D1	751	A	C3'-C2'-O2'	5.15	118.43	110.70
58	D1	2371	A	C2'-C3'-O3'	-5.15	105.97	113.70
58	C1	789	G	C3'-C2'-O2'	-5.15	102.98	110.70
22	Ab	6	U	C5'-C4'-C3'	5.15	122.92	115.20
22	Bb	898	U	C1'-C2'-O2'	5.15	116.12	108.40
58	D1	2450	A	C2'-C3'-O3'	-5.15	101.78	109.50
2	AA	21	ARG	N-CA-C	5.15	116.56	107.61
58	D1	109	U	C4'-C3'-O3'	-5.15	105.28	113.00
58	C1	917	U	C4'-C3'-O3'	-5.14	105.28	113.00
58	C1	2337	C	C1'-C2'-O2'	5.14	116.12	108.40
35	DM	109	LYS	N-CA-C	5.14	119.56	113.28
58	D1	99	G	C4'-C3'-O3'	-5.14	105.28	113.00
28	CB	41	GLY	N-CA-C	-5.14	103.56	111.64
58	C1	574	G	C3'-C2'-O2'	5.14	118.41	110.70
58	C1	1663	A	C4'-C3'-O3'	5.14	117.11	109.40
58	D1	2738	U	C1'-C2'-O2'	-5.14	104.09	111.80
58	D1	2221	C	C3'-C2'-O2'	5.14	118.41	110.70
22	Ab	336	U	C1'-C2'-O2'	5.14	116.11	108.40
58	C1	1005	C	C4'-C3'-O3'	5.14	117.11	109.40
58	C1	2715	C	C3'-C2'-O2'	5.14	118.41	110.70
58	D1	363	A	C1'-C2'-O2'	-5.14	100.69	108.40
58	D1	2098	A	C3'-C2'-O2'	5.14	118.41	110.70
22	Ab	595	A	C3'-C2'-O2'	5.14	118.40	110.70
46	CY	87	LYS	N-CA-C	5.13	116.96	111.36
22	Bb	728	C	C3'-C2'-O2'	5.13	118.40	110.70
58	C1	253	A	N9-C1'-C2'	5.13	121.70	114.00
58	D1	1704	C	C1'-C2'-O2'	5.13	116.10	108.40
58	C1	2801	C	O4'-C4'-C3'	5.13	109.13	104.00
58	D1	1647	U	C3'-C2'-O2'	-5.13	106.91	114.60
22	Bb	6	U	C5'-C4'-C3'	5.13	122.89	115.20
32	CF	168	PRO	N-CA-C	5.13	123.03	112.47
58	D1	1802	G	C1'-C2'-O2'	5.13	116.09	108.40
58	D1	1984	U	C2'-C3'-O3'	5.13	117.19	109.50
58	C1	1520	C	C1'-C2'-O2'	5.12	116.09	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	C1	1539	A	C3'-C2'-O2'	5.12	118.39	110.70
28	DB	101	GLU	N-CA-C	5.12	117.47	110.24
58	D1	2419	U	C3'-C2'-O2'	5.12	118.39	110.70
58	C1	1268	G	C2'-C3'-O3'	5.12	121.38	113.70
58	C1	1330	G	C4'-C3'-O3'	-5.12	105.31	113.00
58	C1	1345	U	C5'-C4'-O4'	5.12	116.78	109.10
58	C1	1745	G	C3'-C2'-O2'	-5.12	106.92	114.60
58	D1	497	A	C1'-C2'-O2'	5.12	116.08	108.40
22	Ab	1402	G	C3'-C2'-O2'	5.12	118.38	110.70
22	Bb	1421	G	C3'-C2'-O2'	5.12	118.38	110.70
32	CF	155	SER	N-CA-C	5.12	121.70	110.80
58	D1	589	A	C2'-C3'-O3'	5.12	121.38	113.70
32	DF	50	VAL	CB-CA-C	-5.12	102.90	111.29
58	C1	872	U	C2'-C3'-O3'	-5.12	106.03	113.70
58	C1	2782	G	C1'-C2'-O2'	5.12	116.07	108.40
59	Cs	15	A	C1'-C2'-O2'	-5.12	104.13	111.80
58	D1	1866	C	C3'-C2'-O2'	5.12	118.37	110.70
22	Bb	289	G	C3'-C2'-O2'	5.11	118.37	110.70
22	Bb	387	G	C3'-C2'-O2'	5.11	118.37	110.70
40	CR	50	SER	N-CA-C	5.11	116.07	108.60
58	D1	722	A	C1'-C2'-O2'	5.11	116.07	108.40
59	Cs	86	G	C3'-C2'-O2'	5.11	118.37	110.70
58	D1	874	U	C4'-C3'-O3'	-5.11	105.33	113.00
22	Bb	782	G	C1'-C2'-O2'	5.11	116.06	108.40
22	Bb	811	U	C2'-C3'-O3'	-5.11	106.04	113.70
58	D1	965	G	C1'-C2'-O2'	5.11	116.07	108.40
58	D1	1968	C	C1'-C2'-O2'	5.11	116.07	108.40
58	D1	482	A	C2'-C3'-O3'	5.11	117.16	109.50
5	AE	48	ALA	CA-C-N	5.11	126.22	119.84
5	AE	48	ALA	C-N-CA	5.11	126.22	119.84
58	D1	1711	A	C1'-C2'-O2'	5.11	116.06	108.40
58	D1	496	A	C2'-C3'-O3'	-5.10	106.05	113.70
58	D1	2034	A	C3'-C2'-O2'	5.10	118.36	110.70
58	C1	518	G	C3'-C2'-O2'	5.10	118.35	110.70
58	C1	2838	C	C2'-C3'-O3'	5.10	121.35	113.70
35	DM	46	VAL	N-CA-C	5.10	119.95	109.34
22	Bb	808	C	C4'-C3'-O3'	5.10	120.65	113.00
58	D1	789	G	C3'-C2'-O2'	-5.10	103.05	110.70
4	BD	8	VAL	N-CA-C	5.10	116.27	111.48
20	BU	74	LYS	CB-CA-C	-5.10	109.72	115.79
42	CT	117	GLN	N-CA-C	5.10	116.48	107.61
58	D1	1566	G	C2'-C3'-O3'	5.10	121.35	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	CY	60	PHE	N-CA-C	5.10	116.98	110.61
58	D1	2793	A	C1'-C2'-O2'	5.10	116.05	108.40
16	AP	3	LYS	N-CA-C	5.10	116.93	109.24
33	CI	62	LYS	N-CA-C	-5.10	107.01	113.43
58	C1	716	A	C2'-C3'-O3'	5.10	117.14	109.50
58	C1	1189	G	C2'-C3'-O3'	-5.10	106.06	113.70
58	C1	2473	U	C3'-C2'-O2'	5.10	118.34	110.70
58	C1	2821	G	C1'-C2'-O2'	5.10	116.04	108.40
58	D1	2754	C	C3'-C2'-O2'	5.09	118.34	110.70
58	D1	1981	A	C1'-C2'-O2'	5.09	116.04	108.40
22	Bb	800	A	C1'-C2'-O2'	5.09	116.04	108.40
58	C1	116	A	C2'-C3'-O3'	5.09	117.14	109.50
58	C1	2684	G	C2'-C3'-O3'	-5.09	106.06	113.70
22	Bb	1051	G	C3'-C2'-O2'	5.09	118.33	110.70
16	BP	20	VAL	N-CA-C	5.09	114.90	107.88
58	C1	385	U	O4'-C1'-C2'	-5.09	102.51	107.60
58	D1	716	A	C1'-C2'-O2'	5.09	119.44	111.80
58	D1	2553	A	C5'-C4'-C3'	5.09	122.83	115.20
42	DT	17	ILE	N-CA-C	5.09	115.75	110.82
10	AJ	62	HIS	N-CA-C	5.09	116.97	108.99
26	C4	30	G	C1'-C2'-O2'	5.09	116.03	108.40
58	C1	1744	A	C4'-C3'-O3'	-5.09	101.77	109.40
32	DF	158	HIS	N-CA-C	5.09	121.63	110.80
22	Ab	1043	C	C2'-C3'-O3'	-5.08	106.07	113.70
22	Bb	652	G	C2'-C3'-O3'	-5.08	106.07	113.70
22	Bb	922	G	C4'-C3'-O3'	-5.08	105.37	113.00
35	CM	21	LYS	N-CA-C	5.08	118.02	110.14
58	C1	242	G	C1'-C2'-O2'	5.08	116.03	108.40
58	D1	2552	A	C3'-C2'-O2'	5.08	118.32	110.70
29	CC	132	HIS	CA-C-N	-5.08	115.09	122.86
29	CC	132	HIS	C-N-CA	-5.08	115.09	122.86
58	C1	2832	A	C3'-C2'-O2'	5.08	118.32	110.70
59	Cs	110	G	C1'-C2'-O2'	5.08	116.02	108.40
58	D1	2863	G	C3'-C2'-O2'	5.08	118.32	110.70
58	D1	782	C	C2'-C3'-O3'	-5.08	106.08	113.70
58	D1	1710	A	N9-C1'-C2'	5.08	119.62	112.00
40	CR	23	ARG	N-CA-C	5.08	121.61	110.80
58	D1	860	C	C3'-C2'-O2'	5.08	118.31	110.70
58	D1	2226	G	C3'-C2'-O2'	5.08	118.31	110.70
26	C4	4	G	C4'-C3'-O3'	5.07	117.01	109.40
40	DR	59	LYS	N-CA-C	5.07	121.61	110.80
22	Ab	1190	C	C1'-C2'-O2'	5.07	116.01	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	DQ	38	VAL	N-CA-CB	5.07	113.92	110.52
58	D1	49	G	C1'-C2'-O2'	-5.07	104.19	111.80
4	AD	9	CYS	CA-CB-SG	5.07	126.06	114.40
25	C3	73	A	C3'-C2'-O2'	5.07	118.30	110.70
57	D0	3	VAL	N-CA-C	5.07	115.99	108.23
22	Ab	495	C	C4'-C3'-O3'	-5.07	101.80	109.40
58	C1	1029	A	C1'-C2'-O2'	5.07	116.00	108.40
58	D1	1233	A	C1'-C2'-O2'	5.07	116.00	108.40
8	BH	79	VAL	N-CA-C	-5.07	106.74	111.45
9	BI	55	ALA	N-CA-C	5.07	116.44	109.15
47	CZ	146	ILE	N-CA-C	5.06	119.87	109.34
46	CY	35	TYR	N-CA-C	5.06	118.11	111.28
58	C1	2260	U	C3'-C2'-O2'	-5.06	107.01	114.60
58	D1	1037	C	C3'-C2'-O2'	5.06	118.29	110.70
22	Bb	1293	G	C3'-C2'-O2'	5.06	118.29	110.70
45	DX	23	GLU	N-CA-C	-5.06	103.25	110.59
58	D1	499	G	C3'-C2'-O2'	-5.06	107.01	114.60
35	CM	5	VAL	N-CA-C	5.06	119.80	108.88
58	C1	1691	G	C1'-C2'-O2'	5.06	115.98	108.40
58	C1	2052	A	C4'-C3'-O3'	-5.06	105.42	113.00
58	D1	190	U	C3'-C2'-O2'	5.06	118.28	110.70
58	C1	2511	U	C2'-C3'-O3'	-5.05	106.12	113.70
58	D1	45	C	C1'-C2'-O2'	5.05	115.98	108.40
58	D1	2636	G	C1'-C2'-O2'	5.05	115.98	108.40
5	AE	26	PHE	N-CA-C	5.05	117.96	110.48
22	Ab	730	A	C3'-C2'-O2'	5.05	118.28	110.70
22	Ab	1251	A	C3'-C2'-O2'	5.05	118.28	110.70
58	C1	2278	A	N9-C1'-C2'	5.05	119.58	112.00
58	C1	38	C	C3'-C2'-O2'	5.05	118.27	110.70
58	D1	481	C	C2'-C3'-O3'	5.05	117.07	109.50
58	C1	906	U	C4'-C3'-O3'	-5.05	105.43	113.00
58	C1	151	G	C3'-C2'-O2'	5.05	118.27	110.70
58	C1	1669	G	C2'-C3'-O3'	-5.05	106.13	113.70
58	D1	147	C	C2'-C3'-O3'	5.05	121.27	113.70
58	D1	1943	G	C1'-C2'-O2'	5.05	115.97	108.40
58	D1	780	A	C2'-C3'-O3'	-5.04	106.13	113.70
58	D1	1298	A	C2'-C3'-O3'	5.04	117.06	109.50
22	Ab	430	U	C1'-C2'-O2'	5.04	115.96	108.40
22	Ab	544	U	C2'-C3'-O3'	5.04	121.26	113.70
28	DB	60	ARG	N-CA-C	5.04	117.61	108.69
54	D7	45	LYS	N-CA-C	5.04	121.54	110.80
58	D1	1227	G	C4'-C3'-O3'	-5.04	105.44	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	D1	1835	U	C2'-C3'-O3'	-5.04	106.14	113.70
40	CR	59	LYS	N-CA-C	5.04	121.53	110.80
58	C1	2083	A	C2'-C3'-O3'	-5.04	101.94	109.50
22	Ab	132	C	C1'-C2'-O2'	5.04	115.96	108.40
22	Ab	1356	G	C1'-C2'-O2'	5.04	115.96	108.40
58	C1	260	A	C1'-C2'-O2'	5.04	115.96	108.40
58	D1	1248	A	N9-C1'-C2'	5.04	121.56	114.00
58	D1	1468	G	C3'-C2'-O2'	5.04	118.26	110.70
58	D1	1691	G	C1'-C2'-O2'	5.04	115.96	108.40
58	D1	2657	C	C3'-C2'-O2'	5.04	118.26	110.70
22	Ab	1355	U	C2'-C3'-O3'	-5.04	106.14	113.70
22	Ab	376	G	C4'-C3'-O3'	5.04	120.55	113.00
22	Ab	700	A	C1'-C2'-O2'	5.04	115.95	108.40
5	BE	67	VAL	N-CA-C	5.04	115.62	108.42
58	C1	2291	G	C3'-C2'-O2'	5.04	118.25	110.70
58	C1	2778	G	C3'-C2'-O2'	5.04	118.25	110.70
58	D1	1878	A	C1'-C2'-O2'	5.04	115.95	108.40
58	D1	2147	A	C2'-C3'-O3'	5.04	117.05	109.50
32	CF	121	ILE	N-CA-C	5.03	115.96	108.46
58	C1	1675	G	C3'-C2'-O2'	5.03	118.25	110.70
58	D1	563	G	C1'-C2'-O2'	5.03	115.95	108.40
22	Bb	60	A	C2'-C3'-O3'	5.03	121.25	113.70
58	C1	2422	A	C1'-C2'-O2'	5.03	115.95	108.40
59	Ds	48	A	C4'-C3'-O3'	5.03	120.55	113.00
58	D1	2710	C	C3'-C2'-O2'	5.03	118.25	110.70
7	AG	73	MET	N-CA-C	5.03	116.84	109.24
22	Ab	1366	C	C2'-C3'-O3'	-5.03	106.16	113.70
22	Bb	434	G	C1'-C2'-O2'	-5.03	104.25	111.80
22	Bb	1454	G	C1'-C2'-O2'	5.03	115.95	108.40
58	D1	2603	G	O5'-P-OP1	5.03	123.09	108.00
58	C1	1732	C	C1'-C2'-O2'	5.03	115.94	108.40
22	Ab	1092	C	C3'-C2'-O2'	5.03	118.24	110.70
22	Bb	316	C	C3'-C2'-O2'	5.03	118.24	110.70
38	CP	12	GLN	N-CA-C	5.03	116.83	109.24
59	Cs	37	C	C3'-C2'-O2'	5.03	118.24	110.70
30	DD	21	ALA	N-CA-C	5.03	121.50	110.80
58	D1	2008	G	C5'-C4'-C3'	-5.03	108.46	116.00
22	Bb	132	C	C3'-C2'-O2'	5.02	118.24	110.70
22	Bb	1323	U	C4'-C3'-O3'	5.02	120.53	113.00
37	CO	23	PRO	N-CA-C	5.02	122.82	112.47
58	D1	1567	G	C3'-C2'-O2'	5.02	118.23	110.70
58	D1	2317	C	C1'-C2'-O2'	5.02	115.93	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	CS	63	VAL	N-CA-C	5.02	115.94	108.46
58	C1	1280	G	C4'-C3'-O3'	-5.02	105.47	113.00
58	D1	82	A	C2'-C3'-O3'	-5.02	101.97	109.50
58	D1	2392	C	C1'-C2'-O2'	5.02	115.93	108.40
58	D1	2837	C	C3'-C2'-O2'	5.02	118.23	110.70
22	Ab	635	C	C3'-C2'-O2'	5.02	118.23	110.70
22	Ab	956	A	C1'-C2'-O2'	5.02	115.93	108.40
58	C1	1627	G	C3'-C2'-O2'	5.02	118.23	110.70
58	C1	1876	G	C3'-C2'-O2'	5.02	118.23	110.70
58	C1	2469	G	C4'-C3'-O3'	5.02	116.92	109.40
58	D1	490	G	N9-C1'-C2'	5.02	119.53	112.00
58	D1	1963	C	C1'-C2'-O2'	5.02	115.92	108.40
58	D1	2275	C	C1'-C2'-O2'	5.02	115.93	108.40
58	D1	2686	A	C3'-C2'-O2'	-5.02	103.17	110.70
58	D1	22	G	C3'-C2'-O2'	5.02	118.22	110.70
58	C1	873	U	C1'-C2'-O2'	-5.01	104.28	111.80
58	D1	327	G	C3'-C2'-O2'	5.01	118.22	110.70
14	AN	34	TYR	N-CA-C	5.01	117.73	109.76
58	C1	825	U	C1'-C2'-O2'	5.01	115.92	108.40
58	D1	158	U	O4'-C4'-C3'	5.01	109.01	104.00
58	D1	424	G	C3'-C2'-O2'	5.01	118.22	110.70
58	C1	1614	G	C2'-C3'-O3'	-5.01	106.19	113.70
58	D1	2345	G	C2'-C3'-O3'	5.01	117.01	109.50
58	C1	1669	G	C1'-C2'-O2'	5.01	115.91	108.40
58	D1	2089	U	C2'-C3'-O3'	-5.01	106.19	113.70
58	D1	16	G	C3'-C2'-O2'	5.01	118.21	110.70
58	D1	2692	C	C3'-C2'-O2'	5.01	122.11	114.60
22	Ab	598	A	C2'-C3'-O3'	5.00	121.20	113.70
22	Ab	1436	G	C3'-C2'-O2'	5.00	118.21	110.70
58	C1	675	G	C3'-C2'-O2'	5.00	118.20	110.70
58	C1	1477	C	C3'-C2'-O2'	5.00	118.21	110.70
22	Ab	823	U	C2'-C3'-O3'	5.00	117.00	109.50
22	Bb	575	U	C1'-C2'-O2'	5.00	115.90	108.40
44	CW	101	SER	N-CA-C	5.00	117.40	109.50

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',C3',C1'
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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Mol	Chain	Res	Type	Group
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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A2	173	0	85	17	0
2	AA	1901	0	1951	38	0
2	BA	1901	0	1951	37	0
3	AC	1612	0	1677	41	0
4	AD	1703	0	1763	56	0
4	BD	1703	0	1763	50	0
5	AE	1147	0	1207	35	0
5	BE	1147	0	1207	24	0
6	AF	843	0	857	7	0
6	BF	843	0	857	18	0
7	AG	1257	0	1296	9	0
7	BG	1257	0	1296	20	0
8	AH	1116	0	1177	15	0
8	BH	1116	0	1177	22	0
9	AI	1011	0	1043	39	0
9	BI	1011	0	1043	33	0
10	AJ	795	0	840	27	0
10	BJ	795	0	840	23	0
11	AK	885	0	904	15	0
11	BK	885	0	904	26	0
12	AL	971	0	1057	28	0
12	BL	971	0	1057	23	0
13	AM	988	0	1059	43	0
13	BM	988	0	1059	33	0
14	AN	492	0	529	23	0
14	BN	492	0	529	16	0
15	AO	734	0	771	9	0
15	BO	734	0	771	13	0
16	AP	701	0	720	16	0
16	BP	701	0	720	20	0
17	AR	824	0	891	15	0
17	BR	824	0	891	22	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	17	0
19	AT	630	0	652	28	0
19	BT	630	0	652	36	0
20	AU	763	0	861	27	0
20	BU	763	0	861	17	0
21	AW	209	0	221	2	0
21	BW	209	0	221	9	0
22	Ab	32329	0	16318	341	0
22	Bb	32329	0	16318	330	1
23	B2	194	0	95	14	0
24	BC	1613	0	1677	34	0
25	C2	1597	0	811	23	0
25	C3	1619	0	822	28	0
25	D3	1619	0	822	46	0
26	C4	1640	0	837	57	0
27	CA	1156	0	755	15	0
28	CB	2105	0	2182	99	0
28	DB	2105	0	2182	100	0
29	CC	1564	0	1629	61	0
29	DC	1564	0	1629	85	0
30	CD	1624	0	1677	64	0
30	DD	1624	0	1677	52	0
31	CE	1474	0	1535	52	0
31	DE	1474	0	1535	57	0
32	CF	1223	0	1282	27	0
32	DF	1223	0	1282	51	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	38	0
35	DM	1105	0	1180	38	0
36	CN	933	0	996	24	0
36	DN	933	0	996	25	0
37	CO	1114	0	1187	91	0
37	DO	1114	0	1187	111	0
38	CP	1122	0	1179	28	0
38	DP	1122	0	1179	39	0
39	CQ	960	0	1021	33	0
39	DQ	960	0	1021	37	0
40	CR	771	0	832	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	DR	771	0	832	31	0
41	CS	1142	0	1202	85	0
41	DS	1142	0	1202	89	0
42	CT	958	0	1018	48	0
42	DT	958	0	1018	48	0
43	CU	779	0	852	47	0
43	DU	779	0	852	46	0
44	CW	896	0	953	25	0
45	CX	726	0	778	19	0
45	DX	726	0	778	21	0
46	CY	776	0	870	51	0
46	DY	776	0	868	61	0
47	CZ	1404	0	1432	38	0
47	DZ	1404	0	1432	26	0
48	Ca	662	0	688	13	0
48	Da	662	0	688	12	0
49	CH	734	0	808	17	0
49	DH	734	0	808	20	0
50	CK	598	0	653	12	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	14	0
53	D6	459	0	477	16	0
54	C7	381	0	390	18	0
54	D7	381	0	390	22	0
55	C8	419	0	467	8	0
55	D8	419	0	467	5	0
56	C9	508	0	576	38	0
56	D9	508	0	576	37	0
57	C0	299	0	326	4	0
57	D0	299	0	324	5	0
58	C1	60459	0	30486	643	0
58	D1	60459	0	30488	738	0
59	Cs	2551	0	1295	19	0
59	Ds	2551	0	1295	28	0
60	D2	416	0	215	8	0
61	D4	1623	0	825	47	0
62	DA	1155	0	757	14	0
63	DW	896	0	956	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
64	DV	1167	0	624	18	0
65	Ab	42	0	45	4	0
65	Bb	42	0	45	3	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	4856	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 10.

All (4856) 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:D1:927:G:O2'	64:DV:19:G:N1	1.81	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
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
22:Ab:1048:U:O2'	22:Ab:1049:C:OP2	1.78	1.02
58:D1:2672:G:H2'	58:D1:2673:A:C2	1.94	1.02
41:CS:13:ARG:CZ	41:CS:13:ARG:HA	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
55:D8:8:ASN:C	55:D8:8:ASN:HD22	1.68	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:Bb:1310:C:OP1	21:BW:21:TYR:OH	1.83	0.96
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
61:D4:74:A:H5'	61:D4:75:C:H5'	1.45	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
22:Ab:1482:G:O2'	22:Ab:1483:G:OP2	1.85	0.93
6:BF:67:MET:HE1	6:BF:75:LEU:HD22	1.51	0.92
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
22:Ab:1037:C:H42	25:C2:34:G:H1'	1.40	0.86
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
29:CC:60:ASN:HB2	58:C1:2820:G:OP1	1.76	0.85
58:C1:2672:G:H2'	58:C1:2673:A:N3	1.90	0.85
47:CZ:53:ILE:HG21	47:CZ:71:VAL:O	1.76	0.85
59:Cs:66:A:O2'	59:Cs:67:G:OP2	1.93	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:Bb:1425:G:N7	22:Bb:1427:A:H2	1.74	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
41:DS:50:ILE:HD11	41:DS:102:ILE:HD11	1.59	0.83
58:D1:2657:C:OP2	58:D1:2744:G:O2'	1.94	0.83
26:C4:5:G:O6	26:C4:69:C:N4	2.12	0.83
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:D1:1346:A:HO2'	58:D1:1347:A:H2'	1.43	0.83
58:C1:2596:U:O2	58:C1:2596:U:H5''	1.78	0.83
61:D4:17:C:H2'	61:D4:18:U:C6	2.13	0.83
58:D1:69:A:C8	58:D1:69:A:H5'	2.14	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
23:B2:18:G:O2'	22:Bb:1384:G:OP1	1.97	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
30:CD:66:PRO:O	30:CD:67:GLN:HB3	1.78	0.82
58:C1:2492:G:HO2'	58:C1:2493:G:P	2.02	0.82
58:D1:1346:A:O2'	58:D1:1347:A:C2'	2.28	0.82
25:C2:19:G:C6	58:C1:927:G:O2'	2.32	0.82
58:C1:1875:G:H2'	58:C1:1876:G:H5'	1.61	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:AU:38:LYS:NZ	22:Ab:1422:C:OP1	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:D1:138:A:H8	58:D1:1453:C:HO2'	1.28	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
22:Ab:1472:G:N7	65:Ab:1601:PAR:N32	2.28	0.81
22:Bb:1425:G:N7	22:Bb:1427:A:C2	2.49	0.80
45:DX:44:GLU:OE1	58:D1:136:G:N2	2.13	0.80
53:D6:3:LYS:O	53:D6:4:HIS:C	2.23	0.80
59:Ds:21:G:O2'	59:Ds:22:U:O4'	1.99	0.80
39:CQ:90:ARG:NH1	58:C1:2889:C:O2'	2.13	0.80
49:CH:29:GLY:O	49:CH:30:VAL:HG22	1.81	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
22:Bb:957:C:H3'	22:Bb:958:C:H5''	1.61	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
22:Bb:1303:C:H3'	22:Bb:1304:C:H5''	1.64	0.80
24:BC:50:ALA:HB1	24:BC:70:VAL:HG11	1.63	0.80
58:C1:2475:C:O2'	58:C1:2476:C:O5'	2.00	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:O2	58:D1:1441:U:H2'	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
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:HE2	54:C7:33:LYS:HA	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:Ab:434:G:O2'	22:Ab:479:U:O4	2.01	0.78
61:D4:2:G:N1	61:D4:73:A:N3	2.14	0.78
42:DT:15:LYS:NZ	58:D1:1261:C:OP2	2.15	0.78
25:C3:8:U:H1'	25:C3:48:C:C2	2.18	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
22:Bb:1279:C:O2'	7:BG:114:ARG:NH2	2.17	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
50:DK:7:ARG:NH2	58:D1:99:G:OP2	2.17	0.78
58:D1:69:A:H5'	58:D1:69:A:H8	1.47	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:CR:63:THR:HG23	59:Cs:50:G:OP1	1.83	0.77
40:DR:89:ARG:O	40:DR:92:TYR:HB3	1.84	0.77
22:Bb:434:G:O2'	22:Bb:479:U:O4	2.01	0.77
58:C1:552:A:O2'	58:C1:553:A:H5'	1.85	0.77
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
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
58:D1:1345:U:O2'	58:D1:1671:G:C2	2.37	0.77
58:D1:2120:U:H2'	58:D1:2120:U:O2	1.84	0.77
41:DS:129:ARG:CZ	41:DS:131:ALA:HB3	2.15	0.77
22:Ab:982:G:H2'	22:Ab:983:A:H4'	1.66	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
32:DF:156:ALA:O	32:DF:157:TYR:C	2.29	0.76
37:DO:25:SER:HB2	58:D1:858:C:H5'	1.67	0.76
4:AD:30:LYS:C	4:AD:32:ALA:H	1.92	0.76
26:C4:61:U:H5''	26:C4:62:C:H5	1.50	0.76
31:CE:70:VAL:O	59:Cs:41:U:C4	2.38	0.76
58:C1:1920:G:N2	58:C1:1923:C:H41	1.84	0.76
13:AM:23:TYR:CE2	22:Ab:1312:U:H4'	2.21	0.76
29:CC:132:HIS:HB3	58:C1:790:G:OP1	1.85	0.76
46:DY:17:SER:O	58:D1:333:A:OP1	2.04	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:D1:276:G:O2'	58:D1:277:G:OP2	2.03	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
5:BE:100:VAL:HG12	5:BE:118:ILE:CG2	2.16	0.75
37:CO:16:ARG:HD3	37:CO:18:ARG:H	1.49	0.75
53:C6:13:LYS:HE2	58:C1:541:C:OP2	1.85	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
37:DO:23:PRO:HB2	37:DO:33:ARG:CD	2.16	0.75
58:D1:1539:A:H2'	58:D1:1540:A:H5''	1.67	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
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
63:DW:64:MET:O	63:DW:65:LEU:HB3	1.84	0.75
58:D1:185:A:C8	58:D1:185:A:H5'	2.21	0.75
22:Ab:1481:A:O2'	22:Ab:1482:G:O5'	2.05	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
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
22:Bb:1427:A:H2'	22:Bb:1427:A:N3	2.02	0.74
58:C1:1908:C:H2'	58:C1:1909:G:H5'	1.69	0.74
59:Ds:21:G:O2'	59:Ds:22:U:O5'	2.03	0.74
39:DQ:9:LYS:O	39:DQ:10:LEU:HD23	1.87	0.74
56:D9:51:ALA:C	56:D9:53:PRO:HD2	2.12	0.74
58:D1:154:C:H3'	58:D1:157:U:P	2.27	0.74
3:AC:4:LYS:NZ	22:Ab:1174:C:OP2	2.20	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
22:Ab:657:G:H2'	22:Ab:658:G:C8	2.23	0.73
31:DE:71:THR:HG21	58:D1:2323:U:O2'	1.88	0.73
58:D1:158:U:H4'	58:D1:159:G:C8	2.22	0.73
16:BP:28:ARG:HG2	16:BP:29:ASP:OD2	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:CI:109:ILE:HG22	33:CI:130:TYR:CZ	2.22	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
53:D6:3:LYS:O	53:D6:4:HIS:O	2.06	0.73
22:Ab:1037:C:N4	25:C2:34:G:H1'	2.04	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
4:BD:25:ARG:C	4:BD:27:TYR:H	1.97	0.72
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
41:CS:28:VAL:O	41:CS:29:ARG:HB2	1.87	0.72
58:C1:267:G:O2'	58:C1:268:G:OP2	2.06	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
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
58:D1:1346:A:O2'	58:D1:1347:A:C3'	2.38	0.72
41:CS:13:ARG:HA	41:CS:13:ARG:NH1	2.04	0.72
22:Ab:1491:A:H2'	22:Ab:1492:C:C6	2.24	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
42:CT:83:LEU:HD12	42:CT:88:ILE:HD11	1.71	0.72
58:C1:1539:A:H2'	58:C1:1540:A:H5''	1.71	0.72
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
58:D1:26:G:N2	58:D1:536:G:HO2'	1.87	0.72
22:Ab:1303:C:H5''	22:Ab:1304:C:H5'	1.71	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
32:DF:41:MET:HE3	32:DF:42:ARG:C	2.15	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
25:C3:48:C:O2'	25:C3:49:C:OP1	2.05	0.71
28:CB:209:ALA:C	28:CB:210:GLY:O	2.29	0.71
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:DO:6:LEU:HG	37:DO:8:PRO:O	1.90	0.71
22:Ab:1241:C:C4	22:Ab:1242:C:O2	2.43	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
4:AD:8:VAL:C	4:AD:10:ARG:H	1.98	0.71
22:Bb:1241:C:C4	22:Bb:1242:C:O2	2.43	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
22:Bb:1037:C:OP2	22:Bb:1179:G:OP2	2.09	0.71
22:Bb:1263:U:H4'	22:Bb:1264:C:OP2	1.90	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
58:C1:2083:A:C4	58:C1:2083:A:H5''	2.25	0.71
31:DE:86:MET:N	31:DE:87:PRO:HD2	2.06	0.71
58:D1:1539:A:N3	58:D1:1539:A:H5'	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
4:AD:30:LYS:C	4:AD:32:ALA:N	2.46	0.71
33:DI:94:ALA:CB	33:DI:114:LEU:HD11	2.20	0.71
58:D1:2782:G:H5''	58:D1:2783:C:OP2	1.91	0.71
22:Bb:430:U:H2'	22:Bb:431:C:C6	2.24	0.71
25:D3:64:A:H2'	25:D3:65:G:C8	2.26	0.71
35:DM:28:THR:HG21	58:D1:1057:U:O4	1.89	0.71
48:Da:23:VAL:HG21	58:D1:903:C:H4'	1.72	0.71
22:Ab:1303:C:H5''	22:Ab:1304:C:C5'	2.20	0.71
28:CB:238:GLY:O	28:CB:239:ARG:HB3	1.91	0.70
32:DF:156:ALA:O	32:DF:158:HIS:N	2.24	0.70
58:D1:1171:A:H8	58:D1:1171:A:OP1	1.73	0.70
43:CU:19:LYS:HG3	43:CU:20:LEU:N	2.04	0.70
49:CH:44:PRO:O	49:CH:46:LEU:HD13	1.90	0.70
58:C1:2450:A:OP1	66:C1:3001:3V6:N	2.23	0.70
58:D1:2902:G:H2'	58:D1:2902:G:N3	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
59:Ds:80:U:O2'	58:D1:963:A:N3	2.21	0.70
58:C1:722:A:H8	58:C1:2090:G:H21	1.40	0.70
37:DO:62:LEU:HB3	58:D1:2404:A:H5'	1.74	0.70
22:Bb:1040:G:H5''	24:BC:154:SER:HB2	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:C4:4:G:O2'	26:C4:5:G:O5'	2.09	0.70
41:CS:2:ASN:O	58:C1:2885:G:OP1	2.10	0.70
28:DB:238:GLY:O	28:DB:239:ARG:HB3	1.91	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
22:Bb:1268:A:H2'	22:Bb:1269:A:H4'	1.74	0.70
25:C3:1:G:O6	25:C3:72:C:N4	2.25	0.70
38:CP:14:ARG:NH1	58:C1:1002:U:OP2	2.24	0.70
57:C0:14:CYS:HG	57:C0:27:CYS:HG	1.37	0.70
31:DE:47:LYS:HA	31:DE:88:ILE:HD13	1.74	0.70
32:DF:41:MET:HE2	32:DF:43:VAL:HG13	1.73	0.70
58:D1:2802:A:H2'	58:D1:2802:A:N3	2.06	0.70
47:CZ:54:HIS:HA	47:CZ:98:MET:HE1	1.72	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
20:AU:65:LYS:NZ	22:Ab:172:C:OP1	2.24	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
35:DM:90:MET:O	35:DM:93:THR:O	2.09	0.69
22:Ab:143:G:O2'	22:Ab:144:A:H5'	1.92	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
56:C9:46:ARG:NH2	58:C1:655:A:OP2	2.25	0.69
58:D1:8:U:C5	58:D1:2640:A:N6	2.60	0.69
22:Bb:438:C:H2'	22:Bb:439:C:C6	2.27	0.69
40:CR:97:ARG:NH2	40:CR:98:VAL:HA	2.06	0.69
38:DP:135:ASP:O	38:DP:138:ASP:OD2	2.09	0.69
58:D1:154:C:C3'	58:D1:157:U:P	2.80	0.69
58:C1:2323:U:H2'	58:C1:2324:C:H5'	1.73	0.69
19:AT:44:MET:HA	19:AT:44:MET:HE3	1.75	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
46:DY:17:SER:OG	46:DY:18:GLY:N	2.20	0.69
56:D9:4:MET:HE3	56:D9:61:LEU:HD22	1.73	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
28:DB:181:GLU:HA	28:DB:272:ALA:HB3	1.74	0.69
58:D1:1498:C:N3	58:D1:1505:G:O6	2.26	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
61:D4:74:A:H5'	61:D4:75:C:C5'	2.21	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:DO:17:LYS:O	37:DO:19:VAL:N	2.26	0.68
58:D1:1538:C:C4	58:D1:2226:G:O2'	2.46	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
22:Ab:932:G:H2'	22:Ab:933:U:C6	2.28	0.68
2:BA:88:ALA:HB2	2:BA:219:VAL:HG13	1.75	0.68
30:CD:101:LEU:HD12	30:CD:102:PRO:HD2	1.73	0.68
58:C1:1908:C:C2'	58:C1:1909:G:H5'	2.23	0.68
41:DS:89:VAL:HG12	41:DS:91:ARG:HG3	1.76	0.68
22:Ab:609:G:H2'	22:Ab:610:U:H6	1.59	0.68
23:B2:20:U:H2'	23:B2:21:C:C6	2.28	0.68
22:Bb:626:A:N3	8:BH:113:SER:OG	2.26	0.68
6:BF:60:PHE:C	6:BF:61:LEU:HD12	2.17	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
22:Ab:802:G:C3'	22:Ab:803:A:H5'	2.23	0.68
22:Bb:951:G:O4'	10:BJ:55:LYS:HG3	1.93	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
38:CP:42:ILE:HD13	38:CP:97:VAL:CG2	2.24	0.68
56:C9:2:PRO:HA	58:C1:613:C:O2	1.92	0.68
22:Ab:1260:U:H5''	22:Ab:1261:A:O4'	1.92	0.68
33:CI:78:THR:HA	33:CI:141:LYS:O	1.94	0.68
61:D4:17:C:C6	61:D4:18:U:C4	2.82	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
22:Ab:816:C:O2'	22:Ab:817:U:P	2.51	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
41:DS:102:ILE:HB	41:DS:110:ILE:CD1	2.24	0.68
58:D1:1850:U:H4'	58:D1:1851:A:OP2	1.94	0.68
22:Ab:1251:A:N1	22:Ab:1294:G:O2'	2.25	0.68
6:BF:50:TYR:OH	18:BS:74:ARG:O	2.10	0.68
55:D8:8:ASN:C	55:D8:8:ASN:ND2	2.40	0.68
37:CO:59:LEU:HA	37:CO:61:ARG:HH11	1.56	0.67
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
26:C4:51:U:C2	26:C4:52:C:C5	2.82	0.67
58:C1:644:G:N3	58:C1:644:G:H5''	2.10	0.67
35:DM:55:VAL:HG22	35:DM:126:PRO:HA	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:D1:841:C:H2'	58:D1:842:C:H6	1.60	0.67
58:D1:2192:A:O2'	58:D1:2193:U:O4'	2.11	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
22:Ab:430:U:H2'	22:Ab:431:C:C6	2.30	0.67
22:Ab:1282:G:O2'	22:Ab:1283:U:P	2.51	0.67
10:BJ:40:LEU:HB2	10:BJ:69:ASN:HB2	1.76	0.67
13:BM:100:GLY:C	13:BM:101:GLN:HG2	2.20	0.67
29:CC:61:ARG:HD3	58:C1:2799:C:O2'	1.95	0.67
30:DD:67:GLN:O	30:DD:67:GLN:HG3	1.95	0.67
12:AL:90:VAL:O	12:AL:92:ASP:N	2.27	0.67
22:Bb:1331:A:H2'	22:Bb:1332:A:H8	1.58	0.67
4:BD:30:LYS:C	4:BD:32:ALA:H	2.00	0.67
58:D1:2050:G:H2'	58:D1:2052:A:OP2	1.94	0.67
37:DO:16:ARG:O	58:D1:707:C:O2'	2.11	0.67
58:D1:1059:U:C2'	58:D1:1060:G:H5'	2.25	0.67
37:CO:23:PRO:HB2	37:CO:33:ARG:HD2	1.76	0.67
37:CO:58:THR:O	37:CO:58:THR:HG22	1.95	0.67
66:C1:3001:3V6:C	66:C1:3001:3V6:CLI	2.79	0.67
30:DD:9:ILE:HG23	30:DD:11:VAL:O	1.95	0.67
39:DQ:3:HIS:HB2	58:D1:1700:A:P	2.35	0.67
45:DX:18:TYR:O	45:DX:20:GLY:N	2.28	0.67
35:CM:45:ASN:HD22	35:CM:45:ASN:H	1.43	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
41:DS:38:ASN:HD22	41:DS:40:THR:H	1.42	0.67
58:D1:2089:U:N3	58:D1:2441:A:H2	1.91	0.67
41:DS:29:ARG:CB	41:DS:85:LYS:HA	2.25	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:HA	41:DS:13:ARG:NH1	2.10	0.67
36:CN:4:PRO:O	36:CN:5:GLN:HB2	1.94	0.66
58:C1:2338:A:H2'	58:C1:2339:A:C8	2.30	0.66
22:Bb:617:G:H5'	22:Bb:618:C:OP2	1.96	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
36:CN:1:MET:HE2	36:CN:32:TYR:CD2	2.30	0.66
40:DR:74:ALA:HB1	40:DR:103:GLU:HB3	1.77	0.66
58:D1:355:A:O2'	58:D1:357:C:OP2	2.12	0.66
58:D1:1059:U:H2'	58:D1:1060:G:H5'	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
46:DY:2:ARG:C	46:DY:4:LYS:H	2.03	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:C1:906:U:H5	58:C1:962:A:N7	1.93	0.66
35:DM:2:LYS:O	35:DM:4:TYR:CZ	2.48	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
17:AR:67:LYS:O	22:Ab:250:G:OP1	2.14	0.66
30:CD:24:LEU:HB3	30:CD:25:PRO:HD2	1.77	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
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
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
54:C7:51:GLU:O	54:C7:52:VAL:HG23	1.94	0.66
30:DD:9:ILE:CG2	30:DD:11:VAL:O	2.44	0.66
58:D1:2083:A:H2'	58:D1:2084:C:O5'	1.96	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
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:D1:2611:A:O3'	66:D1:3001:3V6:H19	1.95	0.66
58:C1:2732:U:O2	58:C1:2732:U:H2'	1.96	0.65
28:DB:24:ILE:HA	28:DB:82:ILE:HG22	1.76	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:CD:53:THR:HG22	30:CD:56:GLU:OE2	1.96	0.65
48:Ca:18:ALA:HB3	48:Ca:20:ARG:HH21	1.60	0.65
58:C1:2209:C:H2'	58:C1:2210:U:C1'	2.26	0.65
61:D4:48:U:H3'	61:D4:49:C:H5'	1.78	0.65
28:DB:62:TYR:CE2	58:D1:1846:G:N7	2.65	0.65
37:DO:106:LEU:HD13	37:DO:112:LEU:HD23	1.78	0.65
49:DH:56:GLN:HA	49:DH:56:GLN:HE21	1.60	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
15:AO:28:GLN:OE1	22:Ab:640:C:O2'	2.05	0.65
42:DT:92:ARG:NE	58:D1:1041:A:H4'	2.11	0.65
58:D1:629:U:H3	58:D1:645:A:H2	1.45	0.65
58:D1:2001:G:O2'	58:D1:2003:C:OP2	2.12	0.65
58:D1:2057:C:H6	58:D1:2057:C:H5'	1.60	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
42:DT:58:ARG:NH1	58:D1:1200:A:OP2	2.30	0.65
56:D9:2:PRO:HB3	58:D1:613:C:O2	1.95	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
37:DO:146:VAL:HG22	37:DO:147:LEU:H	1.60	0.65
49:DH:93:GLU:C	49:DH:95:LEU:H	2.05	0.65
37:CO:18:ARG:HD2	58:C1:708:G:OP1	1.97	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
28:DB:65:ILE:HD11	28:DB:67:PHE:CE2	2.32	0.65
29:DC:144:ARG:CD	58:D1:2583:A:C8	2.80	0.65
58:D1:1254:A:H5'	58:D1:1254:A:H8	1.61	0.65
58:D1:2479:G:O2'	58:D1:2487:A:C8	2.48	0.65
8:BH:103:VAL:HG21	8:BH:110:ALA:HB2	1.78	0.65
25:C2:43:C:OP1	25:C2:43:C:H4'	1.97	0.65
58:C1:91:C:H5'	58:C1:92:G:OP2	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
22:Bb:982:G:H2'	22:Bb:983:A:H4'	1.77	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
58:C1:139:A:C8	58:C1:1453:C:H1'	2.32	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:HA	4:AD:49:ARG:HE	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:CS:28:VAL:O	41:CS:29:ARG:CB	2.45	0.64
12:BL:28:LYS:O	12:BL:29:GLY:C	2.40	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:C1:267:G:O2'	58:C1:268:G:P	2.55	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:D1:1336:C:H2'	58:D1:1337:U:H6	1.62	0.64
58:D1:2318:G:H4'	58:D1:2318:G:OP1	1.96	0.64
22:Bb:1037:C:H42	64:DV:34:G:H1'	1.63	0.64
22:Bb:1418:G:H2'	22:Bb:1419:U:C6	2.33	0.64
58:C1:2412:U:H2'	58:C1:2413:C:H5''	1.78	0.64
32:DF:153:LYS:H	32:DF:153:LYS:HD3	1.62	0.64
58:D1:2083:A:C2'	58:D1:2084:C:O5'	2.45	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
58:C1:2722:A:OP1	58:C1:2724:A:OP1	2.16	0.64
39:DQ:2:ARG:NH2	58:D1:2736:C:OP2	2.30	0.64
53:D6:2:ALA:N	58:D1:2036:A:N3	2.46	0.64
22:Bb:1048:U:O2'	22:Bb:1049:C:OP2	2.10	0.64
36:DN:4:PRO:O	36:DN:5:GLN:HB2	1.96	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
22:Ab:1037:C:O2'	22:Ab:1038:A:H5''	1.98	0.64
22:Ab:1233:A:H2'	22:Ab:1234:A:C8	2.31	0.64
59:Cs:20:C:H2'	59:Cs:21:G:H5'	1.79	0.64
30:DD:89:VAL:O	30:DD:91:GLY:N	2.29	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
38:CP:16:ARG:HH22	58:C1:996:G:P	2.21	0.64
58:C1:2613:A:H4'	58:C1:2613:A:OP2	1.97	0.64
32:DF:43:VAL:HG11	32:DF:52:VAL:HG22	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
56:D9:33:ASN:O	58:D1:2431:C:OP1	2.16	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
22:Bb:1037:C:O2'	22:Bb:1038:A:H5''	1.98	0.63
12:BL:25:PRO:C	12:BL:27:LEU:H	2.06	0.63
28:CB:34:VAL:O	28:CB:35:LYS:C	2.41	0.63
58:C1:2083:A:H5''	58:C1:2083:A:N3	2.13	0.63
32:DF:41:MET:HE2	32:DF:43:VAL:CG1	2.28	0.63
58:D1:1895:G:H5'	58:D1:1896:C:OP2	1.98	0.63
22:Ab:1334:C:H2'	22:Ab:1335:G:C8	2.33	0.63
58:C1:2269:C:H4'	58:C1:2270:G:OP2	1.97	0.63
37:DO:38:GLN:CD	58:D1:987:U:OP2	2.41	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:O2	58:C1:1984:U:H2'	1.97	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:D1:154:C:O2	58:D1:154:C:O4'	2.13	0.63
58:D1:1765:G:C2	58:D1:1767:U:OP2	2.51	0.63
14:AN:27:CYS:C	14:AN:29:ARG:H	2.05	0.63
46:CY:76:CYS:HB3	46:CY:96:ILE:HD11	1.80	0.63
58:C1:154:C:O2	58:C1:154:C:O4'	2.16	0.63
45:DX:12:VAL:HG21	45:DX:17:ALA:HB1	1.80	0.63
58:D1:1920:G:H22	58:D1:1923:C:N4	1.96	0.63
1:A2:17:U:C2'	1:A2:18:G:H5''	2.20	0.63
22:Bb:1120:C:H4'	22:Bb:1121:G:C2	2.34	0.63
4:BD:8:VAL:C	4:BD:10:ARG:H	2.05	0.63
58:C1:355:A:O2'	58:C1:357:C:OP2	2.15	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
42:CT:90:VAL:O	42:CT:91:ASP:C	2.40	0.63
56:D9:33:ASN:O	58:D1:2431:C:P	2.57	0.63
22:Ab:1418:G:H2'	22:Ab:1419:U:C6	2.34	0.63
22:Bb:378:A:H2'	22:Bb:379:A:C8	2.34	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
58:C1:1067:G:O2'	58:C1:1068:U:OP2	2.17	0.63
37:DO:45:LEU:HD23	37:DO:46:LYS:N	2.14	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:D6:35:GLU:O	53:D6:36:CYS:HB3	1.98	0.63
12:AL:28:LYS:O	12:AL:29:GLY:C	2.42	0.63
20:AU:73:HIS:HB3	20:AU:74:LYS:HG2	1.79	0.63
29:CC:61:ARG:CD	58:C1:2799:C:H1'	2.29	0.63
31:DE:71:THR:HG22	31:DE:89:GLY:C	2.24	0.63
37:DO:101:VAL:C	37:DO:103:ALA:H	2.07	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
54:D7:16:CYS:O	54:D7:17:LYS:HB2	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
9:AI:118:LYS:O	9:AI:119:ALA:HB3	1.98	0.62
22:Ab:324:C:O2	22:Ab:324:C:H2'	1.99	0.62
28:CB:24:ILE:O	28:CB:25:THR:C	2.42	0.62
58:C1:2084:C:H2'	58:C1:2085:C:H5'	1.81	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
58:D1:893:U:OP2	58:D1:973:G:O6	2.17	0.62
58:D1:2543:G:O2'	58:D1:2668:A:N6	2.32	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
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
63:DW:64:MET:O	63:DW:65:LEU:CB	2.46	0.62
50:DK:22:GLU:OE2	50:DK:68:ARG:NH2	2.31	0.62
58:D1:1097:C:H3'	58:D1:1097:C:H6	1.65	0.62
13:AM:106:ASN:O	13:AM:107:ALA:HB3	1.99	0.62
22:Bb:1427:A:C6	41:DS:118:ARG:NH2	2.67	0.62
46:DY:60:PHE:HA	46:DY:62:GLU:OE2	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
20:AU:104:LEU:HD23	20:AU:105:SER:N	2.14	0.62
65:Ab:1601:PAR:N64	65:Ab:1601:PAR:H34	2.14	0.62
24:BC:73:PRO:O	24:BC:76:VAL:HG22	1.99	0.62
45:CX:12:VAL:HG12	45:CX:17:ALA:HB1	1.81	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
37:DO:39:LYS:HG3	58:D1:853:U:OP2	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
58:D1:2842:G:H3'	58:D1:2843:G:C5'	2.28	0.62
13:BM:65:LYS:HD2	13:BM:69:GLU:O	2.00	0.62
31:DE:130:ASN:HB3	31:DE:160:VAL:HA	1.81	0.62
32:DF:156:ALA:C	32:DF:158:HIS:N	2.57	0.62
41:DS:96:ARG:NH1	58:D1:1784:C:OP1	2.32	0.62
58:D1:138:A:H8	58:D1:1453:C:O2'	1.82	0.62
22:Ab:1111:C:O2'	22:Ab:1113:A:C8	2.49	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
22:Ab:1375:G:H21	22:Ab:1480:A:H8	1.48	0.62
65:Ab:1601:PAR:O62	65:Ab:1601:PAR:H32	2.00	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
2:AA:111:ARG:HD2	22:Ab:1087:G:OP1	2.00	0.62
5:AE:16:THR:HG21	22:Ab:1063:A:H5'	1.80	0.62
22:Bb:674:G:H2'	22:Bb:675:G:C8	2.35	0.62
24:BC:113:ALA:HB3	24:BC:114:PRO:HD3	1.81	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:D1:1920:G:O2'	58:D1:1921:A:OP2	2.16	0.62
22:Bb:432:C:O2'	22:Bb:433:U:P	2.58	0.62
51:CL:52:HIS:CD2	51:CL:52:HIS:H	2.16	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
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
45:DX:18:TYR:C	45:DX:20:GLY:H	2.08	0.62
12:BL:26:ALA:O	12:BL:27:LEU:O	2.17	0.62
38:CP:85:LYS:HE2	48:Ca:7:LEU:HD13	1.82	0.62
41:CS:10:VAL:O	41:CS:13:ARG:HG2	2.00	0.62
52:C5:60:GLU:O	52:C5:61:VAL:HB	2.00	0.62
33:DI:94:ALA:HB2	33:DI:114:LEU:HD11	1.82	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
22:Bb:921:U:H2'	22:Bb:922:G:H5'	1.81	0.61
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
43:CU:22:VAL:O	43:CU:23:GLU:HB2	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
56:D9:61:LEU:N	56:D9:63:PRO:HD2	2.14	0.61
58:D1:2319:G:O6	58:D1:2321:A:H2'	2.00	0.61
22:Bb:901:A:OP1	5:BE:21:ALA:HB2	2.00	0.61
22:Bb:955:A:O2'	22:Bb:957:C:OP2	2.18	0.61
29:CC:63:LEU:O	29:CC:64:LYS:C	2.42	0.61
22:Bb:1468:C:OP2	65:Bb:1601:PAR:N64	2.33	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
29:DC:36:ARG:HH21	29:DC:88:GLY:HA3	1.64	0.61
34:DJ:10:UNK:CB	58:D1:1091:A:H5''	2.31	0.61
41:DS:80:SER:HB3	41:DS:81:PRO:HD3	1.82	0.61
46:DY:52:SER:C	46:DY:54:LYS:H	2.08	0.61
2:AA:185:ILE:HG22	2:AA:199:TYR:HB2	1.82	0.61
22:Bb:1111:C:O2'	22:Bb:1113:A:N7	2.31	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
37:CO:77:ARG:HB2	37:CO:78:PRO:HD2	1.82	0.61
49:CH:11:ARG:HB2	49:CH:12:PRO:HD2	1.83	0.61
58:C1:2200:C:H4'	58:C1:2200:C:OP1	1.99	0.61
28:DB:35:LYS:O	28:DB:64:ILE:HG22	1.99	0.61
58:D1:2448:U:H2'	58:D1:2449:U:H5'	1.83	0.61
23:B2:20:U:H2'	23:B2:21:C:O4'	2.00	0.61
22:Bb:1282:G:O2'	22:Bb:1283:U:P	2.59	0.61
25:C3:15:G:N3	25:C3:15:G:H2'	2.16	0.61
31:CE:46:ALA:HB2	31:CE:88:ILE:HG12	1.82	0.61
46:CY:8:LYS:HB2	46:CY:28:LYS:NZ	2.14	0.61
51:CL:43:ILE:O	51:CL:47:VAL:HG23	2.00	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
58:C1:1424:A:HO2'	58:C1:1425:G:P	2.23	0.61
37:DO:115:LEU:HA	37:DO:134:ALA:HB2	1.81	0.61
22:Ab:218:U:H2'	22:Ab:219:U:C6	2.36	0.61
22:Bb:1275:G:HO2'	22:Bb:1276:G:H8	1.49	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
35:CM:18:ALA:HB1	35:CM:21:LYS:HB2	1.83	0.61
42:CT:49:HIS:HD2	58:C1:558:U:O2'	1.83	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
7:AG:94:ARG:NH1	22:Ab:1360:A:OP2	2.34	0.61
18:BS:53:ARG:C	18:BS:55:ARG:H	2.09	0.61
27:CA:169:UNK:O	27:CA:171:UNK:N	2.33	0.61
40:CR:89:ARG:HG2	40:CR:89:ARG:HH11	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:29:ASN:HB3	30:DD:112:MET:HE1	1.83	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
22:Ab:781:C:O2'	22:Ab:782:G:H5'	1.99	0.61
48:Ca:18:ALA:HB3	48:Ca:20:ARG:NH2	2.16	0.61
53:C6:33:CYS:O	53:C6:36:CYS:O	2.18	0.61
49:DH:45:ASN:C	49:DH:45:ASN:HD22	2.09	0.61
58:D1:138:A:C8	58:D1:1453:C:O2'	2.52	0.61
66:D1:3001:3V6:OAE	66:D1:3001:3V6:OAG	2.15	0.61
5:AE:16:THR:HG21	22:Ab:1063:A:C5'	2.31	0.61
16:AP:53:VAL:HG12	16:AP:79:VAL:HG22	1.83	0.61
22:Bb:1260:U:H5''	22:Bb:1261:A:O4'	2.00	0.61
4:BD:25:ARG:C	4:BD:27:TYR:N	2.59	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
46:CY:28:LYS:HB3	46:CY:37:VAL:HB	1.83	0.61
50:CK:69:ARG:NH2	58:C1:108:A:H4'	2.16	0.61
56:C9:51:ALA:C	56:C9:53:PRO:HD2	2.25	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
46:DY:28:LYS:HB3	46:DY:37:VAL:HB	1.83	0.61
48:Da:36:ILE:C	48:Da:36:ILE:HD12	2.25	0.61
58:D1:722:A:H8	58:D1:2090:G:H21	1.49	0.61
22:Ab:609:G:H2'	22:Ab:610:U:C6	2.36	0.60
22:Bb:335:C:OP2	36:DN:97:ARG:NH1	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BA:233:SER:HB2	2:BA:234:PRO:HD2	1.83	0.60
37:CO:17:LYS:O	37:CO:17:LYS:CG	2.49	0.60
43:CU:64:HIS:ND1	43:CU:92:THR:HG22	2.17	0.60
58:C1:7:A:H2'	58:C1:8:U:C5	2.35	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
25:C3:25:C:H2'	25:C3:26:A:C8	2.35	0.60
41:CS:38:ASN:HD22	41:CS:40:THR:H	1.49	0.60
56:C9:51:ALA:N	56:C9:53:PRO:HD2	2.16	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
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
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
16:AP:16:HIS:CD2	22:Ab:609:G:H4'	2.37	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
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
58:D1:715:G:H5'	58:D1:715:G:C8	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
37:DO:33:ARG:O	37:DO:34:GLY:C	2.44	0.60
66:D1:3001:3V6:OAG	67:D1:3002:MG:MG	1.44	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
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
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
40:CR:18:ILE:HD11	58:C1:2345:G:N3	2.15	0.60
58:C1:2298:A:H62	58:C1:2355:U:H3	1.48	0.60
35:DM:63:THR:CG2	58:D1:1185:U:H2'	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:D6:2:ALA:HA	58:D1:2036:A:H1'	1.83	0.60
22:Bb:239:A:H4'	22:Bb:240:U:O5'	2.01	0.60
30:CD:74:ARG:HD2	58:C1:720:G:H1'	1.82	0.60
36:CN:23:ARG:NH2	58:C1:2558:U:O2	2.34	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
4:AD:11:LEU:C	4:AD:13:ARG:N	2.60	0.60
5:AE:143:ARG:NH1	8:AH:77:GLU:OE1	2.35	0.60
22:Ab:970:U:H4'	22:Ab:971:G:O5'	2.02	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
22:Bb:970:U:H4'	22:Bb:971:G:O5'	2.02	0.60
22:Bb:1111:C:O2'	22:Bb:1113:A:C8	2.50	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
22:Bb:1210:C:OP1	13:BM:115:LYS:HE3	2.02	0.60
22:Bb:1287:G:C2	22:Bb:1313:G:N3	2.70	0.60
5:BE:10:MET:HB2	5:BE:32:VAL:HG22	1.82	0.60
28:CB:259:THR:HG21	58:C1:1833:A:O3'	2.02	0.60
37:CO:48:PRO:O	37:CO:49:ARG:C	2.44	0.60
47:CZ:28:MET:HE2	47:CZ:90:VAL:HG21	1.83	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
59:Ds:73:A:C4	59:Ds:105:A:C2	2.89	0.60
58:D1:1088:C:H2'	58:D1:1089:G:C8	2.36	0.60
22:Ab:646:G:O2'	22:Ab:820:G:H5'	2.01	0.59
22:Bb:487:C:OP2	12:BL:116:SER:OG	2.18	0.59
22:Bb:1331:A:P	9:BI:118:LYS:HZ3	2.25	0.59
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:H2'	58:C1:2902:G:N3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:AJ:49:VAL:HG21	14:AN:41:ARG:HB2	1.83	0.59
22:Bb:460:G:H2'	22:Bb:461:G:C8	2.37	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
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
58:D1:2319:G:O2'	58:D1:2320:A:OP1	2.18	0.59
41:CS:23:ARG:NH2	58:C1:2858:U:O4	2.33	0.59
61:D4:17:C:H2'	61:D4:18:U:C5	2.36	0.59
32:DF:41:MET:SD	32:DF:53:GLU:O	2.60	0.59
58:D1:1376:A:HO2'	58:D1:1377:G:H8	1.48	0.59
58:D1:1734:U:O2	58:D1:1746:A:H5''	2.03	0.59
22:Ab:348:C:O2'	22:Ab:350:G:OP1	2.17	0.59
22:Bb:1331:A:P	9:BI:118:LYS:NZ	2.75	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:D3:20:U:H2'	25:D3:21:A:H4'	1.84	0.59
25:D3:72:C:OP1	58:D1:1881:U:O2'	2.20	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
58:D1:2083:A:O2'	58:D1:2084:C:H5'	2.02	0.59
22:Ab:831:G:H2'	22:Ab:832:G:H8	1.66	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:34:TRP:CE2	37:CO:12:ALA:HB2	2.37	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
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
22:Bb:1203:G:O3'	19:BT:77:THR:HG21	2.03	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:2:LEU:O	38:CP:70:PRO:HG2	2.01	0.59
38:CP:42:ILE:HD13	38:CP:97:VAL:HG21	1.83	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
31:DE:39:ILE:HG13	31:DE:92:VAL:HG12	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:AL:37:CYS:O	12:AL:79:GLU:O	2.20	0.59
40:CR:96:GLY:O	40:CR:98:VAL:N	2.30	0.59
58:C1:276:G:O2'	58:C1:277:G:P	2.59	0.59
28:DB:35:LYS:HG2	28:DB:63:ARG:HG3	1.84	0.59
39:DQ:10:LEU:HD22	39:DQ:17:ARG:CD	2.33	0.59
51:DL:4:LEU:O	51:DL:36:VAL:HA	2.03	0.59
58:D1:2325:C:O2'	58:D1:2326:G:H5'	2.02	0.59
58:C1:2209:C:H2'	58:C1:2210:U:O4'	2.03	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
39:DQ:38:VAL:HB	39:DQ:39:PRO:HD3	1.85	0.59
57:D0:11:CYS:HB3	57:D0:14:CYS:SG	2.43	0.59
58:D1:567:C:HO2'	58:D1:570:A:P	2.25	0.59
58:D1:570:A:H2'	58:D1:570:A:N3	2.16	0.59
58:D1:2303:C:O2'	58:D1:2304:C:H5'	2.03	0.59
5:AE:6:PHE:HB2	5:AE:34:VAL:HG22	1.85	0.59
22:Ab:1120:C:H4'	22:Ab:1121:G:C2	2.38	0.59
22:Bb:131:C:O2'	16:BP:65:GLN:OE1	2.20	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
33:DI:92:VAL:CG1	33:DI:120:ILE:HB	2.33	0.59
58:D1:935:C:O2	58:D1:935:C:O4'	2.20	0.59
22:Ab:78:G:O2'	22:Ab:79:G:O5'	2.17	0.59
12:BL:90:VAL:O	12:BL:92:ASP:N	2.36	0.59
26:C4:3:C:H2'	26:C4:3:C:O2	2.01	0.59
29:CC:81:ILE:HG22	29:CC:81:ILE:O	2.02	0.59
36:CN:1:MET:HE2	36:CN:32:TYR:CE2	2.38	0.59
46:CY:76:CYS:SG	46:CY:77:PRO:CD	2.91	0.59
50:CK:7:ARG:NH2	58:C1:99:G:OP2	2.36	0.59
28:DB:238:GLY:O	28:DB:239:ARG:CB	2.50	0.59
56:D9:31:HIS:HE1	58:D1:2403:A:OP2	1.86	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
2:BA:47:THR:O	2:BA:51:LEU:HD12	2.03	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:4:VAL:HA	30:CD:19:GLU:HB3	1.85	0.58
30:CD:24:LEU:O	30:CD:26:ALA:N	2.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:AN:44:LEU:C	14:AN:44:LEU:HD12	2.28	0.58
22:Bb:108:U:H2'	22:Bb:109:G:C8	2.38	0.58
41:CS:54:ARG:HA	41:CS:59:THR:HB	1.86	0.58
58:C1:552:A:C2	58:C1:2063:A:H2'	2.37	0.58
58:C1:2147:A:O2'	58:C1:2148:G:OP2	2.19	0.58
31:DE:104:GLU:OE1	52:D5:50:THR:HG22	2.03	0.58
42:DT:13:LYS:HD3	58:D1:1272:G:OP1	2.03	0.58
49:DH:52:ARG:O	49:DH:56:GLN:O	2.21	0.58
58:D1:1540:A:C2	58:D1:1541:A:C2	2.91	0.58
10:AJ:79:ARG:HA	10:AJ:79:ARG:HH11	1.68	0.58
16:AP:28:ARG:NH2	22:Ab:386:C:O3'	2.36	0.58
22:Ab:816:C:O2'	22:Ab:817:U:O5'	2.21	0.58
19:BT:63:THR:O	19:BT:66:MET:HG2	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
48:Ca:43:THR:HG23	48:Ca:43:THR:O	2.03	0.58
58:C1:464:G:O2'	58:C1:465:G:H5'	2.03	0.58
58:C1:1540:A:O4'	58:C1:1540:A:OP1	2.21	0.58
59:Ds:52:A:O2'	59:Ds:53:A:N7	2.35	0.58
15:AO:82:ILE:HD13	15:AO:82:ILE:C	2.29	0.58
16:AP:20:VAL:HG21	16:AP:32:TYR:CG	2.38	0.58
22:Ab:144:A:O2'	22:Ab:145:C:C6	2.55	0.58
45:CX:64:LYS:HE2	58:C1:1381:A:OP2	2.03	0.58
48:Ca:43:THR:HG22	58:C1:2342:G:O3'	2.03	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
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
14:AN:29:ARG:HG2	14:AN:40:CYS:HB2	1.85	0.58
37:CO:38:GLN:CD	58:C1:987:U:OP2	2.47	0.58
41:CS:125:ARG:O	41:CS:128:GLU:HG3	2.04	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
42:DT:31:SER:C	42:DT:33:ARG:H	2.11	0.58
58:D1:1441:U:O2	58:D1:1441:U:C2'	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
10:BJ:58:ASP:O	10:BJ:59:SER:C	2.47	0.58
30:CD:8:GLN:HB3	30:CD:126:VAL:HA	1.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:D1:842:C:H2'	58:D1:843:C:C6	2.39	0.58
2:AA:24:TRP:CZ3	2:AA:26:PRO:HA	2.39	0.58
3:AC:29:TYR:OH	14:AN:54:PRO:O	2.21	0.58
22:Bb:275:A:OP2	17:BR:95:TYR:OH	2.16	0.58
2:BA:88:ALA:HB2	2:BA:219:VAL:CG1	2.33	0.58
25:C2:1:G:N3	25:C2:1:G:H2'	2.18	0.58
28:CB:10:THR:C	28:CB:11:PRO:O	2.47	0.58
49:CH:29:GLY:O	49:CH:30:VAL:CG2	2.51	0.58
46:DY:8:LYS:HB2	46:DY:28:LYS:CE	2.34	0.58
58:D1:1035:A:OP2	58:D1:1036:C:OP2	2.20	0.58
3:AC:154:SER:HB2	22:Ab:1040:G:H5''	1.86	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
58:C1:1098:C:O3'	58:C1:1151:A:P	2.62	0.58
35:DM:18:ALA:HB1	35:DM:21:LYS:HB2	1.85	0.58
37:DO:7:ARG:NH1	37:DO:7:ARG:HA	2.19	0.58
37:DO:23:PRO:HD2	37:DO:33:ARG:NH2	2.18	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:C6:3:LYS:O	53:C6:4:HIS:C	2.46	0.58
40:DR:16:ASN:O	40:DR:19:LYS:HB3	2.04	0.58
49:DH:56:GLN:HE21	49:DH:56:GLN:CA	2.17	0.58
53:D6:42:PRO:HB2	53:D6:43:HIS:CD2	2.39	0.58
22:Ab:1219:C:HO2'	22:Ab:1282:G:H22	1.52	0.58
22:Bb:616:A:C8	22:Bb:617:G:C8	2.92	0.58
22:Bb:1161:A:H5''	9:BI:102:LEU:CD2	2.33	0.58
28:DB:209:ALA:C	28:DB:210:GLY:O	2.43	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
22:Bb:172:C:OP1	20:BU:65:LYS:NZ	2.37	0.57
22:Bb:671:A:O2'	22:Bb:685:C:N4	2.36	0.57
29:CC:70:ALA:O	29:CC:72:VAL:N	2.36	0.57
35:CM:1:MET:HE3	35:CM:3:THR:H	1.69	0.57
41:CS:96:ARG:NH1	58:C1:1784:C:OP1	2.37	0.57
58:C1:1359:C:H5'	58:C1:1359:C:H6	1.67	0.57
42:DT:2:PRO:HA	58:D1:470:C:OP1	2.03	0.57
42:DT:92:ARG:NH2	58:D1:1041:A:OP2	2.36	0.57
46:DY:46:LYS:H	46:DY:62:GLU:HG2	1.68	0.57
59:Ds:52:A:O2'	59:Ds:53:A:C8	2.52	0.57
5:AE:42:GLY:HA3	5:AE:66:MET:HG2	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:AM:102:ARG:NH1	22:Ab:928:U:O5'	2.38	0.57
22:Ab:1037:C:OP2	22:Ab:1179:G:OP2	2.22	0.57
22:Bb:144:A:O2'	22:Bb:145:C:P	2.61	0.57
22:Bb:1311:A:N7	21:BW:7:ARG:NH2	2.52	0.57
37:CO:17:LYS:O	37:CO:19:VAL:N	2.36	0.57
32:DF:83:TYR:HB3	32:DF:134:SER:HA	1.85	0.57
37:DO:64:LYS:HG3	56:D9:25:MET:HE2	1.84	0.57
41:DS:89:VAL:CG1	41:DS:91:ARG:HG3	2.34	0.57
53:D6:43:HIS:HD2	58:D1:2824:C:O2'	1.85	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
22:Ab:144:A:O2'	22:Ab:145:C:H6	1.86	0.57
22:Ab:955:A:H2'	22:Ab:956:A:H5'	1.86	0.57
22:Ab:1275:G:O2'	22:Ab:1276:G:P	2.62	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
56:C9:30:ARG:O	56:C9:31:HIS:HB3	2.05	0.57
58:C1:274:C:O2'	58:C1:275:C:H6	1.87	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
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
43:DU:15:GLU:O	43:DU:16:PRO:C	2.47	0.57
22:Ab:246:A:H4'	22:Ab:247:G:O5'	2.04	0.57
22:Bb:721:A:H2'	22:Bb:722:C:C6	2.39	0.57
19:BT:9:VAL:O	19:BT:11:VAL:N	2.38	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
32:DF:41:MET:CE	32:DF:43:VAL:HG13	2.35	0.57
43:DU:19:LYS:HG3	43:DU:20:LEU:N	2.18	0.57
6:AF:60:PHE:C	6:AF:61:LEU:HD12	2.30	0.57
13:AM:100:GLY:C	13:AM:101:GLN:HG2	2.29	0.57
22:Bb:676:U:OP1	11:BK:124:LYS:CE	2.53	0.57
33:CI:133:HIS:HB2	33:CI:134:PRO:CD	2.35	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
29:DC:134:ILE:C	29:DC:134:ILE:HD12	2.28	0.57
31:DE:132:ASN:HB2	58:D1:2314:G:O2'	2.05	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
40:DR:32:LEU:HD11	59:Ds:30:C:OP2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:DS:92:GLY:O	41:DS:93:ARG:C	2.47	0.57
45:DX:12:VAL:HG11	45:DX:27:THR:OG1	2.04	0.57
48:Da:23:VAL:HA	48:Da:38:VAL:HG22	1.85	0.57
54:D7:28:ARG:O	54:D7:32:ASN:HB3	2.04	0.57
58:D1:1541:A:C8	58:D1:1623:C:O2'	2.57	0.57
12:AL:89:ARG:HA	12:AL:97:ARG:HA	1.86	0.57
22:Ab:324:C:H4'	22:Ab:325:A:H5'	1.86	0.57
22:Ab:845:G:O2'	22:Ab:846:C:H5'	2.04	0.57
22:Ab:1060:G:N2	22:Ab:1063:A:OP2	2.32	0.57
22:Ab:1263:U:H4'	22:Ab:1264:C:OP2	2.04	0.57
22:Bb:955:A:H2'	22:Bb:956:A:H5'	1.87	0.57
9:BI:118:LYS:O	9:BI:119:ALA:HB3	2.05	0.57
28:CB:9:TYR:CD1	28:CB:10:THR:HG22	2.39	0.57
32:CF:20:ALA:HB1	32:CF:21:PRO:HD2	1.85	0.57
39:CQ:3:HIS:HB2	58:C1:1700:A:P	2.44	0.57
58:C1:8:U:C5	58:C1:2640:A:N6	2.72	0.57
58:C1:247:G:H21	58:C1:645:A:H8	1.52	0.57
58:C1:2318:G:N3	58:C1:2318:G:H5''	2.20	0.57
62:DA:36:LYS:HA	62:DA:36:LYS:HE3	1.86	0.57
8:AH:1:MET:HE2	8:AH:2:LEU:H	1.69	0.57
9:AI:28:VAL:HG22	9:AI:63:ILE:HB	1.86	0.57
22:Ab:1143:G:O6	22:Ab:1163:G:C6	2.58	0.57
17:BR:45:HIS:HB2	17:BR:65:ILE:HD13	1.86	0.57
37:CO:39:LYS:HD3	58:C1:852:C:OP2	2.04	0.57
41:CS:28:VAL:HG22	41:CS:46:GLU:HG3	1.85	0.57
49:CH:67:ILE:N	49:CH:68:PRO:HD2	2.20	0.57
58:C1:2332:G:H2'	58:C1:2332:G:N3	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
31:DE:137:GLU:HG2	31:DE:152:LEU:HD23	1.86	0.57
46:DY:17:SER:HA	46:DY:71:LYS:HE2	1.85	0.57
22:Bb:943:A:C2	22:Bb:947:A:C2	2.93	0.57
22:Bb:1374:U:H2'	22:Bb:1375:G:C8	2.40	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:C1:2789:G:H5''	58:C1:2790:A:H5'	1.86	0.57
45:DX:35:THR:HG22	58:D1:1643:C:O3'	2.05	0.57
58:D1:1540:A:N3	58:D1:1541:A:C2	2.73	0.57
22:Ab:33:A:C2	22:Ab:34:A:C5	2.93	0.57
22:Ab:108:U:H2'	22:Ab:109:G:C8	2.39	0.57
4:BD:9:CYS:HA	4:BD:12:CYS:HB2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:BM:82:MET:HG2	13:BM:82:MET:O	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
22:Bb:1301:A:OP2	19:BT:5:LEU:HD23	2.05	0.57
5:BE:76:ILE:HD11	5:BE:142:LEU:HD21	1.86	0.57
37:CO:16:ARG:HH12	58:C1:707:C:H4'	1.70	0.57
46:CY:2:ARG:C	46:CY:4:LYS:H	2.13	0.57
58:C1:1983:C:O5'	58:C1:1983:C:O2'	2.22	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
22:Ab:923:G:H2'	22:Ab:923:G:N3	2.20	0.56
22:Bb:9:A:H62	4:BD:208:SER:HB2	1.69	0.56
9:BI:50:LEU:O	9:BI:53:VAL:HG22	2.05	0.56
14:BN:44:LEU:C	14:BN:44:LEU:HD12	2.30	0.56
58:C1:1539:A:H3'	58:C1:1539:A:N3	2.20	0.56
36:DN:4:PRO:O	36:DN:5:GLN:CB	2.53	0.56
41:DS:54:ARG:HA	41:DS:59:THR:HB	1.86	0.56
58:D1:2744:G:H3'	58:D1:2745:A:C5'	2.34	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
32:CF:156:ALA:O	32:CF:157:TYR:C	2.48	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
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
41:DS:106:SER:C	41:DS:107:ASP:OD1	2.48	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
2:AA:167:PRO:HG3	2:AA:188:ALA:HB2	1.86	0.56
5:AE:51:VAL:HB	5:AE:52:PRO:HD3	1.86	0.56
7:AG:116:ALA:O	7:AG:118:VAL:N	2.38	0.56
16:AP:20:VAL:HG21	16:AP:32:TYR:CD1	2.40	0.56
22:Bb:802:G:O2'	22:Bb:803:A:H5''	2.06	0.56
22:Bb:1043:C:C5	24:BC:2:GLY:HA2	2.40	0.56
4:BD:11:LEU:C	4:BD:13:ARG:N	2.59	0.56
4:BD:30:LYS:C	4:BD:32:ALA:N	2.63	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:BM:67:GLU:OE2	13:BM:68:GLY:N	2.38	0.56
25:C2:72:C:H2'	25:C2:72:C:O2	2.05	0.56
28:CB:210:GLY:O	28:CB:211:ARG:HB3	2.04	0.56
31:CE:70:VAL:O	59:Cs:41:U:O4	2.22	0.56
41:CS:12:SER:O	41:CS:13:ARG:CZ	2.54	0.56
42:CT:47:TYR:HA	42:CT:50:ARG:NH2	2.20	0.56
50:CK:65:ASN:HB3	50:CK:69:ARG:NH2	2.20	0.56
58:C1:669:C:O2	58:C1:669:C:O4'	2.22	0.56
58:C1:1346:A:O2'	58:C1:1347:A:C3'	2.50	0.56
58:C1:2643:A:HO2'	58:C1:2820:G:HO2'	1.51	0.56
61:D4:4:G:H8	61:D4:4:G:H5''	1.71	0.56
61:D4:18:U:H5''	61:D4:19:G:OP2	2.05	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
43:DU:49:THR:HB	43:DU:50:PRO:CD	2.36	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
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
22:Ab:369:A:C2	22:Ab:370:A:C8	2.93	0.56
22:Ab:921:U:C2'	22:Ab:922:G:H5'	2.36	0.56
22:Ab:1282:G:HO2'	22:Ab:1283:U:P	2.26	0.56
10:BJ:49:VAL:HG22	14:BN:41:ARG:HB2	1.87	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
58:C1:1577:C:N4	58:C1:1579:G:OP1	2.38	0.56
61:D4:67:C:H2'	61:D4:68:C:H6	1.70	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
37:DO:13:ASN:C	37:DO:13:ASN:HD22	2.12	0.56
53:D6:16:ARG:NH1	53:D6:17:ASP:OD1	2.39	0.56
22:Ab:432:C:O2'	22:Ab:433:U:P	2.63	0.56
22:Bb:657:G:H2'	22:Bb:658:G:C8	2.39	0.56
22:Bb:798:A:N7	22:Bb:800:A:C4	2.74	0.56
22:Bb:1055:G:H2'	22:Bb:1056:U:C6	2.40	0.56
26:C4:2:G:C2	26:C4:3:C:C5	2.93	0.56
26:C4:73:A:H8	26:C4:73:A:OP2	1.88	0.56
46:CY:76:CYS:SG	46:CY:77:PRO:HD2	2.45	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O2	58:C1:1935:C:O4'	2.23	0.56
28:DB:45:ASN:CG	28:DB:46:GLN:H	2.13	0.56
31:DE:45:GLU:CD	31:DE:45:GLU:H	2.14	0.56
32:DF:20:ALA:HB1	32:DF:21:PRO:HD3	1.87	0.56
47:DZ:7:ALA:HB2	47:DZ:59:LEU:HD22	1.88	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
13:AM:90:LEU:C	13:AM:92:HIS:H	2.14	0.56
22:Ab:68:C:H2'	22:Ab:69:G:C8	2.41	0.56
19:BT:5:LEU:HD12	19:BT:8:GLY:C	2.31	0.56
25:C2:17:C:OP2	25:C2:17:C:H4'	2.05	0.56
29:CC:131:ALA:CB	58:C1:2590:C:O2'	2.54	0.56
35:CM:63:THR:HG21	58:C1:1185:U:H2'	1.87	0.56
43:CU:91:TYR:C	43:CU:91:TYR:HD1	2.14	0.56
58:C1:906:U:O2	58:C1:906:U:O4'	2.22	0.56
49:DH:35:THR:HG21	58:D1:2101:G:OP1	2.05	0.56
58:D1:2083:A:H2'	58:D1:2084:C:H5'	1.87	0.56
9:AI:42:ARG:NH1	9:AI:71:SER:OG	2.39	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
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
22:Ab:1176:U:H2'	22:Ab:1177:C:C6	2.40	0.56
22:Bb:458:A:O2'	16:BP:81:ARG:HA	2.06	0.56
30:CD:167:ALA:HB1	30:CD:173:VAL:HG11	1.87	0.56
41:CS:92:GLY:O	41:CS:93:ARG:C	2.49	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
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
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
20:AU:29:LYS:NZ	22:Ab:171:C:OP1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:Ab:378:A:H2'	22:Ab:379:A:C8	2.40	0.56
24:BC:29:TYR:OH	14:BN:54:PRO:O	2.22	0.56
5:BE:12:LEU:HD13	5:BE:31:LEU:HB3	1.88	0.56
39:CQ:36:THR:HG22	58:C1:1323:A:OP1	2.05	0.56
58:C1:2051:A:H5''	58:C1:2052:A:OP1	2.06	0.56
37:DO:144:GLU:N	37:DO:145:PRO:HD3	2.21	0.56
41:DS:56:GLY:O	41:DS:59:THR:HG23	2.06	0.56
59:Ds:13:A:N1	59:Ds:69:G:O2'	2.29	0.56
58:D1:552:A:C2	58:D1:2064:C:H4'	2.41	0.56
22:Ab:957:C:H3'	22:Ab:958:C:H5''	1.87	0.55
22:Ab:1109:U:OP2	22:Ab:1263:U:O2	2.23	0.55
12:BL:32:PHE:HB3	12:BL:84:LEU:HD21	1.87	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
58:C1:935:C:O2	58:C1:935:C:O4'	2.22	0.55
35:DM:83:LYS:NZ	58:D1:2652:G:OP2	2.26	0.55
38:DP:1:MET:HE1	38:DP:45:GLN:HA	1.87	0.55
39:DQ:20:LEU:HD21	39:DQ:40:LYS:HD3	1.87	0.55
41:DS:3:ARG:O	41:DS:4:GLY:C	2.49	0.55
43:DU:38:LEU:C	43:DU:39:LEU:HD13	2.31	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
22:Bb:1310:C:P	21:BW:21:TYR:OH	2.63	0.55
6:BF:62:TRP:CH2	6:BF:64:GLN:HB2	2.41	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
48:Da:39:ARG:NH2	58:D1:2366:C:O2	2.40	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
22:Bb:1040:G:H5''	24:BC:154:SER:CB	2.36	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:C1:68:G:H2'	58:C1:110:G:O2'	2.05	0.55
28:DB:62:TYR:CZ	58:D1:1846:G:C8	2.95	0.55
45:DX:18:TYR:C	45:DX:20:GLY:N	2.65	0.55
59:Ds:13:A:N6	59:Ds:70:C:H5'	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
26:C4:62:C:H2'	26:C4:63:C:C6	2.41	0.55
31:CE:148:MET:HA	31:CE:148:MET:HE3	1.89	0.55
35:CM:25:ARG:NH2	58:C1:1188:A:OP1	2.39	0.55
30:DD:24:LEU:O	30:DD:26:ALA:N	2.39	0.55
58:D1:1596:C:OP1	58:D1:1764:U:O2'	2.24	0.55
9:AI:125:TYR:HB3	22:Ab:1324:C:H4'	1.89	0.55
22:Bb:559:G:H4'	22:Bb:560:G:H5'	1.89	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
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
56:C9:52:LYS:N	56:C9:53:PRO:HD2	2.20	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
22:Ab:33:A:C2	22:Ab:34:A:C4	2.95	0.55
22:Ab:1303:C:H3'	22:Ab:1304:C:H5''	1.89	0.55
22:Bb:392:G:O2'	22:Bb:394:C:OP1	2.18	0.55
4:BD:25:ARG:O	4:BD:28:SER:N	2.31	0.55
29:CC:111:ARG:HA	39:CQ:2:ARG:HB3	1.89	0.55
30:CD:132:VAL:HG13	30:CD:133:ASN:CG	2.31	0.55
39:CQ:96:ARG:NE	58:C1:2891:A:OP1	2.35	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:C1:670:A:H2'	58:C1:671:G:O4'	2.06	0.55
31:DE:116:ASP:O	31:DE:117:PHE:CB	2.53	0.55
33:DI:133:HIS:HB2	33:DI:134:PRO:HD2	1.89	0.55
36:DN:22:ILE:HD12	58:D1:1973:A:C6	2.41	0.55
36:DN:23:ARG:NH1	58:D1:2573:U:O2'	2.37	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
54:D7:46:HIS:CB	54:D7:47:THR:HG21	2.36	0.55
59:Ds:21:G:O2'	59:Ds:22:U:P	2.65	0.55
58:D1:927:G:O2'	64:DV:19:G:O6	1.98	0.55
58:D1:1539:A:H2'	58:D1:1540:A:C5'	2.36	0.55
58:D1:2203:G:H2'	58:D1:2204:C:C6	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:Ab:802:G:H3'	22:Ab:803:A:H5'	1.88	0.55
22:Bb:969:U:O4	22:Bb:1194:U:O2'	2.25	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
43:CU:91:TYR:C	43:CU:91:TYR:CD1	2.85	0.55
61:D4:48:U:O4'	61:D4:48:U:OP1	2.25	0.55
36:DN:104:ARG:HH21	41:DS:33:LYS:HE2	1.71	0.55
37:DO:7:ARG:CB	37:DO:8:PRO:CD	2.85	0.55
37:DO:47:ASP:HB3	37:DO:48:PRO:C	2.32	0.55
37:DO:63:PRO:HB3	56:D9:13:ARG:HB3	1.88	0.55
46:DY:42:VAL:CG1	46:DY:65:ALA:HB3	2.37	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
3:AC:11:ARG:O	3:AC:12:LEU:C	2.49	0.55
16:AP:28:ARG:HG2	16:AP:29:ASP:OD2	2.06	0.55
22:Ab:1005:G:H2'	22:Ab:1005:G:N3	2.22	0.55
22:Ab:1037:C:N3	25:C2:34:G:H1'	2.22	0.55
22:Bb:932:G:H2'	22:Bb:933:U:C6	2.42	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
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
41:CS:12:SER:O	41:CS:13:ARG:NE	2.40	0.55
58:C1:967:U:H2'	58:C1:968:C:C6	2.42	0.55
40:DR:34:HIS:NE2	40:DR:54:LEU:HB3	2.22	0.55
58:D1:67:C:O2	58:D1:71:A:O2'	2.22	0.55
13:AM:7:VAL:O	13:AM:7:VAL:HG12	2.07	0.55
19:AT:40:ILE:HG21	19:AT:62:ILE:HD11	1.87	0.55
19:AT:58:VAL:HG23	19:AT:58:VAL:O	2.07	0.55
22:Bb:1275:G:O2'	22:Bb:1276:G:H8	1.89	0.55
22:Bb:1355:U:OP1	9:BI:72:GLY:N	2.38	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
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
2:AA:80:ILE:H	2:AA:80:ILE:HD12	1.71	0.55
4:AD:9:CYS:HB2	4:AD:22:LYS:HD2	1.89	0.55
22:Ab:50:U:C2	22:Ab:357:G:N2	2.75	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:Ab:795:C:O2'	22:Ab:879:A:N1	2.40	0.55
22:Bb:144:A:O2'	22:Bb:145:C:OP2	2.24	0.55
22:Bb:765:A:O2'	22:Bb:1500:U:O2	2.23	0.55
22:Bb:1176:U:H2'	22:Bb:1177:C:C6	2.42	0.55
2:BA:77:ALA:HB2	2:BA:211:ILE:HD13	1.87	0.55
61:D4:35:C:O2	61:D4:35:C:H2'	2.07	0.55
37:DO:7:ARG:HA	37:DO:7:ARG:HH11	1.72	0.55
37:DO:41:ARG:NH1	37:DO:45:LEU:HD13	2.22	0.55
54:D7:30:THR:O	54:D7:31:PRO:C	2.49	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
58:D1:2200:C:H4'	58:D1:2200:C:OP1	2.06	0.55
22:Ab:1055:G:H2'	22:Ab:1056:U:C6	2.42	0.54
22:Bb:1241:C:C5	22:Bb:1242:C:O2	2.59	0.54
22:Bb:1361:C:O2	22:Bb:1361:C:H2'	2.08	0.54
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
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
58:D1:431:U:O2	58:D1:431:U:O4'	2.25	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
29:CC:128:SER:OG	29:CC:129:HIS:N	2.36	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:C1:2222:C:O2'	58:C1:2223:C:H5'	2.07	0.54
28:DB:22:SER:O	28:DB:23:GLU:C	2.50	0.54
32:DF:85:LYS:HD2	32:DF:145:ALA:HB2	1.89	0.54
58:D1:439:C:H4'	58:D1:1901:C:O2'	2.07	0.54
58:D1:1009:C:H6	58:D1:1009:C:H5''	1.72	0.54
58:D1:1309:G:H3'	58:D1:1310:A:H5''	1.90	0.54
58:D1:2789:G:H5''	58:D1:2790:A:H5'	1.89	0.54
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
28:CB:70:TRP:CD1	28:CB:70:TRP:C	2.85	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
51:CL:19:GLN:HE22	51:CL:52:HIS:CE1	2.24	0.54
61:D4:33:C:O2	61:D4:33:C:H2'	2.07	0.54
41:DS:104:ASN:HB3	41:DS:105:LEU:HG	1.89	0.54
58:D1:1792:A:O5'	58:D1:1792:A:H8	1.90	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
17:AR:48:GLU:O	17:AR:49:GLU:C	2.50	0.54
22:Bb:802:G:C3'	22:Bb:803:A:H5'	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
61:D4:17:C:O2'	61:D4:18:U:OP1	2.24	0.54
58:D1:113:C:O2'	58:D1:123:A:N3	2.35	0.54
4:AD:31:CYS:C	4:AD:33:MET:H	2.16	0.54
4:AD:36:ARG:NH1	22:Ab:422:G:OP1	2.25	0.54
4:AD:92:VAL:O	4:AD:96:LEU:HD13	2.08	0.54
4:AD:117:ALA:O	4:AD:121:VAL:HG23	2.07	0.54
11:AK:111:ASP:HA	18:AS:84:LYS:HE2	1.90	0.54
22:Ab:557:A:C2	22:Ab:558:A:C2	2.95	0.54
22:Ab:777:U:O2	22:Ab:1494:G:H4'	2.08	0.54
22:Bb:1296:C:OP2	19:BT:6:LYS:HD3	2.07	0.54
37:CO:17:LYS:O	37:CO:17:LYS:HG2	2.08	0.54
53:C6:2:ALA:HA	58:C1:2036:A:H1'	1.89	0.54
58:C1:1066:A:H3'	58:C1:1066:A:H8	1.73	0.54
58:C1:1286:A:C2'	58:C1:1287:A:O5'	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
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
2:AA:185:ILE:HG22	2:AA:199:TYR:CD1	2.42	0.54
22:Bb:424:G:O4'	22:Bb:426:A:C8	2.61	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:C9:61:LEU:CD1	56:C9:62:LEU:HD12	2.36	0.54
59:Cs:74:U:H2'	59:Cs:75:G:O4'	2.08	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:91:ASP:CG	42:DT:96:ALA:HB2	2.33	0.54
42:DT:106:PHE:O	42:DT:109:LEU:HB2	2.07	0.54
22:Ab:1048:U:O2'	22:Ab:1049:C:P	2.65	0.54
22:Bb:434:G:OP1	4:BD:125:HIS:HE1	1.90	0.54
4:BD:168:ARG:N	4:BD:168:ARG:HD2	2.23	0.54
30:CD:9:ILE:HA	30:CD:13:SER:O	2.08	0.54
30:CD:63:LYS:HE2	58:C1:721:A:OP1	2.07	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:C1:1574:A:N7	58:C1:1575:G:C8	2.76	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
58:D1:1538:C:O2	58:D1:1538:C:C2'	2.56	0.54
7:AG:116:ALA:O	7:AG:119:ARG:N	2.36	0.54
22:Ab:324:C:H4'	22:Ab:325:A:C5'	2.37	0.54
22:Ab:775:G:C6	22:Ab:776:A:N7	2.75	0.54
22:Bb:559:G:H4'	22:Bb:560:G:C5'	2.37	0.54
4:BD:12:CYS:SG	4:BD:19:LEU:O	2.65	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:28:VAL:HG21	41:CS:88:ILE:HG13	1.90	0.54
41:CS:129:ARG:HH12	41:CS:131:ALA:HB2	1.72	0.54
58:C1:154:C:C3'	58:C1:157:U:P	2.95	0.54
58:C1:1333:U:H4'	58:C1:1334:C:OP2	2.07	0.54
58:C1:2672:G:H2'	58:C1:2673:A:C4	2.43	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:D1:47:A:H5''	58:D1:49:G:O4'	2.07	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
37:CO:47:ASP:HB3	37:CO:48:PRO:C	2.33	0.54
46:CY:98:VAL:O	46:CY:99:CYS:SG	2.65	0.54
28:DB:47:GLY:HA3	58:D1:819:U:H4'	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:DM:23:LEU:HD23	58:D1:1184:C:OP1	2.08	0.54
41:DS:3:ARG:C	41:DS:5:ALA:N	2.66	0.54
43:DU:17:GLY:HA2	43:DU:96:ILE:HB	1.90	0.54
58:D1:1064:U:O2'	58:D1:1066:A:H2	1.91	0.54
58:D1:1154:C:C5	58:D1:1155:G:C6	2.96	0.54
58:D1:2155:A:N3	58:D1:2155:A:H2'	2.23	0.54
15:AO:82:ILE:HG12	15:AO:87:ILE:HG13	1.89	0.54
22:Ab:677:G:H2'	22:Ab:678:A:O4'	2.07	0.54
22:Bb:1005:G:H2'	22:Bb:1005:G:N3	2.22	0.54
22:Bb:1291:G:C6	22:Bb:1311:A:C2	2.97	0.54
28:CB:20:ASP:C	28:CB:20:ASP:OD1	2.51	0.54
47:CZ:151:HIS:HA	47:CZ:171:ILE:HG12	1.90	0.54
49:CH:41:ARG:HD3	49:CH:43:TYR:OH	2.07	0.54
51:CL:49:LYS:NZ	58:C1:897:U:OP1	2.39	0.54
56:C9:50:LEU:C	56:C9:53:PRO:HD2	2.33	0.54
58:C1:2416:G:O2'	58:C1:2422:A:N6	2.40	0.54
62:DA:58:VAL:HG21	62:DA:166:UNK:H	1.73	0.54
28:DB:30:GLU:HB3	28:DB:35:LYS:HG3	1.89	0.54
38:DP:56:ARG:NH2	58:D1:2481:G:OP1	2.40	0.54
3:AC:172:ARG:HG2	22:Ab:1089:G:H5''	1.90	0.53
4:AD:43:HIS:O	4:AD:45:GLN:N	2.40	0.53
22:Ab:1289:U:H2'	22:Ab:1290:U:C6	2.43	0.53
22:Bb:1469:G:C5	65:Bb:1601:PAR:H51	2.43	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
25:C3:30:G:H2'	25:C3:31:A:C8	2.43	0.53
35:CM:42:TRP:O	42:CT:64:ARG:NH1	2.23	0.53
38:CP:16:ARG:NH2	58:C1:996:G:OP1	2.41	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
49:CH:51:VAL:O	49:CH:57:GLU: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
34:DJ:5:UNK:O	58:D1:1089:G:OP2	2.27	0.53
42:DT:90:VAL:HG21	43:DU:47:VAL:HG21	1.90	0.53
58:D1:659:C:O2'	58:D1:663:U:OP1	2.26	0.53
13:AM:112:GLY:O	13:AM:113:PRO:O	2.27	0.53
22:Bb:378:A:H2'	22:Bb:379:A:H8	1.72	0.53
22:Bb:901:A:O2'	22:Bb:1382:C:OP2	2.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
58:C1:2475:C:O2'	58:C1:2476:C:O4'	2.26	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
13:AM:104:ARG:NH2	22:Ab:930:U:C5	2.77	0.53
26:C4:16:C:O2'	26:C4:62:C:P	2.67	0.53
28:CB:49:ILE:HG23	58:C1:825:U:OP1	2.08	0.53
37:CO:85:LEU:HD23	37:CO:85:LEU:H	1.72	0.53
42:CT:92:ARG:O	42:CT:93:LYS:C	2.51	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:C1:1393:G:H2'	58:C1:1394:A:H5''	1.90	0.53
29:DC:4:ILE:HG12	29:DC:5:LEU:O	2.08	0.53
31:DE:26:GLN:N	31:DE:26:GLN:HE21	2.07	0.53
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:D1:2331:A:N3	58:D1:2331:A:H2'	2.24	0.53
58:D1:2529:A:H5'	58:D1:2529:A:C8	2.43	0.53
20:AU:74:LYS:NZ	22:Ab:127:C:O3'	2.42	0.53
22:Ab:105:G:O6	22:Ab:326:C:N4	2.40	0.53
22:Ab:719:C:H2'	22:Ab:720:C:H6	1.73	0.53
22:Ab:1433:C:OP1	22:Ab:1434:G:N1	2.42	0.53
22:Bb:169:C:H2'	22:Bb:170:C:C6	2.44	0.53
22:Bb:1289:U:H2'	22:Bb:1290:U: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: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
38:DP:56:ARG:NE	58:D1:2480:A:O2'	2.40	0.53
42:DT:90:VAL:O	42:DT:91:ASP:C	2.51	0.53
58:D1:1403:G:O2'	58:D1:1404:A:H5''	2.07	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
38:CP:55:VAL:O	38:CP:56:ARG:C	2.52	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:CW:91:GLY:HA2	58:C1:1659:A:N1	2.24	0.53
56:C9:30:ARG:O	56:C9:30:ARG:HD3	2.08	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:18:ARG:HB3	37:DO:18:ARG:CZ	2.38	0.53
37:DO:144:GLU:N	37:DO:145:PRO:CD	2.71	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
3:AC:177:THR:HG23	22:Ab:1094:A:N1	2.23	0.53
20:AU:96:GLY:O	20:AU:97:ALA:O	2.27	0.53
22:Bb:1269:A:H2'	22:Bb:1270:A:C8	2.44	0.53
22:Bb:1426:G:H3'	22:Bb:1427:A:H5''	1.91	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
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:C1:191:C:H3'	58:C1:192:A:H5''	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:C1:2692:C:H5	58:C1:2737:A:H62	1.55	0.53
22:Ab:60:A:N3	22:Ab:60:A:H2'	2.24	0.53
22:Ab:312:G:OP2	22:Ab:347:G:O2'	2.26	0.53
15:BO:23:GLY:O	15:BO:24:SER:HB3	2.08	0.53
29:CC:119:ARG:HG2	29:CC:160:TYR:HB2	1.90	0.53
30:CD:90:PHE:CD1	58:C1:610:U:H1'	2.44	0.53
37:CO:56:SER:O	37:CO:58:THR:N	2.42	0.53
55:C8:8:ASN:HD22	55:C8:9:ARG:N	2.05	0.53
58:C1:144:G:C2'	58:C1:145:G:H5'	2.38	0.53
28:DB:223:GLY:HA2	28:DB:226:MET:HE3	1.90	0.53
29:DC:69:LYS:C	29:DC:71:GLY:H	2.16	0.53
29:DC:197:ILE:HD11	29:DC:199:ARG:HE	1.74	0.53
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
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
3:AC:164:ARG:NH1	3:AC:166:GLU:OE1	2.41	0.53
19:AT:81:ARG:NE	22:Ab:1208:C:OP1	2.42	0.53
22:Bb:912:C:C6	22:Bb:1326:C:C5	2.97	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:BC:113:ALA:HB3	24:BC:114:PRO:CD	2.39	0.53
15:BO:32:LEU:O	15:BO:33:THR:C	2.51	0.53
37:CO:9:ASN:C	37:CO:11:GLY:N	2.67	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
40:DR:25:ARG:NH2	59:Ds:8:U:O3'	2.41	0.53
63:DW:29:LEU:HD21	63:DW:33:ARG:NH2	2.24	0.53
10:AJ:56:HIS:CE1	22:Ab:1044:G:H1'	2.44	0.53
14:AN:23:ARG:HD2	14:AN:28:GLY:O	2.09	0.53
22:Ab:1107:G:H2'	22:Ab:1128:C:H5	1.74	0.53
13:BM:15:VAL:O	13:BM:19:LEU:HD23	2.09	0.53
47:CZ:51:ALA:O	47:CZ:52:SER:HB3	2.09	0.53
49:CH:46:LEU:HD23	49:CH:61:ARG:HD3	1.91	0.53
58:C1:1066:A:H3'	58:C1:1066:A:C8	2.44	0.53
61:D4:48:U:H3'	61:D4:49:C:C5'	2.39	0.53
37:DO:6:LEU:CG	37:DO:8:PRO:O	2.56	0.53
37:DO:62:LEU:HD23	37:DO:62:LEU:H	1.74	0.53
38:DP:6:ARG:NH2	58:D1:915:G:O3'	2.37	0.53
42:DT:92:ARG:CZ	58:D1:1041:A:OP2	2.57	0.53
48:Da:44:ARG:NH2	58:D1:904:U:OP1	2.42	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
2:AA:100:GLY:O	2:AA:101:MET:C	2.51	0.53
5:AE:25:ARG:HH11	22:Ab:1053:U:P	2.32	0.53
6:AF:100:ASN:HD21	18:AS:23:LYS:HG2	1.74	0.53
12:AL:31:PRO:HG2	22:Ab:359:A:C2	2.43	0.53
19:AT:49:ILE:O	19:AT:60:VAL:HG12	2.08	0.53
22:Ab:1375:G:N2	22:Ab:1480:A:H8	2.06	0.53
10:BJ:90:LEU:N	10:BJ:91:PRO:CD	2.72	0.53
29:CC:137:HIS:HB3	29:CC:138:PRO:CD	2.38	0.53
30:CD:95:ARG:NH2	58:C1:1292:A:OP1	2.42	0.53
40:CR:69:VAL:O	40:CR:72:ALA:HB3	2.09	0.53
40:CR:97:ARG:NE	40:CR:97:ARG:C	2.67	0.53
46:CY:8:LYS:HD3	46:CY:72:VAL:HG23	1.90	0.53
56:C9:62:LEU:HD13	58:C1:230:G:C5'	2.33	0.53
41:DS:60:THR:HG22	41:DS:77:PRO:HA	1.90	0.53
49:DH:90:ILE:O	49:DH:94:LEU:N	2.39	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
22:Ab:921:U:H2'	22:Ab:922:G:H5'	1.91	0.52
22:Bb:125:A:C8	17:BR:63:ARG:HG3	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:Bb:459:G:H4'	16:BP:81:ARG:HH21	1.74	0.52
22:Bb:1135:A:H2'	22:Bb:1136:C:C6	2.44	0.52
22:Bb:1272:G:O2'	9:BI:40:LEU:HD21	2.09	0.52
4:BD:10:ARG:HG2	4:BD:11:LEU:HD23	1.92	0.52
28:CB:24:ILE:HG12	28:CB:25:THR:N	2.23	0.52
35:CM:27:ALA:HB3	35:CM:106:MET:HE3	1.90	0.52
37:CO:114:ILE:HD12	37:CO:115:LEU:N	2.24	0.52
41:CS:117:ASP:O	41:CS:118:ARG:C	2.52	0.52
58:C1:2604:U:H2'	58:C1:2605:C:C6	2.44	0.52
28:DB:238:GLY:O	58:D1:2602:C:OP2	2.27	0.52
29:DC:24:THR:CG2	29:DC:184:VAL:HG23	2.40	0.52
29:DC:188:VAL:O	29:DC:189:PRO:O	2.27	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
58:D1:1895:G:H5'	58:D1:1896:C:P	2.49	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
22:Bb:1464:G:H2'	22:Bb:1465:G:O4'	2.10	0.52
14:BN:15:LYS:O	14:BN:16:PHE:O	2.27	0.52
26:C4:1:C:O2	26:C4:1:C:H2'	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
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
46:DY:28:LYS:O	46:DY:29:GLU:C	2.51	0.52
54:D7:46:HIS:HA	54:D7:47:THR:HG21	1.90	0.52
58:D1:2228:A:H1'	58:D1:2230:G:C4	2.43	0.52
1:A2:19:U:N3	25:C2:37:A:C2	2.77	0.52
22:Ab:1037:C:H42	25:C2:34:G:C1'	2.15	0.52
22:Bb:584:C:H2'	22:Bb:585:C:C6	2.44	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
28:CB:24:ILE:C	28:CB:25:THR:O	2.53	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
56:C9:16:ILE:HD12	56:C9:57:ARG:HG2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:DX:29:TRP:CZ3	45:DX:78:LYS:HB3	2.44	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
22:Ab:1078:U:P	22:Ab:1091:G:H1	2.33	0.52
22:Bb:349:A:H5'	22:Bb:349:A:H8	1.74	0.52
22:Bb:1131:U:OP1	9:BI:7:THR:HG21	2.10	0.52
6:BF:10:LEU:HD13	6:BF:61:LEU:HD13	1.91	0.52
17:BR:53:LEU:CD2	17:BR:82:MET:HE1	2.40	0.52
20:BU:83:ARG:HA	20:BU:86:ARG:HD3	1.91	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
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
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
58:D1:669:C:O2	58:D1:669:C:O4'	2.26	0.52
58:D1:1463:G:OP1	58:D1:1633:C:O2'	2.24	0.52
9:AI:12:GLU:OE1	22:Ab:1233:A:H5''	2.10	0.52
22:Bb:1328:A:H5''	9:BI:120:ARG:HH12	1.73	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
42:CT:92:ARG:HB2	43:CU:11:GLN:NE2	2.25	0.52
58:C1:2554:G:H2'	58:C1:2555:G:C8	2.44	0.52
29:DC:63:LEU:O	29:DC:64:LYS:C	2.51	0.52
37:DO:64:LYS:HD2	56:D9:25:MET:SD	2.50	0.52
37:DO:64:LYS:C	37:DO:66:GLY:N	2.67	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
22:Ab:951:G:H3'	22:Ab:952:A:H5''	1.91	0.52
22:Ab:1291:G:C6	22:Ab:1311:A:C2	2.98	0.52
22:Ab:1331:A:H2'	22:Ab:1332:A:H8	1.75	0.52
22:Bb:258:A:H2'	22:Bb:259:A:C8	2.45	0.52
2:BA:135:GLN:O	2:BA:139:LYS:HG2	2.10	0.52
4:BD:8:VAL:C	4:BD:10:ARG:N	2.64	0.52
58:C1:154:C:H3'	58:C1:157:U:P	2.49	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:C1:1812:C:C4	58:C1:2598:A:N1	2.77	0.52
25:D3:67:C:H2'	25:D3:68:C:C6	2.45	0.52
28:DB:221:VAL:HG23	28:DB:226:MET:HE2	1.91	0.52
35:DM:42:TRP:CD1	42:DT:63:VAL:HG11	2.44	0.52
39:DQ:53:HIS:CD2	58:D1:2849:C:H5''	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
58:D1:1984:U:H4'	58:D1:1985:G:OP1	2.09	0.52
9:AI:47:LEU:C	9:AI:49:PRO:HD2	2.34	0.52
10:AJ:6:ILE:HD11	10:AJ:72:VAL:HB	1.92	0.52
22:Bb:454:G:O6	22:Bb:456:C:H5'	2.09	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
58:C1:676:C:OP2	58:C1:676:C:C6	2.63	0.52
58:C1:2412:U:C2'	58:C1:2413:C:H5''	2.38	0.52
36:DN:43:VAL:HG21	36:DN:52:VAL:CG1	2.40	0.52
37:DO:35:HIS:C	37:DO:36:LYS:HG3	2.33	0.52
46:DY:26:LYS:HG2	46:DY:27:VAL:H	1.74	0.52
50:DK:63:VAL:HA	50:DK:66:GLU:HG2	1.92	0.52
59:Ds:29:A:H2'	59:Ds:30:C:O4'	2.10	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
3:AC:23:TYR:C	3:AC:23:TYR:CD2	2.88	0.52
3:AC:134:ILE:HD11	3:AC:153:VAL:CG2	2.39	0.52
12:AL:91:LYS:HG3	12:AL:91:LYS:O	2.10	0.52
22:Ab:606:A:C8	22:Ab:607:C:C6	2.97	0.52
22:Bb:936:A:O4'	19:BT:55:LYS:NZ	2.41	0.52
28:CB:58:HIS:HD2	28:CB:59:LYS:O	1.93	0.52
28:CB:121:PRO:HB3	28:CB:135:PHE:HE2	1.72	0.52
37:CO:33:ARG:O	37:CO:34:GLY:C	2.53	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
25:D3:25:C:H2'	25:D3:26:A:H8	1.75	0.52
28:DB:239:ARG:HB3	58:D1:2602:C:OP2	2.09	0.52
29:DC:68:ALA:C	29:DC:70:ALA:H	2.18	0.52
39:DQ:77:ARG:NH1	58:D1:1500:U:OP1	2.42	0.52
58:D1:1326:G:H5''	58:D1:1326:G:H8	1.74	0.52
58:D1:2487:A:C2	58:D1:2488:C:C6	2.98	0.52
14:AN:21:TYR:HD2	14:AN:22:THR:O	1.93	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:AU:79:ARG:NH2	22:Ab:257:U:OP2	2.43	0.52
22:Ab:1285:C:H2'	22:Ab:1286:G:H5'	1.91	0.52
22:Bb:36:G:O2'	12:BL:118:SER:O	2.21	0.52
22:Bb:432:C:O2'	22:Bb:433:U:OP2	2.27	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
22:Ab:539:C:H2'	22:Ab:540:C:C6	2.45	0.52
22:Bb:721:A:H2'	22:Bb:722:C:H6	1.74	0.52
22:Bb:1193:U:H5'	22:Bb:1194:U:OP1	2.10	0.52
22:Bb:1241:C:N4	22:Bb:1242:C:O2	2.43	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
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:C1:552:A:C2	58:C1:2064:C:H4'	2.45	0.52
29:DC:11:MET:HE2	58:D1:2693:U:C5	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
58:D1:1066:A:H3'	58:D1:1066:A:C8	2.45	0.52
14:AN:40:CYS:SG	14:AN:43:CYS:N	2.77	0.51
22:Ab:802:G:C2'	22:Ab:803:A:H5'	2.40	0.51
22:Bb:410:A:H5'	22:Bb:410:A:C8	2.45	0.51
22:Bb:958:C:C5'	22:Bb:958:C:H6	2.23	0.51
22:Bb:1446:A:H8	22:Bb:1446:A:O5'	1.93	0.51
16:BP:28:ARG:HG2	16:BP:28:ARG:HH11	1.76	0.51
26:C4:49:C:C2	26:C4:60:A:H1'	2.45	0.51
28:CB:24:ILE:HA	28:CB:82:ILE:HG22	1.92	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:CS:30:VAL:HG21	41:CS:83:ILE:HG13	1.92	0.51
42:CT:59:ARG:HD2	58:C1:1054:A:O4'	2.10	0.51
44:CW:18:ARG:HG2	44:CW:76:VAL:HG13	1.92	0.51
49:CH:90:ILE:O	49:CH:94:LEU:HB2	2.11	0.51
29:DC:77:ILE:HG22	29:DC:78:LEU:HD12	1.92	0.51
37:DO:48:PRO:O	37:DO:50:ARG:N	2.43	0.51
4:AD:86:LYS:HA	4:AD:86:LYS:HE3	1.91	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:1:MET:HE1	43:CU:43:GLU:HG2	1.91	0.51
43:CU:52:VAL:HG13	43:CU:55:ALA:HB3	1.93	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
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
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
58:D1:634:C:C2'	58:D1:635:G:H5'	2.41	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
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
22:Bb:585:C:H2'	22:Bb:586:A:C8	2.45	0.51
18:BS:56:THR:HB	18:BS:58:LEU:HD13	1.91	0.51
35:CM:41:ASP:O	35:CM:42:TRP:C	2.53	0.51
37:CO:16:ARG:CZ	37:CO:18:ARG:HG2	2.41	0.51
46:CY:26:LYS:O	46:CY:27:VAL:O	2.28	0.51
58:C1:636:U:O4'	58:C1:636:U:O2	2.25	0.51
61:D4:76:C:O2'	66:D1:3001:3V6:H8	2.09	0.51
29:DC:24:THR:HG21	29:DC:188:VAL:CG1	2.40	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
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
22:Bb:836:G:O6	22:Bb:847:G:C8	2.64	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:HD1	47:CZ:38:TYR:O	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:C8:8:ASN:HD22	55:C8:8:ASN:C	2.18	0.51
58:C1:2192:A:O2'	58:C1:2193:U:O4'	2.26	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
50:DK:48:HIS:O	50:DK:52:ASP:HB2	2.11	0.51
58:D1:2612:C:O5'	58:D1:2612:C:H6	1.93	0.51
7:AG:116:ALA:O	7:AG:117:ALA:C	2.54	0.51
10:AJ:54:PHE:CE2	10:AJ:55:LYS:HE3	2.45	0.51
17:BR:48:GLU:O	17:BR:49:GLU:C	2.53	0.51
31:CE:71:THR:HG22	31:CE:89:GLY:C	2.35	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:C1:2808:U:O2	58:C1:2808:U:O4'	2.28	0.51
60:D2:55:U:H3'	60:D2:55:U:O2	2.11	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:HD23	37:DO:85:LEU:H	1.74	0.51
43:DU:28:GLU:HB3	43:DU:29:PRO:HD2	1.92	0.51
53:D6:40:LYS:CE	53:D6:46:CYS:HB3	2.41	0.51
58:D1:1530:G:H1'	58:D1:1550:C:N4	2.25	0.51
58:D1:2904:C:H3'	58:D1:2904:C:C6	2.44	0.51
10:AJ:61:GLU:OE1	14:AN:58:LYS:NZ	2.33	0.51
22:Ab:1092:C:H2'	22:Ab:1093:A:O4'	2.11	0.51
22:Ab:1342:A:H2'	22:Ab:1343:G:O4'	2.11	0.51
22:Bb:1308:C:OP1	21:BW:17:THR:OG1	2.23	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
28:CB:45:ASN:CG	28:CB:46:GLN:H	2.18	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
37:CO:66:GLY:O	37:CO:67:MET:HB3	2.09	0.51
41:CS:128:GLU:O	41:CS:130:ALA:N	2.43	0.51
32:DF:158:HIS:HE2	32:DF:170:ARG:C	2.19	0.51
42:DT:31:SER:O	42:DT:33:ARG:N	2.40	0.51
58:D1:2042:C:H4'	58:D1:2043:U:OP2	2.10	0.51
22:Bb:429:C:H2'	22:Bb:430:U:C6	2.45	0.51
22:Bb:1222:U:N3	7:BG:30:ILE:HG22	2.26	0.51
5:BE:20:GLN:O	5:BE:21:ALA:C	2.53	0.51
26:C4:10:G:C5'	26:C4:10:G:H8	2.23	0.51
29:CC:60:ASN:CB	58:C1:2820:G:OP1	2.54	0.51
32:CF:43:VAL:HG11	32:CF:52:VAL:HG22	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:CU:38:LEU:C	43:CU:39:LEU:HD13	2.35	0.51
58:C1:663:U:H2'	58:C1:664:C:C6	2.45	0.51
58:C1:1390:C:O2'	58:C1:1391:G:H5'	2.10	0.51
30:DD:108:LYS:O	30:DD:112:MET:HG3	2.11	0.51
42:DT:92:ARG:HD3	42:DT:94:ASN:HB3	1.92	0.51
56:D9:52:LYS:N	56:D9:53:PRO:CD	2.73	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
4:AD:55:ALA:HB2	22:Ab:493:A:H5''	1.92	0.51
4:AD:110:PHE:N	4:AD:110:PHE:CD1	2.78	0.51
22:Bb:1208:C:H2'	13:BM:103:THR:HB	1.93	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:N	47:CZ:57:ILE:HD12	2.26	0.51
56:C9:43:GLN:C	56:C9:44:LYS:HD2	2.35	0.51
58:C1:1479:A:H61	58:C1:1604:A:N6	2.09	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
58:D1:2239:G:C6	58:D1:2240:C:C4	2.99	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:HG12	19:AT:9:VAL:O	2.11	0.51
22:Ab:33:A:H2'	22:Ab:34:A:C8	2.46	0.51
22:Ab:1491:A:H2'	22:Ab:1492:C:H6	1.74	0.51
22:Bb:62:G:H2'	22:Bb:63:U:O4'	2.10	0.51
18:BS:44:LEU:O	18:BS:45:SER:O	2.29	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:48:MET:HE3	35:CM:48:MET:H	1.74	0.51
35:CM:58:ASP:O	35:CM:60:ILE:N	2.44	0.51
39:CQ:90:ARG:NH1	58:C1:2889:C:O3'	2.42	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:24:LEU:HD21	47:CZ:86:VAL:HG23	1.91	0.51
47:CZ:151:HIS:CB	47:CZ:170:THR:HA	2.41	0.51
49:CH:29:GLY:HA3	58:C1:2407:G:O2'	2.11	0.51
58:C1:2226:G:N2	58:C1:2227:G:H4'	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
58:D1:69:A:H5'	58:D1:71:A:C8	2.46	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
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
22:Bb:921:U:C2'	22:Bb:922:G:H5'	2.41	0.51
22:Bb:1426:G:H3'	22:Bb:1427:A:C5'	2.41	0.51
7:BG:16:LEU:CD1	9:BI:42:ARG:HA	2.40	0.51
33:CI:110:ASP:C	33:CI:112:LYS:H	2.19	0.51
42:CT:92:ARG:NE	58:C1:1041:A:H4'	2.26	0.51
58:C1:2154:G:C6	58:C1:2178:G:O6	2.64	0.51
32:DF:117:PRO:HB3	32:DF:123:PHE:CE1	2.46	0.51
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:14:SER:O	45:DX:15:GLU:C	2.54	0.51
58:D1:2309:A:H2'	58:D1:2310:G:O4'	2.10	0.51
58:D1:2535:G:C5'	58:D1:2535:G:H8	2.24	0.51
4:AD:41:GLY:HA3	22:Ab:526:G:H5'	1.94	0.50
22:Ab:1259:C:H2'	22:Ab:1260:U:H5'	1.93	0.50
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
30:CD:34:TRP:CZ2	37:CO:12:ALA:HB2	2.47	0.50
58:C1:559:C:O2'	58:C1:560:A:H5'	2.10	0.50
58:C1:1697:G:N2	58:C1:2028:C:C2	2.79	0.50
28:DB:62:TYR:OH	58:D1:1846:G:H8	1.93	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
32:DF:138:LYS:O	32:DF:139:GLN:C	2.54	0.50
35:DM:15:LEU:HB2	35:DM:134:ARG:HB2	1.93	0.50
35:DM:41:ASP:OD1	35:DM:41:ASP:N	2.43	0.50
47:DZ:52:SER:OG	47:DZ:53:ILE:N	2.43	0.50
58:D1:2786:C:H2'	58:D1:2787:A:O4'	2.11	0.50
9:AI:53:VAL:O	9:AI:54:ASP:HB2	2.12	0.50
22:Ab:1250:A:N3	22:Ab:1308:C:O2'	2.44	0.50
22:Ab:1258:G:N1	22:Ab:1259:C:O2	2.45	0.50
22:Ab:1320:G:C6	22:Ab:1321:A:C6	3.00	0.50
22:Bb:863:G:O2'	22:Bb:892:A:N1	2.41	0.50
4:BD:80:GLU:O	4:BD:84:LYS:HG2	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
33:CI:6:LEU:O	33:CI:7:GLU:C	2.54	0.50
44:CW:64:MET:O	44:CW:65:LEU:CB	2.58	0.50
51:CL:59:VAL:OXT	51:CL:59:VAL:HG12	2.11	0.50
48:Da:43:THR:HG23	48:Da:43:THR:O	2.11	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
22:Ab:1143:G:H2'	22:Ab:1143:G:N3	2.27	0.50
22:Bb:246:A:H4'	22:Bb:247:G:O5'	2.12	0.50
22:Bb:942:A:OP1	22:Bb:1181:U:OP1	2.29	0.50
28:CB:237:GLU:OE1	58:C1:2611:A:OP2	2.29	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
54:C7:22:ALA:HB2	54:C7:39:TYR:CE2	2.47	0.50
58:C1:1216:G:H5'	58:C1:1217:G:OP2	2.11	0.50
28:DB:259:THR:HG21	58:D1:1833:A:O2'	2.12	0.50
30:DD:132:VAL:HG13	30:DD:133:ASN:CG	2.37	0.50
31:DE:45:GLU:O	31:DE:46:ALA:HB3	2.10	0.50
56:D9:51:ALA:N	56:D9:53:PRO:HD2	2.25	0.50
58:D1:2738:U:O2	58:D1:2738:U:O4'	2.29	0.50
9:AI:43:ALA:C	9:AI:45:ALA:H	2.19	0.50
22:Ab:241:C:O2	22:Ab:279:C:N3	2.45	0.50
22:Ab:1303:C:H5''	22:Ab:1304:C:H5''	1.94	0.50
24:BC:52:LEU:HD23	24:BC:52:LEU:H	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
25:C2:27:G:H2'	25:C2:28:G:C8	2.46	0.50
28:CB:270:ILE:C	28:CB:270:ILE:HD12	2.36	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
58:C1:88:U:O2'	58:C1:89:A:H5''	2.11	0.50
58:C1:275:C:C2'	58:C1:276:G:H5'	2.41	0.50
58:C1:2226:G:N2	58:C1:2227:G:H5'	2.26	0.50
29:DC:77:ILE:HG21	58:D1:2646:C:OP1	2.10	0.50
31:DE:10:LYS:O	31:DE:15:VAL:HG23	2.12	0.50
50:DK:46:GLN:OE1	50:DK:46:GLN:HA	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:DK:71:ASN:OD1	50:DK:71:ASN:O	2.30	0.50
58:D1:7:A:H2'	58:D1:8:U:C6	2.46	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:D1:2057: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
64:DV:43:G:H2'	64:DV:44:A:C8	2.47	0.50
15:AO:25:THR:HG21	15:AO:70:LEU:HB2	1.93	0.50
19:AT:43:GLU:C	19:AT:45:VAL:H	2.20	0.50
22:Ab:1395:C:H2'	22:Ab:1396:A:C8	2.46	0.50
65:Ab:1601:PAR:H34	65:Ab:1601:PAR:HN61	1.75	0.50
22:Bb:951:G:N3	10:BJ:55:LYS:NZ	2.59	0.50
22:Bb:1037:C:N3	64:DV:34:G:H1'	2.26	0.50
2:BA:124:SER:OG	2:BA:125:PRO:HD2	2.10	0.50
33:CI:60:GLU:C	33:CI:62:LYS:H	2.20	0.50
35:CM:46:VAL:O	35:CM:47:ALA:HB3	2.11	0.50
37:CO:107:LYS:C	37:CO:109:GLY:H	2.18	0.50
43:CU:15:GLU:O	43:CU:16:PRO:C	2.54	0.50
46:CY:31:LEU:HB2	46:CY:32:PRO:HA	1.93	0.50
58:C1:2209:C:H2'	58:C1:2210:U:C6	2.47	0.50
58:C1:2596:U:O2	58:C1:2596:U:O4'	2.28	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
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
22:Ab:957:C:C5	22:Ab:958:C:C6	3.00	0.50
22:Ab:1037:C:C4	25:C2:34:G:H1'	2.46	0.50
23:B2:15:A:C2	25:D3:34:G:C6	2.98	0.50
22:Bb:702:G:C8	11:BK:116:HIS:HB3	2.46	0.50
22:Bb:1109:U:OP2	22:Bb:1263:U:O2	2.29	0.50
22:Bb:1135:A:H2'	22:Bb:1136:C:H6	1.77	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
62:DA:78:ALA:HB1	62:DA:82:LYS:HB2	1.93	0.50
28:DB:266:SER:OG	58:D1:1830:C:OP1	2.29	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)
58:D1:516:A:C2'	58:D1:517:G:O5'	2.59	0.50
12:AL:30:ALA:HB1	12:AL:31:PRO:HD2	1.92	0.50
18:AS:43:PHE:C	18:AS:51:LEU:HD12	2.37	0.50
20:AU:16:HIS:O	20:AU:19:SER:HB3	2.12	0.50
22:Bb:585:C:H2'	22:Bb:586:A:H8	1.77	0.50
22:Bb:804:U:H4'	22:Bb:805:G:OP2	2.11	0.50
22:Bb:1346:A:H1'	22:Bb:1348:G:N7	2.27	0.50
30:CD:81:PRO:HD2	58:C1:719:C:H5''	1.94	0.50
35:CM:63:THR:CG2	58:C1:1185:U:H2'	2.40	0.50
47:CZ:17:ALA:O	47:CZ:20:ARG:HG2	2.11	0.50
58:C1:1268:G:H5''	58:C1:1269:C:OP2	2.11	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
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
4:AD:10:ARG:NH2	22:Ab:526:G:OP1	2.45	0.50
5:AE:143:ARG:NH1	8:AH:77:GLU:CD	2.70	0.50
22:Ab:971:G:N3	22:Ab:971:G:H2'	2.27	0.50
22:Ab:1036:G:N7	22:Ab:1182:C:H5'	2.27	0.50
22:Bb:295:G:H2'	22:Bb:296:A:C8	2.47	0.50
22:Bb:1282:G:O2'	22:Bb:1283:U:O5'	2.30	0.50
5:BE:126:ARG:O	5:BE:127:ASN:C	2.54	0.50
12:BL:38:THR:HG21	12:BL:65:GLU:OE2	2.11	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
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
25:D3:16:U:C2	25:D3:19:G:OP2	2.64	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:85:GLY:C	31:DE:87:PRO:HD2	2.37	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
52:D5:42:CYS:SG	52:D5:62:CYS:HB3	2.52	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
13:AM:89:GLY:C	13:AM:90:LEU:O	2.52	0.50
22:Ab:1107:G:H2'	22:Ab:1128:C:C5	2.47	0.50
22:Bb:1161:A:O2'	9:BI:103:THR:HG23	2.12	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
28:CB:245:PRO:O	28:CB:246:PRO:C	2.55	0.50
47:CZ:127:LYS:HE2	47:CZ:164:ALA:HB2	1.94	0.50
58:C1:551:C:O2	58:C1:551:C:O4'	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
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
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
46:DY:2:ARG:C	46:DY:4:LYS:N	2.69	0.50
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
10:AJ:55:LYS:HG3	22:Ab:951:G:O4'	2.12	0.49
22:Ab:460:G:H2'	22:Ab:461:G:H8	1.77	0.49
22:Ab:1111:C:O2'	22:Ab:1113:A:N7	2.34	0.49
22:Bb:802:G:H3'	22:Bb:803:A:H5'	1.94	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
41:CS:67:SER:N	41:CS:70:VAL:O	2.45	0.49
58:C1:267:G:O2'	58:C1:268:G:H8	1.95	0.49
58:C1:516:A:H2'	58:C1:517:G:O4'	2.12	0.49
58:C1:2702:C:O2'	58:C1:2703:C:H5'	2.11	0.49
59:Cs:21:G:O2'	59:Cs:22:U:O4'	2.29	0.49
28:DB:35:LYS:HD3	28:DB:63:ARG:HD2	1.94	0.49
28:DB:210:GLY:O	28:DB:211:ARG:CB	2.60	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
59:Ds:79:C:O5'	59:Ds:79:C:H6	1.94	0.49
58:D1:8:U:C4	58:D1:2640:A:N6	2.80	0.49
22:Ab:144:A:O2'	22:Ab:145:C:P	2.70	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:Ab:658:G:H2'	22:Ab:659:A:H8	1.77	0.49
22:Ab:1259:C:O2'	22:Ab:1261:A:H8	1.94	0.49
22:Bb:1207:A:O3'	19:BT:81:ARG:NH2	2.42	0.49
2:BA:61:LEU:HD23	2:BA:68:ILE:HD11	1.93	0.49
17:BR:33:GLY:O	17:BR:34:LYS:C	2.55	0.49
20:BU:93:GLU:OE1	20:BU:94:ALA:N	2.45	0.49
31:CE:53:LEU:HD22	31:CE:53:LEU:N	2.26	0.49
31:CE:120:LEU:N	31:CE:179:PRO:O	2.34	0.49
58:C1:1540:A:N3	58:C1:1541:A:C2	2.80	0.49
58:C1:2535:G:H8	58:C1:2535:G:C5'	2.24	0.49
25:D3:34:G:N2	25:D3:35:A:N3	2.60	0.49
28:DB:266:SER:C	28:DB:267:SER:O	2.55	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
41:DS:32:TYR:CD2	41:DS:81:PRO:HB2	2.48	0.49
41:DS:57:PHE:O	41:DS:58:ASN:C	2.53	0.49
53:D6:35:GLU:O	53:D6:36:CYS:CB	2.60	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
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
22:Ab:1282:G:O2'	22:Ab:1283:U:O5'	2.29	0.49
22:Bb:58:G:H2'	22:Bb:59:C:C6	2.46	0.49
22:Bb:257:U:O2'	22:Bb:259:A:N7	2.34	0.49
2:BA:19:HIS:HD2	2:BA:189:ASP:OD2	1.95	0.49
4:BD:162:LEU:HD12	4:BD:181:MET:HE2	1.95	0.49
18:BS:37:VAL:O	18:BS:41:LYS:HB2	2.12	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
48:Ca:72:ARG:NH1	48:Ca:75:LEU:HD13	2.27	0.49
58:C1:55:C:H2'	58:C1:56:G:O4'	2.11	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
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
31:DE:2:PRO:HD2	52:D5:51:TYR:CZ	2.48	0.49
54:D7:15:GLU:OE2	54:D7:41:PRO:CG	2.60	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
17:AR:70:ARG:HG2	22:Ab:231:C:H5'	1.94	0.49
22:Bb:781:C:O2'	22:Bb:782:G:H5'	2.12	0.49
4:BD:18:LYS:HE2	4:BD:31:CYS:HB3	1.94	0.49
17:BR:7:THR:CG2	17:BR:58:GLU:HG2	2.42	0.49
29:CC:61:ARG:NH1	58:C1:2819:A:O2'	2.45	0.49
43:CU:28:GLU:CB	43:CU:29:PRO:HD2	2.42	0.49
46:CY:29:GLU:OE1	46:CY:29:GLU:N	2.46	0.49
55:C8:16:HIS:ND1	58:C1:730:G:OP1	2.44	0.49
58:C1:324:G:C4	58:C1:325:C:C5	3.00	0.49
58:C1:2291:G:O2'	58:C1:2399:A:N1	2.40	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
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
37:DO:16:ARG:HD3	37:DO:16:ARG:C	2.37	0.49
56:D9:62:LEU:N	56:D9:63:PRO:CD	2.75	0.49
58:D1:2492:G:C2'	58:D1:2493:G:OP2	2.61	0.49
3:AC:199:LYS:NZ	22:Ab:1042:C:OP2	2.39	0.49
22:Bb:1330:U:H4'	9:BI:120:ARG:HD2	1.94	0.49
9:BI:16:ARG:O	9:BI:63:ILE:HG23	2.12	0.49
9:BI:48:GLU:N	9:BI:49:PRO:HD2	2.27	0.49
28:CB:118:VAL:HG22	28:CB:119:ALA:H	1.77	0.49
28:CB:242:ARG:N	28:CB:242:ARG:HD2	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
38:CP:80:GLU:HA	58:C1:2505:G:O2'	2.12	0.49
50:CK:25:VAL:O	50:CK:26:ARG:C	2.55	0.49
56:C9:62:LEU:N	56:C9:63:PRO:CD	2.75	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
58:C1:1920:G:O2'	58:C1:1921:A:H5''	2.11	0.49
58:C1:2845:U:H2'	58:C1:2846:G:C8	2.48	0.49
25:D3:21:A:N6	25:D3:46:G:N3	2.60	0.49
48:Da:51:VAL:N	48:Da:62:LEU:HD12	2.28	0.49
22:Ab:938:U:H2'	22:Ab:938:U:O2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:Bb:439:C:H2'	22:Bb:440:G:H8	1.76	0.49
4:BD:127:THR:HG23	4:BD:147:ALA:HB3	1.94	0.49
28:CB:2:ALA:O	28:CB:3:VAL:HB	2.13	0.49
36:CN:17:ARG:HB2	36:CN:45:GLU:HG3	1.94	0.49
43:CU:23:GLU:O	43:CU:24:LYS:C	2.55	0.49
46:CY:28:LYS:O	46:CY:38:ILE:HB	2.13	0.49
50:CK:47:ASN:HD22	58:C1:92:G:H21	1.61	0.49
56:C9:33:ASN:O	56:C9:34:TRP:HB3	2.11	0.49
58:C1:534:C:OP1	58:C1:535:U:OP2	2.30	0.49
58:C1:1306:C:C2'	58:C1:1307:A:O5'	2.61	0.49
58:C1:1464:A:O2'	58:C1:1466:G:N7	2.41	0.49
58:C1:2488:C:C2	58:C1:2492:G:O6	2.66	0.49
25:D3:44:G:H2'	25:D3:45:U:O4'	2.13	0.49
28:DB:62:TYR:OH	58:D1:1846:G:C8	2.66	0.49
28:DB:70:TRP:CH2	28:DB:150:LYS:HA	2.48	0.49
30:DD:89:VAL:HG12	30:DD:90:PHE:H	1.78	0.49
36:DN:22:ILE:HD12	58:D1:1973:A:C5	2.48	0.49
58:D1:217:A:H3'	58:D1:218:U:H5'	1.95	0.49
58:D1:2083:A:O2'	58:D1:2084:C:P	2.71	0.49
22:Ab:607:C:C4	22:Ab:608:C:C5	3.00	0.49
22:Bb:1131:U:H2'	22:Bb:1132:C:O4'	2.12	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
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
58:C1:1777:G:H2'	58:C1:1778:G:H5'	1.94	0.49
28:DB:65:ILE:O	28:DB:65:ILE:HD13	2.13	0.49
30:DD:115:ALA:O	30:DD:116:ASP:C	2.56	0.49
32:DF:158:HIS:NE2	32:DF:170:ARG:O	2.46	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
41:DS:31:SER:CA	41:DS:32:TYR:CD2	2.96	0.49
47:DZ:105:VAL:O	47:DZ:141:VAL:HG13	2.12	0.49
49:DH:15:ALA:O	49:DH:40:ARG:HG3	2.12	0.49
54:D7:13:CYS:O	54:D7:21:TYR:HA	2.13	0.49
59:Ds:96:U:N3	59:Ds:97:G:N7	2.61	0.49
66:D1:3001:3V6:C	66:D1:3001:3V6:CLI	2.98	0.49
10:AJ:32:ALA:HB3	10:AJ:76:ASN:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:AS:58:LEU:HD23	18:AS:62:GLU:HB3	1.95	0.49
22:Ab:1385:C:C5	22:Ab:1386:C:C5	3.01	0.49
22:Bb:386:C:O3'	16:BP:28:ARG:NH2	2.46	0.49
22:Bb:1086:C:H5''	2:BA:98:LEU:HD13	1.93	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
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
38:CP:84:GLY:O	38:CP:85:LYS:HB2	2.13	0.49
41:CS:29:ARG:HB3	41:CS:85:LYS:HA	1.94	0.49
28:DB:24:ILE:O	28:DB:25:THR:C	2.48	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
47:DZ:85:HIS:CE1	59:Ds:75:G:H21	2.30	0.49
58:D1:491:A:N3	58:D1:729:C:H1'	2.28	0.49
58:D1:2083:A:C2'	58:D1:2084:C:H5'	2.42	0.49
13:AM:106:ASN:O	13:AM:107:ALA:CB	2.60	0.49
22:Ab:571:G:N2	22:Ab:738:C:OP2	2.46	0.49
22:Ab:1189:G:H2'	22:Ab:1190:C:H6	1.78	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
26:C4:7:G:H8	26:C4:7:G:O5'	1.96	0.49
40:CR:66:ALA:O	40:CR:69:VAL:HG12	2.13	0.49
58:C1:2107:U:H2'	58:C1:2108:G:C8	2.47	0.49
29:DC:95:ILE:HD13	29:DC:95:ILE:N	2.27	0.49
38:DP:1:MET:HE1	38:DP:45:GLN:CA	2.42	0.49
53:D6:57:VAL:C	53:D6:58:LEU:HD12	2.38	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
58:D1:1801:C:H1'	58:D1:1816:A:C8	2.47	0.49
22:Bb:242:A:O2'	17:BR:99:SER:CB	2.61	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
26:C4:10:G:H5'	26:C4:10:G:C8	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:C1:879:U:H2'	58:C1:880:C:C6	2.48	0.49
58:C1:2178:G:O2'	58:C1:2179:A:O5'	2.28	0.49
58:C1:2535:G:C5'	58:C1:2535:G:C8	2.96	0.49
28:DB:49:ILE:HG22	58:D1:825:U:OP1	2.13	0.49
28:DB:254:THR:OG1	58:D1:1854:G:N3	2.45	0.49
31:DE:25:TYR:OH	31:DE:168:GLU:OE1	2.31	0.49
38:DP:21:THR:O	38:DP:21:THR:HG22	2.12	0.49
51:DL:45:GLY:HA3	58:D1:897:U:O2'	2.13	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
58:D1:1095:A:O2'	58:D1:2764:C:H1'	2.13	0.49
58:D1:1097:C:C6	58:D1:1097:C:C3'	2.96	0.49
3:AC:179:ARG:HG2	22:Ab:1095:C:O2	2.13	0.48
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
22:Ab:424:G:O4'	22:Ab:426:A:C8	2.66	0.48
22:Ab:1482:G:O2'	22:Ab:1483:G:P	2.70	0.48
22:Bb:1207:A:H2'	22:Bb:1207:A:N3	2.28	0.48
22:Bb:1382:C:C2	22:Bb:1480:A:N6	2.81	0.48
18:BS:44:LEU:O	18:BS:45:SER:C	2.56	0.48
31:CE:82:LEU:HD21	31:CE:86:MET:HE2	1.94	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
58:C1:173:U:H4'	58:C1:206:A:H4'	1.95	0.48
58:C1:935:C:H1'	58:C1:936:A:O4'	2.13	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:C1:2089:U:N3	58:C1:2441:A:H2	2.10	0.48
58:C1:2402:G:O2'	58:C1:2435:C:N4	2.40	0.48
31:DE:87:PRO:C	31:DE:88:ILE:HD12	2.37	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
43:DU:79:VAL:HG22	58:D1:1232:U:H4'	1.95	0.48
58:D1:1377:G:N2	58:D1:1654:A:HO2'	2.08	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
13:AM:104:ARG:HD2	22:Ab:1208:C:N4	2.28	0.48
22:Ab:378:A:H2'	22:Ab:379:A:H8	1.78	0.48
22:Ab:438:C:H2'	22:Ab:439:C:C6	2.47	0.48
29:CC:61:ARG:NH2	58:C1:2643:A:C2'	2.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:CR:36:TYR:OH	59:Cs:28:C:OP1	2.27	0.48
42:CT:102:GLU:HG3	43:CU:2:PHE:CZ	2.47	0.48
58:C1:139:A:H5''	58:C1:140:C:OP2	2.12	0.48
58:C1:1902:C:H2'	58:C1:1902:C:O2	2.13	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
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
4:AD:9:CYS:CB	4:AD:22:LYS:HD2	2.43	0.48
9:AI:103:THR:HG23	22:Ab:1161:A:O3'	2.12	0.48
12:AL:25:PRO:O	12:AL:27:LEU:HD22	2.13	0.48
13:AM:20:THR:C	13:AM:22:ILE:H	2.22	0.48
19:AT:6:LYS:HG2	19:AT:7:LYS:HE3	1.93	0.48
22:Bb:983:A:O2'	22:Bb:1021:C:O2	2.27	0.48
22:Bb:1291:G:OP1	13:BM:92:HIS:HE1	1.97	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
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
42:CT:66:ASN:ND2	42:CT:70:ARG:HE	2.11	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
35:DM:25:ARG:NH2	58:D1:1188:A:OP1	2.46	0.48
41:DS:85:LYS:NZ	41:DS:85:LYS:HB3	2.28	0.48
58:D1:91:C:O2	58:D1:91:C:H2'	2.13	0.48
58:D1:721:A:C8	58:D1:850:A:C6	3.01	0.48
58:D1:1067:G:O2'	58:D1:1068:U:OP2	2.24	0.48
58:D1:2611:A:H5''	66:D1:3001:3V6:CB	2.43	0.48
4:AD:155:LEU:O	4:AD:156:GLU:C	2.57	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
12:AL:48:PRO:C	12:AL:49:ASN:HD22	2.22	0.48
13:AM:90:LEU:C	13:AM:92:HIS:N	2.72	0.48
22:Ab:923:G:C2	22:Ab:924:A:C8	3.01	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:Bb:1231:C:O2'	9:BI:73:GLN:OE1	2.22	0.48
65:Bb:1601:PAR:N21	65:Bb:1601:PAR:H42	2.28	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
29:CC:111:ARG:HG3	39:CQ:2:ARG:HG2	1.94	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
44:CW:59:VAL:HG12	44:CW:60:ASN:N	2.27	0.48
47:CZ:166:SER:HB2	47:CZ:167:PRO:C	2.38	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:24:GLY:O	35:DM:28:THR:HG22	2.13	0.48
35:DM:128:HIS:CG	35:DM:128:HIS:O	2.66	0.48
53:D6:4:HIS:HB2	53:D6:5:PRO:HD3	1.96	0.48
1:A2:19:U:C2	25:C2:37:A:C2	3.02	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
22:Bb:614:G:H2'	22:Bb:615:G:H5'	1.94	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
28:CB:24:ILE:CG1	28:CB:25:THR:N	2.75	0.48
28:CB:58:HIS:CD2	58:C1:1613:A:H5'	2.48	0.48
37:CO:10:PRO:O	37:CO:11:GLY:C	2.56	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
58:C1:8:U:O2'	58:C1:9:G:P	2.72	0.48
58:C1:1344:G:H5''	58:C1:1345:U:OP1	2.14	0.48
58:C1:1441:U:H2'	58:C1:1441:U:O2	2.13	0.48
58:C1:1479:A:H61	58:C1:1604:A:H62	1.61	0.48
28:DB:264:LYS:NZ	58:D1:1830:C:OP1	2.44	0.48
31:DE:5:VAL:HG22	31:DE:8:LYS:HB2	1.96	0.48
32:DF:156:ALA:C	32:DF:158:HIS:H	2.20	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
46:DY:27:VAL:C	46:DY:29:GLU:OE1	2.55	0.48
58:D1:31:C:O2'	58:D1:32:U:H5'	2.14	0.48
58:D1:1156:A:O2'	58:D1:1157:G:C1'	2.62	0.48
4:AD:8:VAL:C	4:AD:10:ARG:N	2.71	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:AU:103:GLY:H	22:Ab:199:U:H4'	1.79	0.48
22:Ab:715:G:OP1	22:Ab:750:A:H1'	2.13	0.48
22:Ab:1032:U:H1'	22:Ab:1183:A:N7	2.29	0.48
22:Bb:201:C:OP1	20:BU:61:SER:OG	2.31	0.48
22:Bb:445:G:N7	22:Bb:466:G:C6	2.82	0.48
22:Bb:1300:A:C1'	19:BT:37:ARG:HH21	2.27	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
39:CQ:23:ASN:ND2	58:C1:1339:U:O2'	2.47	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
41:DS:82:LEU:HD12	41:DS:82:LEU:N	2.28	0.48
50:DK:16:LEU:HD13	50:DK:20:GLU:HG3	1.95	0.48
51:DL:52:HIS:H	51:DL:52:HIS:CD2	2.30	0.48
58:D1:202:G:O2'	58:D1:203:G:O4'	2.25	0.48
58:D1:2450:A:C5'	58:D1:2450:A:C8	2.95	0.48
58:D1:2723:U:C5'	58:D1:2723:U:O2	2.61	0.48
58:D1:2807:G:H2'	58:D1:2807:G:N3	2.27	0.48
58:D1:2890:C:N3	58:D1:2891:A:N7	2.61	0.48
3:AC:154:SER:OG	3:AC:155:GLY:N	2.47	0.48
18:AS:30:ASP:C	18:AS:32:ARG:H	2.22	0.48
22:Ab:1241:C:N4	22:Ab:1242:C:O2	2.47	0.48
22:Bb:955:A:C2'	22:Bb:956:A:H5'	2.44	0.48
22:Bb:1206:G:H4'	13:BM:102:ARG:NH1	2.29	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
29:CC:96:PHE:HA	29:CC:100:GLU:OE1	2.13	0.48
29:CC:111:ARG:CZ	39:CQ:2:ARG:HH21	2.27	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
42:CT:66:ASN:C	42:CT:66:ASN:HD22	2.22	0.48
43:CU:4:ILE:O	43:CU:4:ILE:HG22	2.14	0.48
58:C1:2535:G:H5''	58:C1:2535:G:C8	2.45	0.48
61:D4:14:A:C5	61:D4:23:G:C6	3.02	0.48
28:DB:221:VAL:CG2	28:DB:226:MET:HE2	2.44	0.48
30:DD:53:THR:HG22	30:DD:56:GLU:CD	2.38	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
37:DO:33:ARG:CZ	58:D1:609:C:H2'	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
48:Da:53:MET:HG3	48:Da:59:LEU:HD23	1.94	0.48
58:D1:217:A:H3'	58:D1:218:U:C5'	2.43	0.48
2:AA:67:THR:HG21	2:AA:155:LEU:HD21	1.96	0.48
5:AE:92:LYS:HB3	5:AE:119:LEU:HB2	1.96	0.48
18:AS:44:LEU:O	18:AS:45:SER:C	2.57	0.48
22:Ab:174:A:H2'	22:Ab:175:U:C6	2.49	0.48
22:Ab:1287:G:C2	22:Ab:1313:G:N3	2.82	0.48
22:Ab:1385:C:C4	22:Ab:1386:C:C5	3.02	0.48
22:Bb:1427:A:C5	41:DS:118:ARG:CZ	2.97	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
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
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
56:D9:61:LEU:HD12	56:D9:62:LEU:H	1.78	0.48
58:D1:2449:U:H3'	58:D1:2449:U:H6	1.78	0.48
58:D1:2666:G:O2'	58:D1:2675:G:N1	2.43	0.48
2:AA:80:ILE:O	2:AA:80:ILE:HG22	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
22:Ab:342:G:OP1	41:CS:41:ARG:NH1	2.46	0.48
22:Bb:953:A:H5'	22:Bb:953:A:H8	1.76	0.48
22:Bb:994:A:H2'	22:Bb:995:A:C8	2.49	0.48
7:BG:116:ALA:O	7:BG:117:ALA:C	2.57	0.48
8:BH:4:ASP:CG	8:BH:85:ARG:HH21	2.21	0.48
14:BN:13:THR:N	14:BN:14:PRO:HD3	2.29	0.48
19:BT:58:VAL:HG23	19:BT:58:VAL:O	2.13	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
37:CO:64:LYS:C	37:CO:66:GLY:N	2.72	0.48
48:Ca:36:ILE:C	48:Ca:36:ILE:HD12	2.39	0.48
50:CK:45:SER:O	50:CK:46:GLN:NE2	2.46	0.48
50:CK:47:ASN:O	50:CK:48:HIS:C	2.57	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
29:DC:7:VAL:HG11	41:DS:1:MET:SD	2.54	0.48
32:DF:55:PRO:O	32:DF:56:SER:C	2.57	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:DR:19:LYS:HG2	40:DR:19:LYS:O	2.14	0.48
40:DR:95:HIS:CG	40:DR:96:GLY:N	2.81	0.48
59:Ds:41:U:H2'	59:Ds:42:C:OP1	2.13	0.48
58:D1:247:G:H21	58:D1:645:A:H8	1.62	0.48
58:D1:1540:A:N3	58:D1:1540:A:H2'	2.28	0.48
58:D1:2346:A:C8	58:D1:2348:G:N7	2.82	0.48
13:AM:66:LEU:H	13:AM:70:LEU:HD12	1.78	0.48
22:Ab:1036:G:H4'	22:Ab:1037:C:H5'	1.96	0.48
22:Ab:1275:G:O2'	22:Ab:1276:G:H8	1.96	0.48
22:Bb:459:G:H2'	22:Bb:460:G:H8	1.79	0.48
22:Bb:1036:G:N7	22:Bb:1182:C:H5''	2.29	0.48
17:BR:7:THR:HG22	17:BR:58:GLU:HG2	1.96	0.48
27:CA:212:UNK:O	27:CA:213:UNK:CB	2.61	0.48
28:CB:13:ARG:NH1	58:C1:775:G:OP2	2.45	0.48
32:CF:106:THR:HG22	32:CF:112:PRO:HB3	1.96	0.48
33:CI:6:LEU:C	33:CI:15:VAL:HG12	2.39	0.48
41:CS:129:ARG:HD2	41:CS:129:ARG:C	2.38	0.48
43:CU:76:LYS:O	43:CU:79:VAL:HG12	2.14	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
59:Cs:20:C:C2'	59:Cs:21:G:H5'	2.41	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:HE21	39:DQ:71:GLN:HA	1.78	0.48
39:DQ:90:ARG:NH1	58:D1:2889:C:O2'	2.38	0.48
40:DR:30:ARG:HD2	40:DR:31:SER:O	2.14	0.48
42:DT:76:TYR:HE2	58:D1:1197:C:HO2'	1.60	0.48
47:DZ:119:GLU:OE1	47:DZ:122:ARG:HD2	2.14	0.48
55:D8:38:GLY:O	55:D8:39:ARG:C	2.55	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
58:D1:2612:C:H5''	66:D1:3001:3V6:CLJ	2.50	0.48
22:Ab:798:A:N7	22:Ab:800:A:C4	2.81	0.47
22:Bb:859:G:OP2	12:BL:12:ARG:NH2	2.47	0.47
22:Bb:920:G:H21	9:BI:124:GLN:NE2	2.12	0.47
22:Bb:1078:U:H5''	22:Bb:1092:C:O2	2.14	0.47
22:Bb:1334:C:H2'	22:Bb:1335:G:C8	2.49	0.47
28:CB:165:ILE:HD13	28:CB:175:LEU:CD2	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:CH:61:ARG:NH2	58:C1:1409:G:OP2	2.47	0.47
58:C1:1345:U:O2'	58:C1:1671:G:C2	2.60	0.47
58:C1:1538:C:O2	58:C1:1538:C:C2'	2.60	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
54:D7:12:GLU:HA	54:D7:23:THR:HA	1.96	0.47
59:Ds:66:A:O2'	59:Ds:67:G:OP2	2.27	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
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
11:BK:54:ARG:NH2	25:D3:39:U:O2'	2.47	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
58:C1:257:U:O2	58:C1:257:U:H2'	2.15	0.47
58:C1:1538:C:C5	58:C1:2226:G:O2'	2.66	0.47
58:C1:2830:A:OP2	58:C1:2831:G:OP2	2.32	0.47
28:DB:259:THR:CG2	58:D1:1828:U:H5'	2.41	0.47
37:DO:107:LYS:HB2	37:DO:108:LYS:CE	2.44	0.47
42:DT:13:LYS:CD	58:D1:1272:G:OP1	2.61	0.47
42:DT:77:SER:OG	58:D1:1056:G:H5''	2.14	0.47
58:D1:2752:A:H2'	58:D1:2753:A:C8	2.49	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
22:Ab:434:G:H4'	22:Ab:435:A:OP1	2.15	0.47
22:Ab:1049:C:C2'	22:Ab:1050:A:H5'	2.43	0.47
22:Bb:243:G:OP2	17:BR:99:SER:HB2	2.13	0.47
22:Bb:938:U:O2	22:Bb:938:U:H2'	2.13	0.47
22:Bb:953:A:H5'	22:Bb:953:A:C8	2.48	0.47
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
29:CC:153:GLY:O	29:CC:154:LYS:C	2.57	0.47
30:CD:53:THR:HG23	30:CD:55:GLY:H	1.80	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:O	40:CR:26:LEU:HD23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:CY:2:ARG:NH2	58:C1:103:C:O2'	2.39	0.47
49:CH:23:LYS:HD3	49:CH:28:GLY:HA3	1.95	0.47
54:C7:17:LYS:HB2	54:C7:18:ARG:HH12	1.80	0.47
58:C1:859:U:H2'	58:C1:860:C:C6	2.49	0.47
58:C1:1540:A:H2'	58:C1:1541:A:C2	2.49	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
37:DO:146:VAL:HG13	37:DO:147:LEU:N	2.28	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
49:DH:90:ILE:CG2	49:DH:94:LEU:HD12	2.43	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
58:D1:2611:A:C6	58:D1:2612:C:N4	2.83	0.47
58:D1:2778:G:N3	58:D1:2778:G:H2'	2.29	0.47
3:AC:58:GLU:O	3:AC:59:ARG:HG3	2.14	0.47
3:AC:195:VAL:CG2	22:Ab:1187:U:O2'	2.63	0.47
5:AE:61:TYR:O	5:AE:64:ARG:HB3	2.13	0.47
22:Bb:1002:G:H2'	22:Bb:1002:G:N3	2.29	0.47
22:Bb:1209:A:H2'	22:Bb:1210:C:O5'	2.14	0.47
26:C4:3:C:N4	26:C4:4:G:N7	2.63	0.47
26:C4:52:C:O2	26:C4:52:C:H2'	2.14	0.47
35:CM:57:ALA:O	35:CM:58:ASP:C	2.57	0.47
41:CS:89:VAL:CG1	41:CS:91:ARG:HG3	2.45	0.47
56:C9:6:THR:HG21	58:C1:231:U:OP1	2.14	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
61:D4:68:C:O2	61:D4:68:C:H2'	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
58:D1:863:C:O2'	58:D1:885:U:OP1	2.25	0.47
17:AR:57:VAL:HG12	17:AR:76:LEU:HA	1.97	0.47
22:Ab:84:A:H5''	22:Ab:86:U:O2	2.14	0.47
22:Ab:984:A:C6	22:Ab:1004:U:H1'	2.49	0.47
22:Bb:103:A:H2'	22:Bb:322:G:N2	2.30	0.47
11:BK:48:ILE:HD11	11:BK:64:ALA:HA	1.97	0.47
25:C3:9:A:O4'	25:C3:46:G:N2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C1:179:A:H2'	58:C1:180:C:C6	2.49	0.47
58:C1:820:A:O2'	58:C1:821:G:OP2	2.26	0.47
58:C1:2168:G:H2'	58:C1:2169:G:O4'	2.14	0.47
35:DM:3:THR:O	35:DM:5:VAL:N	2.47	0.47
35:DM:57:ALA:C	35:DM:58:ASP:O	2.56	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
39:DQ:107:ASP:C	39:DQ:107:ASP:OD2	2.58	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
58:D1:1578:C:O2'	58:D1:1579:G:N2	2.44	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:5:ARG:HB2	22:Ab:372:G:OP1	2.15	0.47
16:AP:19:ILE:HG22	16:AP:36:ILE:HG13	1.95	0.47
22:Ab:90:U:O2'	22:Ab:91:G:P	2.73	0.47
22:Ab:460:G:H2'	22:Ab:461:G:C8	2.50	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
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: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
61:D4:16:C:O2	61:D4:61:U:H4'	2.14	0.47
38:DP:26:TYR:HE1	38:DP:28:ALA:HB2	1.76	0.47
38:DP:134:ARG:HA	38:DP:137:TYR:CD1	2.49	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
58:D1:1905:A:H2'	58:D1:1906:A:H5''	1.95	0.47
2:AA:11:LEU:HD12	2:AA:217:ARG:NH2	2.30	0.47
2:AA:69:LEU:HD12	2:AA:70:PHE:N	2.29	0.47
2:AA:233:SER:CB	2:AA:234:PRO:CD	2.93	0.47
4:AD:110:PHE:N	4:AD:110:PHE:HD1	2.11	0.47
4:AD:195:ALA:O	6:BF:16:GLN:HG3	2.15	0.47
9:AI:15:ALA:HB2	9:AI:65:VAL:HG23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:AJ:23:ILE:HG23	10:AJ:85:LEU:HD22	1.96	0.47
10:AJ:55:LYS:NZ	22:Ab:951:G:C4	2.82	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
22:Ab:837:A:H2'	22:Ab:838:A:O4'	2.15	0.47
22:Ab:1241:C:C5	22:Ab:1242:C:O2	2.67	0.47
22:Bb:339:U:O2	22:Bb:343:G:C2	2.67	0.47
22:Bb:853:C:O2'	8:BH:14:ARG:NH1	2.47	0.47
22:Bb:952:A:OP2	14:BN:41:ARG:NH1	2.47	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
27:CA:77:ILE:HG23	27:CA:77:ILE:O	2.15	0.47
27:CA:82:LYS:HB3	27:CA:86:ALA:HB2	1.97	0.47
28:CB:220:HIS:C	28:CB:220:HIS:CD2	2.92	0.47
29:CC:6:GLY:HA2	29:CC:51:PHE:CZ	2.49	0.47
31:CE:110:ALA:HB1	31:CE:140:ILE:CD1	2.44	0.47
37:CO:39:LYS:HG3	58:C1:853:U:OP2	2.14	0.47
38:CP:133:ARG:O	38:CP:134:ARG:HG2	2.14	0.47
39:CQ:3:HIS:HB2	58:C1:1700:A:OP1	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
46:CY:26:LYS:O	46:CY:27:VAL:C	2.57	0.47
46:CY:28:LYS:O	46:CY:29:GLU:C	2.58	0.47
46:CY:87:LYS:O	46:CY:88:LYS:HB2	2.14	0.47
47:CZ:127:LYS:HB2	47:CZ:162:GLU:HG3	1.96	0.47
51:CL:6:VAL:O	51:CL:34:GLU:HA	2.14	0.47
53:C6:33:CYS:SG	53:C6:40:LYS:CE	3.03	0.47
54:C7:15:GLU:O	54:C7:16:CYS:C	2.58	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
58:C1:565:C:H2'	58:C1:566:C:C6	2.50	0.47
58:C1:1345:U:HO2'	58:C1:1671:G:N2	2.11	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
58:C1:2890:C:C2	58:C1:2891:A:C8	3.03	0.47
59:Cs:40:U:C2	59:Cs:43:C:OP2	2.68	0.47
61:D4:4:G:H8	61:D4:4:G:C5'	2.27	0.47
28:DB:127:VAL:HA	28:DB:193:VAL:HG13	1.96	0.47
28:DB:242:ARG:HD2	28:DB:242:ARG:N	2.29	0.47
29:DC:44:TYR:O	29:DC:45:THR:CB	2.62	0.47
29:DC:134:ILE:C	29:DC:134:ILE:CD1	2.88	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:DE:126:ASP:O	31:DE:128:ARG:N	2.48	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
37:DO:41:ARG:HH11	37:DO:45:LEU:HD13	1.80	0.47
38:DP:118:LEU:HD12	38:DP:131:ILE:CG2	2.44	0.47
40:DR:54:LEU:HD22	40:DR:57:LYS:HA	1.96	0.47
41:DS:27:THR:OG1	41:DS:28:VAL:N	2.45	0.47
42:DT:97:ASP:C	42:DT:97:ASP:OD1	2.56	0.47
43:DU:91:TYR:C	43:DU:91:TYR:CD1	2.93	0.47
51:DL:8:LEU:HD13	51:DL:31:LEU:HD23	1.97	0.47
56:D9:4:MET:HE2	58:D1:615:G:C1'	2.44	0.47
58:D1:13:A:O5'	58:D1:13:A:H8	1.97	0.47
58:D1:1069:G:H3'	58:D1:1070:G:H5''	1.96	0.47
58:D1:1727:G:O2'	58:D1:1792:A:H2'	2.13	0.47
58:D1:1898:A:H5''	58:D1:1899:G:OP2	2.14	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
18:AS:50:ILE:CD1	18:AS:70:ILE:HG21	2.45	0.47
22:Ab:239:A:H4'	22:Ab:240:U:O5'	2.15	0.47
22:Ab:1036:G:N7	22:Ab:1182:C:C5'	2.78	0.47
22:Ab:1190:C:H2'	22:Ab:1191:C:C6	2.50	0.47
22:Ab:1287:G:N2	22:Ab:1313:G:O2'	2.35	0.47
22:Bb:1193:U:H4'	22:Bb:1194:U:OP1	2.14	0.47
22:Bb:1233:A:H2'	22:Bb:1234:A:C8	2.49	0.47
16:BP:20:VAL:HG23	16:BP:35:LYS:HA	1.96	0.47
21:BW:5:ASP:C	21:BW:7:ARG:H	2.23	0.47
26:C4:10:G:C5'	26:C4:10:G:C8	2.97	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
54:C7:33:LYS:HA	54:C7:33:LYS:CE	2.40	0.47
58:C1:1540:A:N3	58:C1:1540:A:H2'	2.30	0.47
61:D4:76:C:H6	61:D4:76:C:H5''	1.79	0.47
28:DB:108:PRO:HB3	28:DB:143:HIS:CE1	2.50	0.47
30:DD:66:PRO:O	30:DD:67:GLN:HB3	2.13	0.47
30:DD:179:GLU:OE1	30:DD:179:GLU:N	2.48	0.47
32:DF:137:ASP:HB3	32:DF:140:LYS:HB2	1.97	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
47:DZ:19:ARG:HH22	59:Ds:77:U:P	2.38	0.47
50:DK:25:VAL:HG21	50:DK:61:LEU:CD1	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:D9:30:ARG:CZ	58:D1:2430:U:O4	2.63	0.47
58:D1:551:C:O2	58:D1:551:C:O4'	2.32	0.47
58:D1:2269:C:H4'	58:D1:2270:G:OP2	2.15	0.47
3:AC:23:TYR:CD2	3:AC:24:ALA:N	2.83	0.47
3:AC:53:ALA:HB2	3:AC:115:LEU:HD21	1.96	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
22:Ab:1048:U:C2'	22:Ab:1049:C:OP2	2.61	0.47
23:B2:20:U:O2'	23:B2:21:C:H5'	2.15	0.47
22:Bb:715:G:OP1	22:Bb:750:A:H1'	2.14	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
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
58:C1:2450:A:C5'	58:C1:2450:A:C8	2.98	0.47
28:DB:270:ILE:C	28:DB:271:ILE:HG13	2.38	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
39:DQ:9:LYS:C	39:DQ:10:LEU:HG	2.39	0.47
39:DQ:16:HIS:CE1	58:D1:1320:A:C4	3.03	0.47
42:DT:102:GLU:HG3	43:DU:2:PHE:CE1	2.50	0.47
51:DL:17:LYS:HG2	58:D1:1013:U:OP1	2.15	0.47
58:D1:1884:A:H2'	58:D1:1885:G:O4'	2.15	0.47
58:D1:2904:C:C6	58:D1:2904:C:C3'	2.97	0.47
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
22:Bb:529:C:O2'	22:Bb:533:C:OP1	2.32	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
28:CB:266:SER:C	28:CB:267:SER:O	2.55	0.47
31:CE:60:LEU:O	31:CE:60:LEU:HD13	2.15	0.47
38:CP:16:ARG:NH2	58:C1:996:G:P	2.88	0.47
40:CR:91:PRO:O	40:CR:92:TYR:C	2.58	0.47
43:CU:18:LEU:N	43:CU:18:LEU:CD1	2.78	0.47
46:CY:47:LYS:HB3	58:C1:508:A:O4'	2.15	0.47
58:C1:1346:A:C4'	58:C1:1347:A:OP1	2.59	0.47
58:C1:2044:G:H5'	58:C1:2628:C:H4'	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:C1:2487:A:C2	58:C1:2488:C:H6	2.33	0.47
60:D2:42:C:H42	64:DV:28:G:H1	1.61	0.47
28:DB:31:LYS:O	28:DB:32:SER:C	2.55	0.47
58:D1:894:G:O6	58:D1:973:G:H2'	2.14	0.47
58:D1:1423:A:O2'	58:D1:1424:A:H5''	2.15	0.47
2:AA:104:ASN:OD1	2:AA:107:THR:OG1	2.33	0.46
5:AE:106:PRO:O	5:AE:110:LEU:HG	2.15	0.46
19:AT:6:LYS:C	19:AT:7:LYS:HE3	2.40	0.46
21:AW:10:ARG:NH2	22:Ab:1225:C:OP2	2.49	0.46
22:Ab:812:A:H2'	22:Ab:813:G:O5'	2.14	0.46
22:Ab:1113:A:C2	22:Ab:1129:A:C4	3.04	0.46
22:Bb:67:G:H4'	22:Bb:168:U:C5	2.50	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
31:CE:91:ARG:HD2	31:CE:91:ARG:C	2.40	0.46
36:CN:104:ARG:NE	41:CS:33:LYS:HE3	2.31	0.46
38:CP:71:ASP:OD2	58:C1:953:C:O2'	2.29	0.46
45:CX:38:GLU:OE2	58:C1:142:C:H4'	2.15	0.46
33:DI:81:VAL:HG21	33:DI:88:ILE:CG2	2.45	0.46
36:DN:68:GLU:H	36:DN:68:GLU:CD	2.23	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
39:DQ:36:THR:HG22	58:D1:1323:A:OP1	2.15	0.46
40:DR:90:GLY:C	40:DR:92:TYR:H	2.23	0.46
58:D1:98:G:HO2'	58:D1:98:G:H8	1.60	0.46
3:AC:76:VAL:HG23	3:AC:77:ILE:HG13	1.96	0.46
16:AP:74:LEU:O	16:AP:79:VAL:HG23	2.15	0.46
22:Ab:1426:G:H2'	41:CS:118:ARG:HD2	1.97	0.46
22:Bb:617:G:H8	22:Bb:617:G:H5''	1.80	0.46
22:Bb:995:A:H2'	22:Bb:996:G:O4'	2.14	0.46
10:BJ:50:ILE:HG22	10:BJ:60:ARG:HB3	1.97	0.46
29:CC:120:TRP:O	29:CC:121:ASN:HB2	2.15	0.46
33:CI:114:LEU:O	33:CI:115:ALA:HB2	2.16	0.46
37:CO:57:THR:O	37:CO:58:THR:HB	2.14	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
54:C7:18:ARG:HD2	54:C7:43:CYS:SG	2.55	0.46
58:C1:321:G:H5'	58:C1:322:A:OP1	2.15	0.46
58:C1:2480:A:H2	58:C1:2492:G:H21	1.62	0.46
29:DC:81:ILE:O	29:DC:82:ARG:C	2.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
58:D1:157:U:OP2	58:D1:157:U:H6	1.98	0.46
58:D1:579:U:H2'	58:D1:580:G:C8	2.49	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
22:Ab:1189:G:C5	22:Ab:1190:C:C5	3.04	0.46
22:Bb:1331:A:H2'	22:Bb:1332:A:C8	2.46	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
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
38:CP:123:HIS:CG	58:C1:2478:C:H4'	2.51	0.46
56:C9:61:LEU:H	56:C9:61:LEU:HG	1.27	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
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
25:D3:19:G:O2'	58:D1:2133:G:H1'	2.15	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
58:D1:1766:A:O2'	58:D1:1767:U:H5'	2.16	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
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
20:AU:84:LEU:CD1	20:AU:84:LEU:C	2.89	0.46
22:Ab:989:G:C2	22:Ab:999:U:H1'	2.50	0.46
22:Bb:627:C:H5'	8:BH:31:PHE:CE1	2.50	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:CO:50:ARG:HH11	58:C1:240:G:P	2.38	0.46
40:CR:74:ALA:HB1	40:CR:103:GLU:HB2	1.97	0.46
40:CR:74:ALA:HB1	40:CR:103:GLU:CB	2.46	0.46
40:CR:97:ARG:HH21	40:CR:98:VAL:HG22	1.81	0.46
47:CZ:52:SER:OG	47:CZ:53:ILE:N	2.48	0.46
47:CZ:151:HIS:HB3	47:CZ:170:THR:HA	1.98	0.46
56:C9:31:HIS:HE1	58:C1:2403:A:OP2	1.98	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
58:C1:2502:U:H4'	58:C1:2581:G:OP1	2.16	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
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
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
22:Ab:147:A:N6	22:Ab:165:U:C2	2.83	0.46
22:Ab:1411:A:H2'	22:Ab:1412:C:C6	2.50	0.46
22:Bb:923:G:H2'	22:Bb:923:G:N3	2.31	0.46
2:BA:167:PRO:HD3	2:BA:188:ALA:HB2	1.97	0.46
10:BJ:6:ILE:HG13	10:BJ:72:VAL:O	2.16	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
40:CR:18:ILE:HD11	58:C1:2345:G:H21	1.81	0.46
48:Ca:11:ARG:O	48:Ca:14:ARG:NH2	2.49	0.46
58:C1:918:A:C6	58:C1:951:G:C2	3.04	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
58:D1:2801:C:OP1	58:D1:2801:C:H4'	2.15	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
22:Ab:1037:C:O2	22:Ab:1037:C:H2'	2.15	0.46
22:Bb:1154:C:H2'	22:Bb:1155:G:H8	1.81	0.46
22:Bb:1179:G:OP1	22:Bb:1180:G:OP2	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:Bb:1303:C:C3'	22:Bb:1304:C:H5''	2.42	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
47:CZ:149:SER:HB2	47:CZ:173:ALA:HA	1.98	0.46
58:C1:179:A:H2'	58:C1:180:C:H6	1.81	0.46
58:C1:552:A:N1	58:C1:2064:C:O5'	2.49	0.46
58:C1:826:G:H8	58:C1:826:G:O5'	1.98	0.46
58:C1:2487:A:N1	58:C1:2488:C:C5	2.84	0.46
25:D3:34:G:C2	25:D3:35:A:N3	2.84	0.46
28:DB:24:ILE:C	28:DB:25:THR:O	2.54	0.46
30:DD:128:ALA:O	30:DD:142:TRP:NE1	2.48	0.46
31:DE:40:ASN:CG	58:D1:2324:C:O4'	2.59	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
49:DH:67:ILE:N	49:DH:68:PRO:HD2	2.30	0.46
56:D9:29:LYS:HD3	56:D9:44:LYS:HD3	1.97	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
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
22:Bb:159:U:H2'	22:Bb:160:C:C6	2.50	0.46
22:Bb:971:G:H2'	22:Bb:971:G:N3	2.29	0.46
22:Bb:1282:G:C2'	22:Bb:1283:U:OP2	2.63	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
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
58:C1:274:C:O2'	58:C1:275:C:P	2.73	0.46
58:C1:2443:A:H2'	58:C1:2444:A:C8	2.51	0.46
28:DB:34:VAL:HG23	28:DB:35:LYS:N	2.30	0.46
29:DC:24:THR:HG23	29:DC:184:VAL:HG23	1.98	0.46
29:DC:105:THR:OG1	29:DC:199:ARG:NH2	2.45	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
42:DT:76:TYR:O	42:DT:77:SER:C	2.59	0.46
59:Ds:96:U:C2	59:Ds:97:G:C8	3.03	0.46
58:D1:906:U:O2	58:D1:906:U:O4'	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:D1:1254:A:H5'	58:D1:1254:A:C8	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
10:AJ:57:LYS:O	10:AJ:57:LYS:HG3	2.15	0.46
12:AL:47:LYS:HB3	12:AL:48:PRO:HD3	1.98	0.46
14:AN:27:CYS:C	14:AN:29:ARG:N	2.70	0.46
22:Bb:160:C:H2'	22:Bb:161:G:C8	2.51	0.46
22:Bb:348:C:O2'	22:Bb:350:G:OP1	2.31	0.46
22:Bb:961:A:H3'	22:Bb:961:A:N3	2.31	0.46
22:Bb:1101:C:H1'	22:Bb:1161:A:C4	2.51	0.46
22:Bb:1282:G:HO2'	22:Bb:1283:U:P	2.38	0.46
11:BK:86:GLY:H	11:BK:112:THR:HG1	1.54	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
32:CF:110:SER:HB2	58:C1:2664:U:O2'	2.16	0.46
37:CO:23:PRO:HD2	37:CO:33:ARG:NH2	2.31	0.46
58:C1:2612:C:P	66:C1:3001:3V6:H19	2.55	0.46
58:C1:2697:G:C2	58:C1:2736:C:O2	2.69	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
49:DH:84:GLY:O	49:DH:85:LEU:C	2.58	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
58:D1:2249:G:H2'	58:D1:2249:G:N3	2.31	0.46
17:AR:17:LYS:HZ2	22:Ab:252:U:P	2.38	0.46
19:AT:81:ARG:HB3	22:Ab:1208:C:H5''	1.98	0.46
22:Ab:485:C:H2'	22:Ab:486:G:H8	1.81	0.46
22:Ab:1430:C:C4	22:Ab:1431:U:C4	3.03	0.46
22:Bb:90:U:O2'	22:Bb:91:G:P	2.74	0.46
22:Bb:250:G:OP1	17:BR:67:LYS:O	2.34	0.46
22:Bb:407:A:OP2	4:BD:25:ARG:NH2	2.49	0.46
4:BD:11:LEU:O	4:BD:12:CYS:C	2.57	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
28:CB:76:PRO:HA	28:CB:118:VAL:HG23	1.97	0.46
28:CB:221:VAL:HG22	28:CB:226:MET:HE2	1.98	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
30:CD:115:ALA:O	30:CD:116:ASP:C	2.59	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:CF:150:ALA:O	32:CF:151:ILE:C	2.58	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
47:CZ:63:ASP:C	47:CZ:65:GLN:H	2.23	0.46
53:C6:35:GLU:O	53:C6:36:CYS:HB2	2.15	0.46
58:C1:144:G:O2'	58:C1:145:G:H5'	2.15	0.46
58:C1:298:G:OP1	58:C1:298:G:O4'	2.34	0.46
58:C1:2083:A:C4	58:C1:2083:A:C5'	2.98	0.46
58:C1:2124:C:O2	58:C1:2208:G:C2	2.69	0.46
36:DN:77:ILE:HD12	41:DS:74:ARG:HG2	1.97	0.46
37:DO:108:LYS:O	37:DO:110:TYR:N	2.49	0.46
38:DP:26:TYR:CD1	38:DP:26:TYR:C	2.94	0.46
46:DY:31:LEU:HD23	46:DY:36:ALA:HB3	1.98	0.46
49:DH:93:GLU:C	49:DH:95:LEU:N	2.73	0.46
54:D7:24:GLU:OE2	58:D1:2357:A:C8	2.69	0.46
58:D1:99:G:C8	58:D1:99:G:H5''	2.51	0.46
58:D1:162:C:H5'	58:D1:163:G:OP2	2.15	0.46
4:AD:25:ARG:C	4:AD:27:TYR:H	2.24	0.46
9:AI:48:GLU:N	9:AI:49:PRO:CD	2.79	0.46
22:Bb:442:G:H2'	22:Bb:470:G:N2	2.30	0.46
22:Bb:627:C:H5'	8:BH:31:PHE:CD1	2.51	0.46
22:Bb:1259:C:H3'	22:Bb:1259:C:H6	1.81	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:O	19:BT:58:VAL:CG2	2.63	0.46
35:CM:3:THR:O	35:CM:5:VAL:N	2.48	0.46
37:CO:110:TYR:O	37:CO:111:ARG:C	2.59	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
42:CT:55:ARG:HD2	58:C1:1200:A:OP1	2.16	0.46
45:CX:12:VAL:HB	45:CX:17:ALA:HB1	1.98	0.46
54:C7:24:GLU:OE2	58:C1:2357:A:O2'	2.27	0.46
58:C1:139:A:H8	58:C1:1640:G:H21	1.60	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
29:DC:151:TYR:O	58:D1:2630:C:H4'	2.15	0.46
35:DM:131:GLN:OE1	35:DM:131:GLN:HA	2.16	0.46
36:DN:17:ARG:HB2	36:DN:45:GLU:HG3	1.98	0.46
54:D7:37:ARG:NH1	58:D1:2355:U:C5	2.83	0.46
58:D1:821:G:C4	58:D1:840:G:C8	3.03	0.46
17:AR:63:ARG:HG3	22:Ab:125:A:C8	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
22:Ab:39:G:C2	22:Ab:393:A:C2	3.04	0.45
22:Ab:333:C:H2'	22:Ab:334:A:C8	2.51	0.45
22:Ab:1329:G:N2	22:Ab:1356:G:H2'	2.31	0.45
22:Bb:1113:A:C2	22:Bb:1129:A:C4	3.04	0.45
22:Bb:1312:U:C5	22:Bb:1313:G:C5	3.04	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
28:CB:211:ARG:NH1	58:C1:1612:A:OP1	2.49	0.45
47:CZ:24:LEU:HB2	47:CZ:41:LEU:HG	1.98	0.45
58:C1:25:G:C6	58:C1:26:G:N1	2.83	0.45
58:C1:1319:A:N3	58:C1:1342:C:H1'	2.31	0.45
58:C1:1636:G:H5''	58:C1:1636:G:C8	2.47	0.45
25:D3:30:G:C2	25:D3:41:C:N3	2.84	0.45
28:DB:28:GLU:HB2	28:DB:29:PRO:HD3	1.99	0.45
29:DC:1:MET:HG2	29:DC:83:ASP:O	2.16	0.45
29:DC:181:LEU:HD21	41:DS:7:ILE:CG2	2.46	0.45
33:DI:129:THR:HG22	33:DI:130:TYR:H	1.80	0.45
46:DY:29:GLU:OE1	46:DY:29:GLU:N	2.49	0.45
47:DZ:68:PRO:O	47:DZ:91:LEU:HD12	2.16	0.45
52:D5:61:VAL:HG13	52:D5:65:CYS:SG	2.56	0.45
58:D1:668:A:O2'	58:D1:669:C:H5'	2.15	0.45
58:D1:1004:A:H5''	58:D1:1005:C:OP2	2.16	0.45
10:AJ:38:ILE:HG13	10:AJ:71:LEU:HB3	1.97	0.45
22:Ab:262:G:H5'	22:Ab:262:G:C8	2.50	0.45
22:Ab:1101:C:H1'	22:Ab:1161:A:C4	2.50	0.45
4:BD:13:ARG:O	4:BD:15:GLU:N	2.48	0.45
4:BD:61:LYS:NZ	4:BD:72:GLU:OE2	2.49	0.45
28:CB:25:THR:C	28:CB:27:THR:H	2.24	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
32:CF:17:VAL:O	32:CF:45:VAL:HG22	2.15	0.45
37:CO:35:HIS:C	37:CO:36:LYS:HG3	2.41	0.45
44:CW:84:ARG:NE	58:C1:1368:U:OP1	2.50	0.45
50:CK:16:LEU:O	50:CK:17:SER:HB3	2.16	0.45
55:C8:8:ASN:C	55:C8:8:ASN:ND2	2.75	0.45
58:C1:1698:A:O3'	58:C1:1699:G:H8	1.99	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
37:DO:17:LYS:C	37:DO:19:VAL:N	2.74	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:DY:49:VAL:O	46:DY:50:ARG:HB2	2.17	0.45
56:D9:2:PRO:O	56:D9:3:LYS:CB	2.64	0.45
58:D1:534:C:OP1	58:D1:535:U:OP2	2.34	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
13:BM:28:ALA:O	13:BM:30:ALA:N	2.49	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
38:CP:51:ARG:O	38:CP:52:VAL:C	2.59	0.45
39:CQ:84:ALA:HB3	39:CQ:85:PRO:HD3	1.98	0.45
41:CS:58:ASN:C	41:CS:58:ASN:HD22	2.25	0.45
41:CS:89:VAL:HG12	41:CS:91:ARG:HG3	1.97	0.45
42:CT:2:PRO:HA	58:C1:470:C:OP1	2.16	0.45
42:CT:49:HIS:CD2	58:C1:558:U:O2'	2.66	0.45
58:C1:1326:G:H8	58:C1:1326:G:H5''	1.81	0.45
58:C1:1777:G:C2'	58:C1:1778:G:H5'	2.47	0.45
58:C1:1984:U:O2	58:C1:1984:U:C2'	2.62	0.45
58:C1:2200:C:N4	58:C1:2203:G:O6	2.49	0.45
59:Cs:87:G:H3'	59:Cs:88:C:H5''	1.98	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
59:Ds:71:C:C4	59:Ds:72:G:N7	2.84	0.45
58:D1:552:A:O2'	58:D1:553:A:H5'	2.16	0.45
58:D1:1766:A:N6	58:D1:1769:A:C2	2.85	0.45
58:D1:1813:A:C2	58:D1:2598:A:C5	3.04	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
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
4:AD:73:ARG:NH2	22:Ab:397:C:OP2	2.49	0.45
5:AE:16:THR:O	5:AE:17:ALA:HB2	2.17	0.45
12:AL:115:LYS:HG3	22:Ab:522:G:OP2	2.17	0.45
17:AR:66:SER:OG	17:AR:69:LYS:HB2	2.16	0.45
20:AU:103:GLY:N	22:Ab:199:U:H4'	2.31	0.45
22:Ab:1037:C:O2	22:Ab:1037:C:C2'	2.64	0.45
22:Bb:39:G:C2	22:Bb:393:A:C2	3.05	0.45
22:Bb:1273:G:O3'	9:BI:39:GLY:HA3	2.16	0.45
10:BJ:82:ILE:O	10:BJ:86:MET:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
37:CO:108:LYS:C	37:CO:110:TYR:N	2.75	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
48:Ca:53:MET:HA	48:Ca:58:THR:O	2.16	0.45
58:C1:264:U:H2'	58:C1:265:C:C6	2.51	0.45
58:C1:393:C:O2	58:C1:393:C:H2'	2.16	0.45
58:C1:2124:C:O2	58:C1:2208:G:N2	2.49	0.45
29:DC:156:MET:SD	58:D1:2630:C:O2'	2.71	0.45
39:DQ:103:ARG:HD3	63:DW:40:ASN:ND2	2.31	0.45
41:DS:58:ASN:C	41:DS:58:ASN:HD22	2.25	0.45
46:DY:17:SER:HB2	46:DY:71:LYS:HE2	1.99	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
58:D1:139:A:C8	58:D1:1453:C:H1'	2.52	0.45
58:D1:516:A:H2'	58:D1:517:G:O4'	2.17	0.45
58:D1:1156:A:O2'	58:D1:1157:G:C4'	2.64	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
8:AH:113:SER:OG	22:Ab:626:A:N3	2.45	0.45
11:AK:84:VAL:HG23	11:AK:110:ASP:OD1	2.16	0.45
13:AM:7:VAL:HG23	31:CE:115:ARG:HG3	1.97	0.45
22:Ab:30:G:H5'	22:Ab:292:U:OP1	2.17	0.45
22:Ab:67:G:H4'	22:Ab:168:U:C5	2.51	0.45
22:Bb:774:A:OP1	61:D4:39:A:O2'	2.33	0.45
22:Bb:1211:A:H2'	22:Bb:1212:C:C6	2.52	0.45
5:BE:76:ILE:HG22	5:BE:93:PRO:HB3	1.98	0.45
19:BT:31:ILE:HG23	19:BT:31:ILE:O	2.17	0.45
25:C3:61:C:H2'	25:C3:62:C:C5	2.51	0.45
28:CB:9:TYR:C	28:CB:10:THR:HG22	2.41	0.45
28:CB:52:ARG:NH1	58:C1:1854:G:OP1	2.45	0.45
29:CC:14:ILE:HB	41:CS:14:TYR:CZ	2.51	0.45
31:CE:9:ARG:C	31:CE:11:TYR:H	2.25	0.45
35:CM:58:ASP:C	35:CM:60:ILE:H	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:CP:98:LYS:HB3	38:CP:99:PRO:CD	2.47	0.45
38:CP:137:TYR:CE2	47:CZ:81:ARG:NH1	2.85	0.45
58:C1:646:G:O2'	58:C1:647:G:H5'	2.16	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
58:C1:2723:U:H1'	58:C1:2724:A:C8	2.52	0.45
30:DD:169:ASN:ND2	58:D1:345:A:H3'	2.31	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
46:DY:52:SER:C	46:DY:54:LYS:N	2.68	0.45
52:D5:36:VAL:O	52:D5:52:SER:O	2.35	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:D1:566:C:O2'	58:D1:567:C:OP1	2.21	0.45
58:D1:2057:C:H6	58:D1:2057:C:C5'	2.29	0.45
58:D1:2562:C:H2'	58:D1:2563:U:C6	2.50	0.45
5:AE:76:ILE:HD11	5:AE:142:LEU:HD21	1.98	0.45
6:AF:72:VAL:CG1	22:Ab:721:A:O2'	2.64	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:83:ASP:C	13:AM:85:GLY:N	2.74	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
22:Bb:1252:C:O5'	22:Bb:1252:C:H6	1.99	0.45
36:CN:101:PRO:HG3	41:CS:67:SER:CB	2.47	0.45
46:CY:7:VAL:HB	46:CY:8:LYS:CD	2.47	0.45
46:CY:74:PRO:O	46:CY:80:GLY:HA2	2.16	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
25:D3:34:G:N1	25:D3:35:A:N3	2.64	0.45
29:DC:69:LYS:C	29:DC:71:GLY:N	2.75	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
50:DK:71:ASN:OD1	50:DK:71:ASN:C	2.59	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
4:AD:9:CYS:SG	4:AD:31:CYS:C	2.84	0.45
11:AK:99:GLN:HG2	11:AK:105:VAL:HG21	1.97	0.45
13:AM:64:TRP:CD1	13:AM:64:TRP:H	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:Ab:662:U:H2'	22:Ab:663:C:C6	2.51	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
28:CB:45:ASN:CG	28:CB:46:GLN:N	2.74	0.45
29:CC:70:ALA:O	29:CC:71:GLY:C	2.59	0.45
30:CD:103:LYS:HA	30:CD:106:ARG:HG3	1.98	0.45
31:CE:71:THR:HA	59:Cs:41:U:O4	2.15	0.45
41:CS:28:VAL:HG22	41:CS:46:GLU:CG	2.47	0.45
41:CS:129:ARG:NH1	41:CS:131:ALA:HB2	2.32	0.45
48:Ca:39:ARG:HH21	58:C1:2366:C:H1'	1.82	0.45
49:CH:66:HIS:O	49:CH:67:ILE:C	2.59	0.45
57:C0:19:ARG:O	57:C0:20:HIS:HB2	2.17	0.45
58:C1:552:A:C2	58:C1:2064:C:C5'	3.00	0.45
58:C1:1540:A:O4'	58:C1:1540:A:P	2.75	0.45
25:D3:61:C:H2'	25:D3:62:C:H6	1.82	0.45
28:DB:70:TRP:CD1	28:DB:70:TRP:C	2.95	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
29:DC:109:LYS:HE2	58:D1:2829:A:C8	2.51	0.45
32:DF:68:THR:O	32:DF:69:ARG:C	2.60	0.45
41:DS:3:ARG:CZ	58:D1:2885:G:O3'	2.65	0.45
41:DS:92:GLY:C	41:DS:94:ALA:N	2.75	0.45
43:DU:5:VAL:HG22	43:DU:6:LYS:N	2.32	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
50:DK:29:LYS:HD3	50:DK:57:ILE:HD13	1.98	0.45
51:DL:10:LYS:HB3	51:DL:53:LEU:HD23	1.98	0.45
56:D9:8:LYS:HB3	56:D9:12:LYS:HE3	1.99	0.45
58:D1:554:G:O4'	58:D1:554:G:N3	2.49	0.45
58:D1:1092:G:OP1	58:D1:1092:G:H4'	2.11	0.45
58:D1:1451:U:H2'	58:D1:1452:C:C6	2.52	0.45
3:AC:60:ALA:HB2	10:AJ:91:PRO:O	2.17	0.45
4:AD:61:LYS:HE2	4:AD:62:GLN:HE21	1.82	0.45
13:AM:115:LYS:HE3	22:Ab:1210:C:OP1	2.17	0.45
23:B2:19:U:P	23:B2:19:U:O4'	2.74	0.45
22:Bb:469:G:H4'	22:Bb:470:G:O5'	2.16	0.45
22:Bb:676:U:H5	11:BK:26:ASN:HD21	1.64	0.45
22:Bb:775:G:C6	22:Bb:776:A:N7	2.85	0.45
22:Bb:1095:C:O2	24:BC:179:ARG:HG2	2.17	0.45
22:Bb:1480:A:H2	22:Bb:1483:G:H1	1.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
26:C4:75:C:O5'	26:C4:75:C:H6	1.99	0.45
28:CB:130:ALA:C	28:CB:131:LEU:HD12	2.42	0.45
28:CB:226:MET:HB3	28:CB:230:ASP:HB2	1.99	0.45
28:CB:241:PRO:O	28:CB:242:ARG:C	2.59	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
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
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
58:C1:1625:A:H5'	58:C1:1625:A:H8	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
29:DC:70:ALA:O	29:DC:71:GLY:C	2.59	0.45
29:DC:74:PRO:O	29:DC:75:VAL:C	2.59	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
59:Ds:71:C:C2	59:Ds:72:G:C8	3.05	0.45
58:D1:715:G:H5'	58:D1:715:G:H8	1.81	0.45
58:D1:1357:U:C2	58:D1:1648:A:C2	3.04	0.45
58:D1:1510:C:HO2'	58:D1:1573:A:H8	1.65	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
2:AA:55:PHE:O	2:AA:56:ARG:C	2.59	0.45
3:AC:154:SER:CB	22:Ab:1040:G:H5''	2.47	0.45
10:AJ:50:ILE:HA	10:AJ:60:ARG:HB2	1.99	0.45
22:Ab:251:G:O6	22:Ab:262:G:O6	2.34	0.45
22:Ab:369:A:N3	22:Ab:370:A:C8	2.85	0.45
22:Ab:993:A:H2'	22:Ab:994:A:C8	2.52	0.45
22:Ab:995:A:O5'	22:Ab:995:A:H8	2.00	0.45
22:Ab:1275:G:HO2'	22:Ab:1276:G:P	2.40	0.45
22:Bb:741:U:OP1	22:Bb:806:C:O2'	2.35	0.45
22:Bb:1048:U:HO2'	22:Bb:1049:C:P	2.33	0.45
2:BA:105:PHE:O	2:BA:106:LYS:C	2.59	0.45
2:BA:185:ILE:CG2	2:BA:199:TYR:HB2	2.46	0.45
13:BM:16:ASP:HA	13:BM:34:LEU:HD11	1.99	0.45
13:BM:117:VAL:O	13:BM:118:ALA:HB2	2.16	0.45
19:BT:23:ASN:O	19:BT:25:LYS:N	2.50	0.45
43:CU:38:LEU:HD23	43:CU:38:LEU:C	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:CY:31:LEU:CB	46:CY:32:PRO:HA	2.46	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
58:C1:271:U:H3'	58:C1:271:U:H6	1.82	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
61:D4:17:C:HO2'	61:D4:18:U:P	2.39	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
63:DW:17:VAL:O	63:DW:18:ARG:C	2.58	0.45
58:D1:154:C:O3'	58:D1:157:U:OP1	2.35	0.45
58:D1:495:A:H2'	58:D1:496:A:O4'	2.17	0.45
58:D1:2714:C:C2	58:D1:2715:C:C5	3.05	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
4:AD:134:ASP:OD2	22:Ab:603:U:N3	2.44	0.45
13:AM:63:THR:HG22	13:AM:64:TRP:N	2.32	0.45
22:Ab:432:C:O2'	22:Ab:433:U:OP2	2.32	0.45
22:Ab:904:G:C6	22:Ab:1483:G:C6	3.05	0.45
22:Bb:144:A:HO2'	22:Bb:145:C:H6	1.62	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:8:LEU:HD23	10:BJ:96:ILE:CG2	2.46	0.45
10:BJ:23:ILE:O	10:BJ:23:ILE:HG22	2.17	0.45
30:CD:8:GLN:O	30:CD:9:ILE:C	2.59	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: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
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:38:GLN:OE1	58:D1:987:U:OP2	2.35	0.45
37:DO:48:PRO:O	37:DO:49:ARG:C	2.60	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:DU:47:VAL:HB	43:DU:49:THR:O	2.16	0.45
52:D5:40:ILE:HA	52:D5:57:ILE:HB	1.99	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
58:D1:1538:C:C5	58:D1:2226:G:O2'	2.62	0.45
58:D1:1636:G:H5''	58:D1:1636:G:C8	2.49	0.45
4:AD:108:LEU:HB3	4:AD:110:PHE:CE1	2.52	0.44
5:AE:146:ALA:O	5:AE:147:ASP:C	2.60	0.44
6:AF:9:VAL:HB	6:AF:87:ARG:HB2	1.99	0.44
9:AI:112:LYS:HD3	22:Ab:1351:G:OP2	2.17	0.44
12:AL:84:LEU:HB2	12:AL:104:VAL:HG11	1.99	0.44
19:AT:36:ARG:HD3	22:Ab:1202:G:O3'	2.17	0.44
22:Bb:1324:C:O2'	22:Bb:1325:G:H5'	2.16	0.44
17:BR:67:LYS:HA	17:BR:70:ARG:HH12	1.82	0.44
29:CC:102:VAL:HG12	29:CC:199:ARG:O	2.17	0.44
39:CQ:24:GLN:HE22	39:CQ:36:THR:HG21	1.82	0.44
40:CR:14:VAL:O	40:CR:15:ARG:C	2.60	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:C1:353:A:H2	58:C1:1254:A:H2'	1.82	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
37:DO:101:VAL:C	37:DO:103:ALA:N	2.75	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
47:DZ:73:GLN:NE2	59:Ds:103:G:O2'	2.48	0.44
58:D1:745:A:H2'	58:D1:746:G:O4'	2.18	0.44
58:D1:2723:U:O2	58:D1:2723:U:H5'	2.17	0.44
4:AD:170:VAL:O	4:AD:171:GLY:C	2.60	0.44
13:AM:19:LEU:O	13:AM:22:ILE:HD12	2.17	0.44
17:AR:69:LYS:NZ	22:Ab:251:G:OP1	2.45	0.44
22:Ab:324:C:H4'	22:Ab:325:A:O5'	2.17	0.44
22:Ab:524:G:H2'	22:Ab:525:G:O4'	2.17	0.44
22:Ab:630:U:H2'	22:Ab:631:C:C6	2.52	0.44
22:Bb:1278:C:H5''	22:Bb:1279:C:OP2	2.17	0.44
2:BA:233:SER:CB	2:BA:234:PRO:HD2	2.47	0.44
12:BL:25:PRO:C	12:BL:27:LEU:N	2.75	0.44
28:CB:88:ARG:NH2	58:C1:1847:G:OP1	2.50	0.44
29:CC:77:ILE:HG22	29:CC:78:LEU:N	2.32	0.44
36:CN:6:THR:HA	58:C1:1713:G:OP1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:CQ:75:LEU:O	39:CQ:75:LEU:HD13	2.18	0.44
57:C0:22:ARG:HB2	57:C0:24:TYR:HE1	1.81	0.44
58:C1:635:G:H8	58:C1:635:G:H5''	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
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
60:D2:46:G:O2'	60:D2:47:U:O5'	2.33	0.44
28:DB:28:GLU:O	28:DB:29:PRO:C	2.60	0.44
32:DF:43:VAL:CG1	32:DF:52:VAL:HA	2.47	0.44
36:DN:7:TYR:C	36:DN:8:LEU:HD22	2.42	0.44
36:DN:47:ILE:O	36:DN:48:PRO:C	2.60	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
46:DY:26:LYS:O	46:DY:27:VAL:C	2.59	0.44
59:Ds:20:C:H2'	59:Ds:21:G:H5'	1.99	0.44
58:D1:2535:G:C5'	58:D1:2535:G:C8	3.00	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
22:Bb:917:G:H5''	7:BG:102:ARG:NH2	2.32	0.44
22:Bb:1328:A:C5'	9:BI:120:ARG:HH12	2.29	0.44
22:Bb:1351:G:OP1	9:BI:111:ARG:NH2	2.49	0.44
5:BE:72:GLN:O	5:BE:73:ASN:HB2	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:O	38:CP:58:PHE:CD1	2.69	0.44
58:C1:88:U:H2'	58:C1:88:U:O2	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:C1:2001:G:O2'	58:C1:2003:C:OP2	2.35	0.44
58:C1:2221:C:O2'	58:C1:2238:A:N1	2.46	0.44
61:D4:24:C:H2'	61:D4:25:U:C6	2.52	0.44
29:DC:58:ARG:HH22	58:D1:2840:G:P	2.40	0.44
29:DC:144:ARG:O	58:D1:2074:G:H5'	2.16	0.44
39:DQ:38:VAL:O	39:DQ:41:ALA:HB3	2.18	0.44
41:DS:18:ASP:N	41:DS:18:ASP:OD1	2.49	0.44
41:DS:29:ARG:CG	41:DS:85:LYS:HA	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:DS:56:GLY:O	41:DS:59:THR:CG2	2.64	0.44
63:DW:15:ARG:NH2	58:D1:1311:G:O4'	2.47	0.44
58:D1:1991:A:H5''	58:D1:1992:A:OP1	2.17	0.44
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
64:DV:46:U:H2'	64:DV:47:C:C6	2.52	0.44
4:AD:64:LEU:HD12	4:AD:64:LEU:O	2.18	0.44
14:AN:5:ALA:HB2	22:Ab:1198:G:H5''	1.99	0.44
22:Ab:1427:A:C2	41:CS:118:ARG:NH2	2.85	0.44
22:Bb:952:A:H8	22:Bb:952:A:OP1	2.01	0.44
24:BC:11:ARG:O	24:BC:12:LEU:C	2.59	0.44
13:BM:82:MET:O	13:BM:82:MET:CG	2.65	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:C1:65:U:H2'	58:C1:66:G:C8	2.53	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:O2	58:C1:2732:U:C2'	2.64	0.44
66:C1:3001:3V6:CLI	66:C1:3001:3V6:O	2.72	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
29:DC:51:PHE:C	29:DC:74:PRO:HB3	2.43	0.44
32:DF:43:VAL:HG11	32:DF:52:VAL:HA	1.99	0.44
32:DF:158:HIS:CE1	32:DF:169:VAL:O	2.71	0.44
35:DM:3:THR:O	35:DM:5:VAL:HG12	2.18	0.44
42:DT:92:ARG:O	42:DT:93:LYS:C	2.61	0.44
56:D9:4:MET:HE2	58:D1:615:G:O4'	2.16	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
3:AC:2:GLY:HA2	22:Ab:1043:C:C5	2.53	0.44
4:AD:61:LYS:HD3	4:AD:206:PHE:CE2	2.53	0.44
19:AT:43:GLU:O	19:AT:45:VAL:N	2.46	0.44
22:Ab:1055:G:H2'	22:Ab:1056:U:H6	1.81	0.44
22:Bb:136:A:H1'	22:Bb:177:U:O2	2.17	0.44
22:Bb:199:U:H2'	22:Bb:200:C:C6	2.52	0.44
22:Bb:319:U:O3'	20:BU:22:ARG:HD3	2.18	0.44
22:Bb:1295:U:P	19:BT:6:LYS:HG3	2.58	0.44
24:BC:150:LYS:HG3	24:BC:169:ALA:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:BT:6:LYS:CG	19:BT:7:LYS:HE3	2.45	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
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
58:C1:69:A:H3'	58:C1:69:A:OP2	2.18	0.44
58:C1:1090:A:H3'	58:C1:1090:A:N3	2.33	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:N	40:DR:36:TYR:CD1	2.86	0.44
41:DS:5:ALA:HB2	58:D1:2884:C:H4'	1.99	0.44
42:DT:76:TYR:CE2	58:D1:1198:C:H5'	2.51	0.44
46:DY:12:THR:HG22	46:DY:75:ILE:HG23	1.99	0.44
46:DY:42:VAL:HG23	46:DY:67:LEU:CD1	2.48	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
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
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
22:Ab:89:G:O2'	22:Ab:90:U:H5'	2.18	0.44
22:Ab:1032:U:H4'	22:Ab:1033:G:OP2	2.18	0.44
22:Bb:324:C:H4'	22:Bb:325:A:O5'	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
6:BF:98:LEU:HA	18:BS:30:ASP:HA	2.00	0.44
14:BN:12:ARG:HB3	14:BN:14:PRO:HD3	2.00	0.44
20:BU:50:GLU:CG	20:BU:100:ILE:HB	2.48	0.44
28:CB:35:LYS:HD2	28:CB:36:PRO:CA	2.47	0.44
41:CS:2:ASN:O	58:C1:2885:G:P	2.76	0.44
42:CT:66:ASN:HD21	42:CT:70:ARG:NH2	2.15	0.44
58:C1:624:G:N2	58:C1:702:G:C5	2.86	0.44
58:C1:1066:A:C8	58:C1:1066:A:C3'	3.01	0.44
58:C1:2595:U:O2	58:C1:2595:U:O4'	2.36	0.44
59:Cs:78:A:C2	59:Cs:100:A:C4	3.06	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
37:DO:10:PRO:O	37:DO:11:GLY:C	2.59	0.44
48:Da:51:VAL:HG22	48:Da:81:VAL:HG23	1.99	0.44
54:D7:28:ARG:HA	54:D7:32:ASN:HD22	1.82	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:O2	58:D1:2097:U:H2'	2.17	0.44
64:DV:25:C:H2'	64:DV:26:A:H8	1.83	0.44
3:AC:110:ASN:O	3:AC:141:VAL:HG22	2.17	0.44
22:Ab:487:C:O5'	22:Ab:487:C:H6	2.01	0.44
22:Ab:917:G:H2'	22:Ab:918:C:C6	2.52	0.44
22:Ab:1109:U:H2'	22:Ab:1110:G:O5'	2.18	0.44
23:B2:19:U:N3	64:DV:37:A:C2	2.86	0.44
22:Bb:338:C:H2'	22:Bb:339:U:O4'	2.18	0.44
22:Bb:1037:C:N4	64:DV:34:G:H1'	2.29	0.44
22:Bb:1259:C:H2'	22:Bb:1260:U:H5'	1.98	0.44
5:BE:36:ASP:O	5:BE:38:GLN:HG2	2.18	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:53:ARG:NH1	58:C1:559:C:O3'	2.50	0.44
42:CT:112:ARG:NH2	43:CU:46:VAL:HG11	2.32	0.44
49:CH:23:LYS:O	49:CH:24:ALA:C	2.60	0.44
58:C1:875:A:N7	58:C1:2258:A:O2'	2.49	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
28:DB:24:ILE:HD13	28:DB:25:THR:N	2.32	0.44
31:DE:40:ASN:ND2	58:D1:2324:C:C4'	2.80	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
58:D1:107:G:C6	58:D1:108:A:N7	2.86	0.44
58:D1:303:C:C2	58:D1:384:G:N2	2.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:AT:36:ARG:HA	19:AT:71:LEU:HB2	2.00	0.44
22:Ab:1261:A:O2'	22:Ab:1263:U:OP2	2.21	0.44
22:Ab:1282:G:O2'	22:Ab:1283:U:OP2	2.30	0.44
22:Bb:175:U:H2'	22:Bb:176:G:H5'	2.00	0.44
22:Bb:544:U:O2'	22:Bb:545:U:OP2	2.21	0.44
22:Bb:1426:G:O2'	41:DS:122:ASP:OD2	2.34	0.44
16:BP:28:ARG:CG	16:BP:29:ASP:OD2	2.62	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
26:C4:53:G:HO2'	26:C4:54:G:P	2.41	0.44
30:CD:2:LYS:O	30:CD:3:GLU:HB3	2.17	0.44
30:CD:113:ALA:HB1	30:CD:186:ILE:HG21	1.99	0.44
32:CF:137:ASP:O	32:CF:138:LYS:HB2	2.18	0.44
35:CM:96:GLU:OE2	35:CM:96:GLU:N	2.38	0.44
37:CO:16:ARG:HH11	37:CO:16:ARG:C	2.26	0.44
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
49:CH:3:LYS:HE2	58:C1:1409:G:N7	2.33	0.44
50:CK:59:ARG:HD3	58:C1:75:C:OP1	2.17	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
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
61:D4:17:C:C2'	61:D4:18:U:C5	3.01	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
54:D7:46:HIS:CA	54:D7:47:THR:HG21	2.48	0.44
58:D1:1052:C:OP2	58:D1:1053:C:O2'	2.30	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
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:94:ARG:CZ	19:AT:81:ARG:HG2	2.48	0.44
22:Ab:469:G:H4'	22:Ab:470:G:O5'	2.18	0.44
22:Ab:503:C:H2'	22:Ab:504:A:O4'	2.18	0.44
22:Ab:661:U:H3	22:Ab:697:G:H22	1.65	0.44
22:Ab:686:A:H3'	22:Ab:687:G:H5'	1.99	0.44
13:BM:13:LYS:HA	13:BM:44:ARG:HH11	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
43:CU:78:LYS:NZ	58:C1:595:G:OP2	2.50	0.44
58:C1:553:A:H62	58:C1:2062:U:H3	1.66	0.44
58:C1:906:U:C5	58:C1:962:A:N7	2.81	0.44
58:C1:1094:C:C4	58:C1:1156:A:C2	3.06	0.44
25:D3:2:C:O2'	25:D3:3:C:O5'	2.36	0.44
25:D3:36:A:H2'	25:D3:37:A:O5'	2.18	0.44
28:DB:34:VAL:O	28:DB:35:LYS:C	2.60	0.44
29:DC:164:ARG:NH2	58:D1:2785:C:OP1	2.49	0.44
37:DO:47:ASP:HB3	37:DO:48:PRO:CA	2.48	0.44
63:DW:15:ARG:NH1	58:D1:1311:G:C5	2.86	0.44
63:DW:18:ARG:NH1	58:D1:542:G:H4'	2.33	0.44
50:DK:2:LYS:HB2	58:D1:95:C:H5''	2.00	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
4:AD:88:VAL:O	4:AD:92:VAL:HG23	2.17	0.43
8:AH:21:LYS:O	8:AH:65:TYR:OH	2.30	0.43
9:AI:77:ILE:O	9:AI:81:ILE:HG12	2.17	0.43
16:AP:71:ARG:O	16:AP:72:ARG:C	2.61	0.43
20:AU:13:LEU:O	20:AU:14:LYS:C	2.60	0.43
22:Ab:1067:G:OP1	22:Ab:1069:U:C4	2.71	0.43
22:Ab:1141:C:O2	22:Ab:1141:C:C2'	2.66	0.43
22:Ab:1189:G:C6	22:Ab:1190:C:C4	3.06	0.43
22:Bb:372:G:OP2	16:BP:67:THR:HG21	2.18	0.43
22:Bb:1330:U:H2'	22:Bb:1331:A:H8	1.83	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
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:16:ARG:HD3	37:CO:16:ARG:C	2.42	0.43
37:CO:55:ARG:NH1	58:C1:879:U:O2	2.50	0.43
37:CO:125:VAL:HG11	37:CO:138:LEU:HD21	1.99	0.43
40:CR:95:HIS:HD2	59:Cs:48:A:H4'	1.83	0.43
46:CY:76:CYS:HB3	46:CY:96:ILE:CD1	2.47	0.43
58:C1:139:A:C5'	58:C1:140:C:OP2	2.66	0.43
58:C1:1006:G:OP1	58:C1:1007:U:OP2	2.36	0.43
58:C1:2301:G:C2	58:C1:2354:C:O2	2.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
58:D1:99:G:OP1	58:D1:99:G:C4'	2.66	0.43
58:D1:1087:G:N3	58:D1:1087:G:H2'	2.33	0.43
58:D1:1217:G:H5'	58:D1:1218:A:O5'	2.18	0.43
6:AF:97:PHE:HD2	18:AS:31:LEU:HD21	1.82	0.43
9:AI:4:TYR:CE2	9:AI:88:TYR:CB	3.01	0.43
9:AI:9:ARG:CG	9:AI:14:VAL:HG13	2.48	0.43
22:Ab:1049:C:H2'	22:Ab:1050:A:H5'	1.99	0.43
22:Bb:1302:C:H5'	19:BT:70:LYS:HG2	2.01	0.43
22:Bb:1491:A:H2'	22:Bb:1492:C:C6	2.53	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
13:BM:70:LEU:O	13:BM:71:ARG:C	2.61	0.43
16:BP:28:ARG:NH1	16:BP:29:ASP:OD1	2.50	0.43
37:CO:63:PRO:HB3	56:C9:13:ARG:HB3	2.00	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
48:Ca:36:ILE:HD12	48:Ca:37:LEU:N	2.33	0.43
58:C1:68:G:C2'	58:C1:110:G:O2'	2.66	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
58:C1:1547:C:H6	58:C1:1547:C:H5''	1.82	0.43
58:C1:2319:G:O2'	58:C1:2320:A:OP1	2.28	0.43
28:DB:35:LYS:HD2	28:DB:36:PRO:HA	1.99	0.43
30:DD:179:GLU:N	30:DD:179:GLU:CD	2.76	0.43
31:DE:60:LEU:O	31:DE:64:THR:HG22	2.19	0.43
35:DM:55:VAL:O	35:DM:56:ASN:C	2.61	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
52:D5:37:PRO:O	52:D5:55:PRO:HG3	2.18	0.43
54:D7:37:ARG:HG3	58:D1:2355:U:O2'	2.17	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:AU:105:SER:HB3	22:Ab:198:G:N3	2.33	0.43
22:Ab:174:A:C2	22:Ab:175:U:C2	3.06	0.43
22:Ab:335:C:H2'	22:Ab:336:U:C6	2.52	0.43
22:Ab:918:C:H2'	22:Ab:919:G:H8	1.83	0.43
22:Ab:1200:C:H2'	22:Ab:1201:U:C6	2.53	0.43
22:Bb:742:G:H5'	22:Bb:858:C:H1'	1.99	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
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
28:CB:22:SER:O	28:CB:23:GLU:C	2.60	0.43
40:CR:89:ARG:O	40:CR:92:TYR:HB3	2.18	0.43
55:C8:9:ARG:NH2	58:C1:1355:G:OP2	2.50	0.43
58:C1:874:U:O2	58:C1:874:U:H3'	2.17	0.43
58:C1:2671:A:C5'	58:C1:2672:G:H21	2.32	0.43
29:DC:92:THR:O	29:DC:95:ILE:HG12	2.18	0.43
29:DC:137:HIS:HB3	29:DC:138:PRO:CD	2.47	0.43
30:DD:95:ARG:NH2	58:D1:1292:A:OP1	2.51	0.43
30:DD:188:ARG:HA	37:DO:7:ARG:HD3	2.01	0.43
31:DE:111:LEU:O	31:DE:114:ILE:HB	2.18	0.43
33:DI:6:LEU:O	33:DI:15:VAL:HG12	2.18	0.43
33:DI:142:VAL:HG12	33:DI:143:SER:H	1.83	0.43
38:DP:133:ARG:O	38:DP:134:ARG:HG2	2.19	0.43
42:DT:65:ILE:HD11	42:DT:96:ALA:HB3	1.99	0.43
42:DT:88:ILE:O	42:DT:88:ILE:HG13	2.16	0.43
43:DU:38:LEU:O	43:DU:39:LEU:HD13	2.18	0.43
48:Da:24:LYS:HG3	48:Da:36:ILE:HD11	1.99	0.43
58:D1:1849:A:H4'	58:D1:1850:U:O5'	2.17	0.43
17:AR:53:LEU:CD2	17:AR:82:MET:HE1	2.48	0.43
22:Bb:741:U:H2'	22:Bb:742:G:O4'	2.18	0.43
22:Bb:932:G:H2'	22:Bb:933:U:H6	1.82	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
16:BP:43:LYS:C	16:BP:45:THR:H	2.26	0.43
25:C2:16:U:H3'	25:C2:17:C:H5'	1.99	0.43
27:CA:74:VAL:HB	27:CA:91:ALA:CB	2.49	0.43
41:CS:106:SER:C	41:CS:107:ASP:OD1	2.61	0.43
44:CW:36:LEU:HD12	44:CW:48:ALA:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:CY:2:ARG:NH2	58:C1:103:C:H1'	2.33	0.43
48:Ca:24:LYS:HG3	48:Ca:36:ILE:HD11	2.01	0.43
49:CH:35:THR:HG21	58:C1:2101:G:OP1	2.18	0.43
54:C7:11:LEU:HD21	54:C7:51:GLU:HB2	2.00	0.43
58:C1:164:G:O2'	58:C1:165:G:H5'	2.18	0.43
58:C1:666:G:C8	58:C1:666:G:H3'	2.53	0.43
58:C1:1064:U:H3	58:C1:1187:A:H62	1.65	0.43
58:C1:1254:A:H5'	58:C1:1254:A:H8	1.84	0.43
58:C1:1734:U:H1'	58:C1:1747:A:C6	2.53	0.43
58:C1:2810:A:H2'	58:C1:2810:A:N3	2.34	0.43
62:DA:36:LYS:HA	62:DA:36:LYS:CE	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
56:D9:2:PRO:HB3	58:D1:613:C:H1'	2.00	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
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:HG22	13:AM:116:THR:O	2.18	0.43
14:AN:21:TYR:CE1	22:Ab:959:U:H5'	2.53	0.43
22:Ab:1109:U:C2'	22:Ab:1110:G:O5'	2.67	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
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
40:CR:16:ASN:OD1	40:CR:16:ASN:C	2.60	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:C1:676:C:OP2	58:C1:676:C:C5	2.71	0.43
58:C1:2095:U:H2'	58:C1:2096:U:C6	2.53	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
38:DP:138:ASP:OD1	47:DZ:122:ARG:NH1	2.52	0.43
41:DS:28:VAL:HG22	41:DS:46:GLU:HG3	2.00	0.43
56:D9:30:ARG:O	56:D9:31:HIS:HB3	2.19	0.43
58:D1:2529:A:H5'	58:D1:2529:A:H8	1.82	0.43
64:DV:55:C:H6	64:DV:55:C:O5'	2.00	0.43
8:AH:17:THR:HB	8:AH:78:GLN:OE1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:AM:81:LEU:O	13:AM:89:GLY:HA3	2.17	0.43
20:AU:24:LEU:HD13	20:AU:24:LEU:C	2.44	0.43
22:Ab:604:C:H2'	22:Ab:605:A:O4'	2.18	0.43
22:Bb:546:C:C4	22:Bb:862:U:C5	3.06	0.43
22:Bb:1427:A:N3	22:Bb:1427:A:C2'	2.78	0.43
4:BD:31:CYS:C	4:BD:33:MET:H	2.24	0.43
4:BD:166:LYS:HG3	4:BD:178:VAL:HG11	2.00	0.43
11:BK:107:SER:C	11:BK:108:ILE:HD12	2.44	0.43
28:CB:28:GLU:HB2	28:CB:29:PRO:HD3	2.00	0.43
28:CB:186:HIS:HD2	28:CB:188:GLU:H	1.65	0.43
29:CC:59:VAL:HG13	29:CC:63:LEU:HG	2.01	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
46:CY:46:LYS:NZ	58:C1:505:A:OP2	2.49	0.43
58:C1:82:A:N1	58:C1:96:G:O2'	2.45	0.43
58:C1:566:C:H2'	58:C1:567:C:OP1	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
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
38:DP:27:VAL:HG23	38:DP:137:TYR:CD1	2.53	0.43
55:D8:5:TRP:CH2	58:D1:732:G:N7	2.87	0.43
56:D9:6:THR:HG22	56:D9:63:PRO:HD3	2.01	0.43
56:D9:51:ALA:CA	56:D9:53:PRO:HD2	2.48	0.43
58:D1:849:U:O2'	58:D1:850:A:H5'	2.18	0.43
58:D1:1887:G:O2'	58:D1:1906:A:N6	2.46	0.43
2:AA:236:TYR:O	2:AA:237:ALA:C	2.61	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
22:Bb:258:A:C6	22:Bb:259:A:C6	3.07	0.43
22:Bb:1219:C:O2'	22:Bb:1282:G:N2	2.44	0.43
2:BA:60:ASP:HB3	2:BA:64:ARG:NH2	2.34	0.43
24:BC:126:ARG:O	24:BC:127:ARG:C	2.60	0.43
17:BR:59:ILE:CG2	17:BR:71:PHE:HB3	2.48	0.43
31:CE:126:ASP:HB3	58:C1:2314:G:H5''	2.00	0.43
32:CF:41:MET:HE3	32:CF:42:ARG:C	2.44	0.43
35:CM:1:MET:HG2	35:CM:2:LYS:N	2.34	0.43
41:CS:82:LEU:O	41:CS:83:ILE:O	2.37	0.43
42:CT:92:ARG:HD2	43:CU:11:GLN:CD	2.44	0.43
54:C7:30:THR:O	54:C7:31:PRO:C	2.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:C9:29:LYS:HG3	56:C9:29:LYS:O	2.19	0.43
58:C1:1578:C:O2'	58:C1:1579:G:N2	2.52	0.43
62:DA:55:ASP:HB2	62:DA:56:GLN:HE21	1.83	0.43
29:DC:166:THR:OG1	58:D1:2785:C:OP1	2.35	0.43
32:DF:92:ILE:C	32:DF:94:TYR:H	2.26	0.43
36:DN:31:LYS:CE	58:D1:2017:C:OP1	2.67	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
43:DU:28:GLU:CB	43:DU:29:PRO:HD2	2.49	0.43
45:DX:66:LEU:HD23	45:DX:66:LEU:C	2.43	0.43
58:D1:2277:A:C2	58:D1:2283:U:C5	3.06	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
2:AA:83:MET:O	2:AA:85:ALA:N	2.52	0.43
2:AA:118:LEU:CB	2:AA:142:LEU:HD12	2.48	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
22:Ab:1233:A:H1'	22:Ab:1352:C:O2'	2.19	0.43
22:Bb:910:C:H4'	7:BG:4:ARG:NH2	2.34	0.43
24:BC:11:ARG:O	24:BC:13:GLY:N	2.51	0.43
33:CI:123:LEU:HD23	33:CI:124:GLY:H	1.83	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
54:C7:20:ASN:O	54:C7:21:TYR:CD1	2.72	0.43
56:C9:33:ASN:N	56:C9:33:ASN:ND2	2.65	0.43
58:C1:865:A:C4	58:C1:1233:A:C2	3.06	0.43
58:C1:1095:A:C2	58:C1:2763:G:C4	3.07	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:H1'	2.53	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
30:DD:84:VAL:O	30:DD:85:GLY:C	2.61	0.43
37:DO:6:LEU:CD1	37:DO:8:PRO:O	2.67	0.43
37:DO:105:LEU:O	37:DO:106:LEU:HB3	2.19	0.43
41:DS:26:ASP:OD2	41:DS:26:ASP:C	2.61	0.43
63:DW:10:VAL:O	63:DW:11:ARG:CB	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:DY:2:ARG:NH2	58:D1:317:A:O2'	2.52	0.43
46:DY:7:VAL:HB	46:DY:8:LYS:HE3	2.00	0.43
58:D1:510:C:O2'	58:D1:511:C:H5'	2.19	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
2:AA:185:ILE:HG22	2:AA:199:TYR:HD1	1.82	0.43
4:AD:138:TYR:C	4:AD:138:TYR:CD2	2.96	0.43
20:AU:55:ILE:O	20:AU:56:MET:C	2.61	0.43
22:Ab:708:G:C2	22:Ab:709:G:C8	3.07	0.43
22:Ab:1135:A:H2'	22:Ab:1136:C:C6	2.54	0.43
22:Bb:751:A:H2'	22:Bb:752:A:O4'	2.18	0.43
22:Bb:1055:G:H2'	22:Bb:1056:U:H6	1.81	0.43
4:BD:129:ASN:HD22	4:BD:129:ASN:N	2.16	0.43
12:BL:48:PRO:C	12:BL:49:ASN:HD22	2.26	0.43
18:BS:67:ALA:O	18:BS:68:LYS:C	2.60	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
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
58:C1:934:C:H2'	58:C1:935:C:H5'	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
28:DB:25:THR:O	28:DB:26:LYS:C	2.61	0.43
32:DF:84:SER:O	32:DF:133:VAL:O	2.36	0.43
33:DI:27:ARG:HD3	49:DH:71:TYR:CE1	2.54	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
49:DH:93:GLU:O	49:DH:95:LEU:N	2.51	0.43
50:DK:28:LYS:HB3	50:DK:53:LEU:HD21	2.01	0.43
50:DK:42:GLY:O	50:DK:44:LEU:N	2.52	0.43
58:D1:1066:A:C8	58:D1:1066:A:C3'	3.02	0.43
58:D1:2342:G:O2'	58:D1:2347:A:N1	2.45	0.43
1:A2:20:U:O2'	1:A2:21:C:H5'	2.19	0.43
6:AF:62:TRP:CD1	18:AS:35:ARG:CZ	3.01	0.43
8:AH:11:THR:HG22	8:AH:15:ASN:ND2	2.33	0.43
8:AH:103:VAL:HG21	8:AH:110:ALA:HB2	2.01	0.43
9:AI:96:LEU:HD12	9:AI:101:PHE:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:AI:126:SER:OG	22:Ab:1213:G:O3'	2.37	0.43
10:AJ:55:LYS:NZ	22:Ab:951:G:N3	2.66	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
22:Ab:351:C:C4	22:Ab:352:A:N7	2.87	0.43
22:Ab:802:G:O2'	22:Ab:803:A:C5'	2.67	0.43
22:Ab:831:G:C4	22:Ab:832:G:C8	3.07	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
13:BM:64:TRP:CD1	13:BM:64:TRP:H	2.36	0.43
27:CA:21:THR:O	27:CA:21:THR:OG1	2.34	0.43
28:CB:166:GLN:NE2	28:CB:166:GLN:HA	2.31	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
41:CS:3:ARG:C	41:CS:5:ALA:N	2.75	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
56:C9:6:THR:CG2	58:C1:231:U:OP1	2.67	0.43
56:C9:50:LEU:O	56:C9:51:ALA:HB3	2.19	0.43
58:C1:2413:C:C2'	58:C1:2414:C:H5'	2.48	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
42:DT:57:PHE:O	42:DT:58:ARG:C	2.62	0.43
46:DY:81:LYS:HE2	46:DY:97:ARG:HE	1.83	0.43
49:DH:3:LYS:HD3	58:D1:1409:G:OP2	2.19	0.43
56:D9:4:MET:CE	56:D9:61:LEU:HD22	2.46	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
3:AC:193:TYR:HA	22:Ab:1188:G:O2'	2.19	0.42
5:AE:102:ALA:HB2	5:AE:120:THR:OG1	2.18	0.42
9:AI:118:LYS:NZ	22:Ab:1331:A:OP2	2.52	0.42
9:AI:125:TYR:HD2	9:AI:126:SER:N	2.16	0.42
17:AR:25:ARG:HH22	22:Ab:234:G:P	2.42	0.42
22:Ab:117:C:OP1	22:Ab:307:C:O2'	2.24	0.42
22:Ab:955:A:C2'	22:Ab:956:A:H5'	2.48	0.42
22:Ab:1332:A:C2	22:Ab:1333:U:C2	3.07	0.42
23:B2:19:U:H4'	23:B2:19:U:OP2	2.18	0.42
22:Bb:242:A:O2'	17:BR:99:SER:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:Bb:559:G:C5	22:Bb:859:G:C2	3.07	0.42
22:Bb:1342:A:O2'	22:Bb:1343:G:H5'	2.19	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
28:CB:242:ARG:H	28:CB:242:ARG:CD	2.32	0.42
37:CO:18:ARG:NH2	58:C1:1292:A:OP2	2.52	0.42
38:CP:16:ARG:C	38:CP:17:LEU:HD23	2.44	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
50:CK:8:LYS:O	50:CK:9:GLN:C	2.62	0.42
58:C1:921:G:N2	58:C1:948:C:C2	2.87	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
61:D4:12:G:C5	61:D4:13:C:C5	3.07	0.42
28:DB:62:TYR:CZ	58:D1:1846:G:N7	2.87	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
30:DD:90:PHE:HB3	58:D1:610:U:H1'	2.00	0.42
36:DN:61:VAL:O	36:DN:61:VAL:HG13	2.18	0.42
37:DO:66:GLY:O	37:DO:67:MET:HB3	2.18	0.42
37:DO:110:TYR:O	37:DO:111:ARG:C	2.62	0.42
63:DW:84:ARG:O	63:DW:95:ILE:HA	2.18	0.42
59:Ds:25:A:C2'	59:Ds:26:A:O5'	2.66	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
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
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
22:Ab:811:U:O5'	22:Ab:811:U:H6	2.02	0.42
22:Ab:1223:G:H2'	22:Ab:1224:C:C6	2.54	0.42
22:Ab:1482:G:HO2'	22:Ab:1483:G:P	2.41	0.42
22:Bb:1058:C:OP1	2:BA:179:LYS:NZ	2.34	0.42
22:Bb:1129:A:H2'	22:Bb:1130:C:O5'	2.19	0.42
22:Bb:1309:C:OP1	21:BW:21:TYR:HD1	2.02	0.42
22:Bb:1331:A:OP2	9:BI:118:LYS:NZ	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
26:C4:10:G:H8	26:C4:10:G:H5'	1.84	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
44:CW:60:ASN:ND2	58:C1:511:C:H4'	2.33	0.42
45:CX:80:ILE:HD13	45:CX:80:ILE:O	2.19	0.42
46:CY:2:ARG:C	46:CY:4:LYS:N	2.77	0.42
53:C6:55:ARG:C	53:C6:56:LYS:HD3	2.44	0.42
58:C1:932:C:C2	58:C1:935:C:N4	2.87	0.42
58:C1:1539:A:C2'	58:C1:1540:A:H5''	2.44	0.42
58:C1:1877:A:N3	58:C1:1877:A:H2'	2.34	0.42
58:C1:2667:U:H3	58:C1:2676:A:H2	1.65	0.42
59:Cs:28:C:H2'	59:Cs:29:A:O4'	2.19	0.42
32:DF:89:ILE:HD11	32:DF:94:TYR:O	2.19	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
37:DO:108:LYS:C	37:DO:110:TYR:H	2.27	0.42
38:DP:14:ARG:NH2	58:D1:1000:G:OP2	2.52	0.42
38:DP:16:ARG:O	38:DP:17:LEU:HD23	2.19	0.42
40:DR:98:VAL:HG12	40:DR:100:ALA:HB2	2.00	0.42
43:DU:34:GLU:HG2	43:DU:56:SER:HB2	2.00	0.42
43:DU:35:LEU:HB2	43:DU:57:VAL:CG1	2.49	0.42
48:Da:55:ARG:HE	48:Da:55:ARG:HB2	1.65	0.42
58:D1:69:A:H3'	58:D1:69:A:OP2	2.20	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
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
19:AT:6:LYS:HD3	22:Ab:1296:C:OP2	2.19	0.42
20:AU:26:ASN:HB2	20:AU:71:THR:HG23	2.01	0.42
22:Ab:741:U:OP1	22:Ab:806:C:O2'	2.33	0.42
22:Ab:798:A:C8	22:Ab:800:A:C8	3.07	0.42
22:Bb:719:C:H2'	22:Bb:720:C:H6	1.85	0.42
22:Bb:959:U:H5'	14:BN:21:TYR:CE1	2.54	0.42
22:Bb:1427:A:C5	41:DS:118:ARG:NH2	2.87	0.42
24:BC:70:VAL:HG12	24:BC:71:ALA:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:28:VAL:HG22	41:CS:46:GLU:HA	1.99	0.42
41:CS:29:ARG:HG3	41:CS:30:VAL:HG13	2.01	0.42
44:CW:49:LYS:NZ	58:C1:514:G:N7	2.66	0.42
46:CY:19:LYS:HB3	46:CY:20:TYR:CD1	2.53	0.42
58:C1:275:C:O2'	58:C1:276:G:H5'	2.18	0.42
58:C1:1008:C:O2'	58:C1:2284:A:N3	2.45	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:C1:2782:G:C5'	58:C1:2783:C:OP2	2.65	0.42
25:D3:16:U:H3'	25:D3:17:C:C5'	2.50	0.42
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
47:DZ:113:ALA:HB1	58:D1:941:A:C2	2.54	0.42
54:D7:46:HIS:CB	54:D7:47:THR:CG2	2.97	0.42
59:Ds:40:U:H1'	59:Ds:45:A:N6	2.34	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
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
2:AA:102:LEU:HD12	2:AA:102:LEU:N	2.35	0.42
5:AE:68:GLU:O	5:AE:68:GLU:CG	2.65	0.42
8:AH:86:ILE:HG13	8:AH:133:LEU:HD22	2.01	0.42
10:AJ:54:PHE:CZ	10:AJ:55:LYS:NZ	2.87	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
16:AP:67:THR:HG21	22:Ab:372:G:OP2	2.18	0.42
19:AT:39:THR:HG22	19:AT:40:ILE:N	2.34	0.42
22:Ab:454:G:O6	22:Ab:456:C:H5''	2.20	0.42
22:Ab:770:G:C2	22:Ab:781:C:C2	3.08	0.42
22:Ab:802:G:C3'	22:Ab:803:A:C5'	2.94	0.42
22:Ab:1040:G:C5	22:Ab:1186:A:C2	3.07	0.42
23:B2:19:U:OP2	23:B2:19:U:C4'	2.66	0.42
22:Bb:372:G:H2'	22:Bb:373:G:O5'	2.19	0.42
24:BC:18:TRP:C	24:BC:20:SER:H	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:BP:23:ASP:OD1	16:BP:24:ALA:N	2.53	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
39:CQ:48:VAL:O	39:CQ:49:ASP:C	2.61	0.42
41:CS:88:ILE:HG22	41:CS:89:VAL:CG2	2.43	0.42
47:CZ:8:TYR:CD1	47:CZ:8:TYR:N	2.87	0.42
47:CZ:145:GLU:HG3	47:CZ:146:ILE:CD1	2.49	0.42
58:C1:267:G:C2'	58:C1:268:G:OP2	2.67	0.42
58:C1:2623:C:C4	58:C1:2624:U:H5	2.37	0.42
29:DC:14:ILE:HG12	29:DC:21:VAL:HG22	2.02	0.42
29:DC:75:VAL:C	29:DC:77:ILE:H	2.28	0.42
32:DF:158:HIS:CE1	32:DF:170:ARG:HA	2.54	0.42
37:DO:64:LYS:CG	56:D9:25:MET:HE2	2.49	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:98:LEU:O	42:DT:101:ARG:O	2.37	0.42
49:DH:3:LYS:CD	58:D1:1409:G:OP2	2.67	0.42
59:Ds:102:A:H2'	59:Ds:103:G:O4'	2.20	0.42
58:D1:634:C:H2'	58:D1:635:G:H5'	1.99	0.42
58:D1:2201:U:O2	58:D1:2201:U:H2'	2.19	0.42
58:D1:2595:U:O2	58:D1:2595:U:O4'	2.36	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
11:AK:119:CYS:HB3	22:Ab:761:A:H2	1.84	0.42
12:AL:86:ARG:HB2	12:AL:101:VAL:HG23	2.01	0.42
17:AR:31:LEU:HD11	22:Ab:548:C:C5	2.54	0.42
22:Ab:89:G:C6	22:Ab:90:U:C4	3.08	0.42
22:Ab:1116:G:N3	22:Ab:1125:G:N2	2.67	0.42
22:Ab:1361:C:O2	22:Ab:1361:C:H2'	2.19	0.42
22:Bb:419:G:H2'	22:Bb:420:G:O4'	2.19	0.42
22:Bb:1300:A:H4'	19:BT:10:PHE:HB2	2.02	0.42
11:BK:37:GLY:O	11:BK:39:PRO:HD3	2.18	0.42
13:BM:108:ARG:N	13:BM:108:ARG:HD2	2.34	0.42
28:CB:43:ARG:HD2	28:CB:44:ASN:OD1	2.19	0.42
28:CB:224:ALA:O	28:CB:225:ALA:CB	2.67	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
31:CE:143:GLU:OE2	52:C5:52:SER:HB2	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:112:ARG:CZ	43:CU:46:VAL:HG11	2.50	0.42
48:Ca:12:ASN:O	48:Ca:14:ARG:N	2.52	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
58:C1:26:G:C4	58:C1:536:G:N2	2.87	0.42
58:C1:209:A:H4'	58:C1:210:A:O5'	2.20	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
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
45:DX:35:THR:CG2	58:D1:1643:C:O3'	2.66	0.42
46:DY:7:VAL:HG21	46:DY:8:LYS:NZ	2.34	0.42
56:D9:53:PRO:O	56:D9:54:GLU:C	2.62	0.42
58:D1:556:A:N7	58:D1:2042:C:O2'	2.41	0.42
1:A2:20:U:H2'	1:A2:21:C:O5'	2.20	0.42
2:AA:25:ASN:C	2:AA:25:ASN:OD1	2.62	0.42
16:AP:55:ARG:O	16:AP:56:ALA:C	2.62	0.42
22:Ab:13:U:H4'	22:Ab:510:C:O2'	2.20	0.42
22:Ab:982:G:C2'	22:Ab:983:A:H4'	2.45	0.42
22:Ab:1282:G:C2'	22:Ab:1283:U:OP2	2.68	0.42
22:Bb:460:G:H2'	22:Bb:461:G:H8	1.83	0.42
22:Bb:600:G:C2	22:Bb:601:G:N7	2.87	0.42
22:Bb:1032:U:H1'	22:Bb:1183:A:N7	2.35	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
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
30:CD:139:PHE:CD2	30:CD:139:PHE:C	2.97	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
58:C1:1311:G:O2'	58:C1:2033:G:O6	2.30	0.42
25:D3:9:A:C2	25:D3:45:U:C4	3.07	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:D4:50:G:N2	61:D4:67:C:C2	2.87	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:2:PRO:HD2	52:D5:51:TYR:CE2	2.54	0.42
31:DE:166:ASP:OD1	31:DE:166:ASP:N	2.52	0.42
32:DF:88:LEU:HD22	32:DF:88:LEU:N	2.35	0.42
45:DX:39:ILE:O	45:DX:40:LYS:C	2.63	0.42
56:D9:60:LEU:C	56:D9:63:PRO:HD2	2.45	0.42
58:D1:2192:A:O2'	58:D1:2193:U:C6	2.72	0.42
58:D1:2517:U:O2	58:D1:2517:U:C2'	2.66	0.42
5:AE:25:ARG:NH1	22:Ab:1052:C:O3'	2.52	0.42
20:AU:10:LEU:O	20:AU:13:LEU:HD12	2.19	0.42
22:Ab:483:A:H4'	22:Ab:484:G:OP1	2.19	0.42
22:Ab:917:G:C6	22:Ab:918:C:N4	2.87	0.42
22:Bb:294:A:H2'	22:Bb:295:G:O4'	2.20	0.42
22:Bb:837:A:H2'	22:Bb:838:A:O4'	2.19	0.42
22:Bb:917:G:H2'	22:Bb:918:C:C6	2.55	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
27:CA:56:GLN:NE2	27:CA:168:UNK:CB	2.83	0.42
30:CD:51:THR:HB	30:CD:88:VAL:HG11	2.02	0.42
30:CD:126:VAL:HG23	30:CD:127:GLU:N	2.34	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
44:CW:18:ARG:O	44:CW:19:LEU:C	2.63	0.42
44:CW:40:ASN:C	44:CW:41:LYS:HG2	2.45	0.42
56:C9:28:GLY:O	56:C9:32:LEU:HG	2.20	0.42
58:C1:894:G:H2'	58:C1:895:A:C8	2.54	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:N3	58:C1:2125:G:O4'	2.53	0.42
58:C1:2479:G:H22	58:C1:2492:G:C2'	2.31	0.42
37:DO:107:LYS:C	37:DO:109:GLY:N	2.78	0.42
39:DQ:11:ASN:CG	39:DQ:12:ARG:H	2.18	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
50:DK:61:LEU:HD12	50:DK:61:LEU:HA	1.89	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:D7:15:GLU:OE2	54:D7:41:PRO:HG3	2.19	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
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
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
9:AI:104:ARG:HD2	22:Ab:1101:C:OP1	2.19	0.42
11:AK:22:HIS:HB3	11:AK:29:ILE:HG23	2.02	0.42
11:AK:108:ILE:O	18:AS:87:ARG:N	2.49	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
22:Ab:915:A:C2	22:Ab:1362:G:O6	2.73	0.42
22:Ab:1331:A:C4	22:Ab:1332:A:C8	3.08	0.42
23:B2:18:G:O2'	22:Bb:1384:G:P	2.77	0.42
22:Bb:174:A:H2'	22:Bb:175:U:C6	2.54	0.42
22:Bb:524:G:H2'	22:Bb:525:G:O4'	2.20	0.42
22:Bb:658:G:H2'	22:Bb:659:A:H8	1.85	0.42
22:Bb:982:G:C2'	22:Bb:983:A:H4'	2.49	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
26:C4:17:C:C4	26:C4:18:U:C4	3.07	0.42
29:CC:104:VAL:HG11	29:CC:188:VAL:CG2	2.50	0.42
37:CO:58:THR:O	37:CO:58:THR:CG2	2.66	0.42
44:CW:62:HIS:O	44:CW:63:ASP:C	2.62	0.42
45:CX:54:VAL:C	45:CX:55:ASN:HD22	2.28	0.42
47:CZ:8:TYR:HB2	47:CZ:38:TYR:CE1	2.55	0.42
58:C1:2666:G:O2'	58:C1:2675:G:N1	2.50	0.42
31:DE:26:GLN:HE21	31:DE:26:GLN:H	1.67	0.42
31:DE:116:ASP:O	31:DE:117:PHE:HB2	2.20	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
54:D7:46:HIS:HB2	54:D7:47:THR:HG21	2.01	0.42
58:D1:195:A:H2'	58:D1:196:C:O4'	2.19	0.42
58:D1:978:G:N3	58:D1:978:G:H2'	2.33	0.42
58:D1:1477:C:H2'	58:D1:1478:U:O5'	2.20	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
15:AO:83:GLU:C	15:AO:85:LEU:H	2.27	0.42
22:Ab:1465:G:H8	22:Ab:1465:G:O5'	2.03	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:Bb:676:U:OP1	11:BK:124:LYS:HE2	2.20	0.42
22:Bb:1221:A:H4'	22:Bb:1222:U:H5''	2.01	0.42
22:Bb:1310:C:P	21:BW:21:TYR:HH	2.37	0.42
5:BE:76:ILE:CG1	5:BE:77:PRO:HD2	2.49	0.42
5:BE:139:LEU:HA	5:BE:142:LEU:CD1	2.50	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
26:C4:53:G:O2'	26:C4:54:G:H8	2.02	0.42
32:CF:92:ILE:C	32:CF:94:TYR:H	2.27	0.42
37:CO:124:LYS:HD3	37:CO:124:LYS:HA	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:C1:576:U:C4	58:C1:577:U:C4	3.08	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
60:D2:43:C:H4'	60:D2:43:C:OP1	2.20	0.42
30:DD:12:LEU:O	30:DD:13:SER:C	2.62	0.42
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:9:GLU:OE1	36:DN:9:GLU:HA	2.20	0.42
41:DS:96:ARG:NH1	58:D1:1784:C:P	2.93	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
49:DH:86:SER:HB2	49:DH:89:GLU:HB2	2.02	0.42
58:D1:88:U:O2	58:D1:88:U:H2'	2.18	0.42
58:D1:552:A:N1	58:D1:2063:A:H2'	2.34	0.42
58:D1:1098:C:O3'	58:D1:1151:A:P	2.77	0.42
58:D1:1151:A:P	58:D1:1151:A:O4'	2.78	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
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
22:Ab:376:G:C2	22:Ab:380:G:C6	3.08	0.42
22:Ab:379:A:OP1	22:Ab:449:C:O2'	2.35	0.42
22:Bb:640:C:O2'	15:BO:28:GLN:OE1	2.26	0.42
22:Bb:742:G:H8	22:Bb:742:G:O5'	2.02	0.42
22:Bb:748:C:H2'	22:Bb:749:G:O4'	2.19	0.42
2:BA:194:PRO:O	2:BA:195:ASP:C	2.63	0.42
8:BH:8:ASP:O	8:BH:9:MET:C	2.63	0.42
15:BO:55:GLY:O	15:BO:56:LEU:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:BS:67:ALA:HA	18:BS:70:ILE:HG13	2.01	0.42
29:CC:93:VAL:O	29:CC:95:ILE:N	2.53	0.42
29:CC:111:ARG:HG3	39:CQ:2:ARG:CG	2.50	0.42
30:CD:34:TRP:CD2	37:CO:12:ALA:HB2	2.54	0.42
32:CF:136:ILE:HD12	32:CF:136:ILE:N	2.35	0.42
33:CI:91:SER:HB2	33:CI:119:PRO:O	2.19	0.42
38:CP:110:THR:HG23	38:CP:113:GLN:HB2	2.02	0.42
41:CS:5:ALA:HB3	58:C1:2884:C:O2'	2.20	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:C1:1315:C:O2'	58:C1:1694:C:OP2	2.30	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:C1:1792:A:H8	58:C1:1792:A:O5'	2.02	0.42
25:D3:7:A:N6	25:D3:49:C:N4	2.67	0.42
41:DS:24:PRO:CA	41:DS:49:VAL:HG13	2.49	0.42
41:DS:128:GLU:O	41:DS:129:ARG:C	2.62	0.42
42:DT:25:TRP:CZ3	58:D1:16:G:H4'	2.55	0.42
42:DT:66:ASN:HD21	42:DT:70:ARG:HE	1.67	0.42
42:DT:85:LYS:C	42:DT:87:GLY:N	2.76	0.42
43:DU:19:LYS:HG2	43:DU:94:LEU:HB2	2.01	0.42
50:DK:64:LEU:HD23	50:DK:64:LEU:O	2.19	0.42
56:D9:14:VAL:HG21	56:D9:22:VAL:HG13	2.01	0.42
58:D1:420:A:C6	58:D1:421:U:C4	3.07	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:H8	58:D1:2675:G:O5'	2.03	0.42
2:AA:32:ILE:CD1	2:AA:40:HIS:CD2	3.03	0.41
3:AC:206:GLU:O	3:AC:207:VAL:C	2.63	0.41
9:AI:118:LYS:O	9:AI:119:ALA:CB	2.64	0.41
22:Ab:580:C:O2	22:Ab:580:C:H2'	2.20	0.41
22:Bb:257:U:H2'	22:Bb:259:A:OP2	2.20	0.41
22:Bb:1275:G:O2'	22:Bb:1276:G:P	2.78	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:O	19:BT:9:VAL:HG12	2.20	0.41
29:CC:101:ARG:HD2	29:CC:169:ASN:ND2	2.34	0.41
29:CC:107:THR:HG22	29:CC:107:THR:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:CF:149:ARG:HA	32:CF:162:ILE:HG13	2.02	0.41
37:CO:108:LYS:C	37:CO:110:TYR:H	2.27	0.41
45:CX:36:LYS:HB2	58:C1:1643:C:H5'	2.02	0.41
56:C9:30:ARG:CZ	58:C1:2430:U:O4	2.68	0.41
58:C1:271:U:H2'	58:C1:272:G:OP2	2.20	0.41
58:C1:754:C:C6	58:C1:754:C:H5''	2.55	0.41
58:C1:1575:G:H2'	58:C1:1575:G:N3	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
58:C1:2527:G:C6	58:C1:2528:C:N4	2.87	0.41
30:DD:37:VAL:O	30:DD:38:ARG:C	2.63	0.41
32:DF:44:VAL:O	32:DF:45:VAL:C	2.63	0.41
37:DO:146:VAL:HG13	37:DO:147:LEU:HB2	2.02	0.41
49:DH:63:ALA:O	49:DH:64:ALA:C	2.63	0.41
58:D1:157:U:OP2	58:D1:157:U:C6	2.73	0.41
58:D1:193:G:O2'	58:D1:194:U:P	2.78	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:D1:1729:C:H2'	58:D1:1730:C:H6	1.85	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
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
11:AK:20:TYR:CD1	22:Ab:691:C:H4'	2.55	0.41
22:Ab:539:C:H2'	22:Ab:540:C:H6	1.86	0.41
22:Bb:1434:G:H2'	22:Bb:1435:G:O4'	2.20	0.41
33:CI:81:VAL:HG22	33:CI:82:ARG:N	2.35	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
49:CH:44:PRO:O	49:CH:46:LEU:N	2.54	0.41
51:CL:40:THR:OG1	51:CL:43:ILE:HG12	2.20	0.41
56:C9:22:VAL:HB	56:C9:53:PRO:HB3	2.02	0.41
58:C1:552:A:H2	58:C1:2064:C:H5'	1.84	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
25:D3:34:G:N1	25:D3:35:A:C6	2.88	0.41
28:DB:65:ILE:HD13	28:DB:65:ILE:C	2.45	0.41
28:DB:158:ALA:O	28:DB:159:ALA:C	2.62	0.41
28:DB:245:PRO:O	28:DB:246:PRO:C	2.63	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:DP:123:HIS:CD2	58:D1:2478:C:H4'	2.54	0.41
39:DQ:21:TYR:HB3	39:DQ:47:PHE:CD2	2.55	0.41
59:Ds:38:C:O2	59:Ds:48:A:H1'	2.20	0.41
58:D1:906:U:C5	58:D1:962:A:N7	2.89	0.41
58:D1:949:C:H2'	58:D1:950:U:C6	2.55	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
3:AC:53:ALA:HB2	3:AC:115:LEU:CD2	2.50	0.41
9:AI:118:LYS:NZ	22:Ab:1331:A:P	2.93	0.41
18:AS:33:ASP:O	18:AS:40:LEU:HD11	2.20	0.41
22:Ab:1305:G:H4'	22:Ab:1345:C:N3	2.36	0.41
22:Bb:199:U:H2'	22:Bb:200:C:H6	1.84	0.41
22:Bb:342:G:H2'	22:Bb:342:G:N3	2.35	0.41
22:Bb:1193:U:C4'	22:Bb:1194:U:OP1	2.68	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
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
39:CQ:85:PRO:C	39:CQ:87:TYR:H	2.28	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
44:CW:80:PRO:HB3	58:C1:25:G:OP1	2.20	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
56:C9:4:MET:HE3	56:C9:61:LEU:HD22	2.01	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
58:C1:2450:A:C8	58:C1:2450:A:H5''	2.55	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
37:DO:46:LYS:HE2	58:D1:184:A:O4'	2.21	0.41
63:DW:64:MET:O	63:DW:109:GLU:CD	2.63	0.41
46:DY:17:SER:CA	46:DY:71:LYS:HE2	2.49	0.41
58:D1:821:G:C5	58:D1:840:G:C8	3.08	0.41
58:D1:1032:G:O2'	58:D1:1045:A:N3	2.47	0.41
58:D1:1549:C:HO2'	58:D1:1550:C:H5'	1.80	0.41
58:D1:2045:G:H2'	58:D1:2046:C:C6	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A2:15:A:OP2	22:Ab:1483:G:H2'	2.21	0.41
2:AA:185:ILE:HG22	2:AA:199:TYR:CB	2.50	0.41
4:AD:128:VAL:O	4:AD:129:ASN:C	2.63	0.41
16:AP:19:ILE:HG22	16:AP:36:ILE:CG1	2.50	0.41
22:Ab:500:U:O4	22:Ab:517:A:OP2	2.38	0.41
22:Ab:802:G:O2'	22:Ab:803:A:H5''	2.19	0.41
22:Bb:734:G:N3	15:BO:23:GLY:HA3	2.36	0.41
22:Bb:761:A:C2	22:Bb:762:G:H1'	2.56	0.41
22:Bb:1046:C:H3'	22:Bb:1047:G:H2'	2.03	0.41
2:BA:90:MET:HE2	2:BA:90:MET:HA	2.01	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
14:BN:27:CYS:C	14:BN:29:ARG:H	2.28	0.41
15:BO:62:GLN:O	15:BO:63:ARG:C	2.62	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
28:CB:270:ILE:C	28:CB:270:ILE:CD1	2.93	0.41
33:CI:74:ASN:OD1	33:CI:75:LEU:N	2.54	0.41
37:CO:13:ASN:C	37:CO:13:ASN:HD22	2.27	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
47:CZ:135:GLU:O	47:CZ:136:PHE:C	2.63	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
38:DP:12:GLN:HE21	38:DP:73:PRO:HD2	1.85	0.41
39:DQ:11:ASN:CG	39:DQ:12:ARG:N	2.75	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
59:Ds:49:C:H6	59:Ds:49:C:O5'	2.03	0.41
58:D1:670:A:H2'	58:D1:671:G:O4'	2.20	0.41
58:D1:799:C:O5'	58:D1:799:C:H6	2.02	0.41
58:D1:928:G:H2'	58:D1:929:G:C8	2.56	0.41
58:D1:2272:C:O2'	58:D1:2273:U:H5'	2.21	0.41
58:D1:2597:C:H6	58:D1:2597:C:O5'	2.04	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
22:Ab:671:A:N3	22:Ab:672:G:H1'	2.36	0.41
22:Ab:820:G:C6	22:Ab:829:G:C6	3.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:Ab:945:C:H6	22:Ab:945:C:O5'	2.03	0.41
8:BH:6:ILE:O	8:BH:9:MET:HB3	2.20	0.41
25:C3:10:G:N2	25:C3:26:A:H1'	2.34	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
41:CS:128:GLU:O	41:CS:129:ARG:C	2.64	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
56:C9:4:MET:HB2	56:C9:61:LEU:HD13	2.01	0.41
58:C1:497:A:C8	58:C1:497:A:H3'	2.56	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
59:Cs:21:G:O2'	59:Cs:22:U:O5'	2.38	0.41
59:Cs:66:A:C2'	59:Cs:67:G:OP2	2.67	0.41
29:DC:182:LEU:C	29:DC:183:LEU:HD12	2.46	0.41
32:DF:20:ALA:CB	32:DF:21:PRO:CD	2.94	0.41
41:DS:38:ASN:ND2	41:DS:40:THR:H	2.15	0.41
46:DY:20:TYR:O	46:DY:21:LYS:C	2.62	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
58:D1:1090:A:H3'	58:D1:1090:A:N3	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
64:DV:15:G:H4'	64:DV:16:U:OP1	2.21	0.41
4:AD:25:ARG:C	4:AD:27:TYR:N	2.78	0.41
9:AI:59:PHE:CD1	9:AI:59:PHE:N	2.88	0.41
12:AL:60:LEU:HD22	12:AL:60:LEU:N	2.35	0.41
17:AR:53:LEU:HD22	17:AR:82:MET:HE1	2.02	0.41
22:Ab:1036:G:N7	22:Ab:1181:U:H3'	2.36	0.41
22:Bb:1050:A:N3	22:Bb:1051:G:H1'	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
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
30:CD:96:ASP:OD1	30:CD:96:ASP:C	2.64	0.41
31:CE:18:GLU:O	31:CE:22:ARG:HB2	2.20	0.41
33:CI:5:LEU:HD22	33:CI:9:LEU:HD13	2.01	0.41
33:CI:98:ALA:HA	33:CI:109:ILE:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:CT:97:ASP:OD1	42:CT:97:ASP:C	2.63	0.41
54:C7:13:CYS:HB2	54:C7:22:ALA:HB3	2.03	0.41
58:C1:710:C:H4'	58:C1:985:A:OP1	2.19	0.41
58:C1:966:G:C6	58:C1:967:U:C4	3.09	0.41
58:C1:1092:G:OP1	58:C1:1092:G:H4'	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:N3	58:C1:2640:A:H2'	2.36	0.41
62:DA:77:ILE:HG23	62:DA:77:ILE:O	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:3:GLU:HA	30:DD:24:LEU:HB3	2.03	0.41
30:DD:157:VAL:HG11	30:DD:181:LEU:HD13	2.01	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
43:DU:75:PHE:CD1	43:DU:75:PHE:C	2.98	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
48:Da:41:ARG:NH2	58:D1:2398:U:O2'	2.51	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:O2	58:D1:2518:C:H2'	2.20	0.41
58:D1:2801:C:N3	58:D1:2902:G:O6	2.53	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
16:AP:53:VAL:O	16:AP:54:GLU:C	2.62	0.41
20:AU:69:GLY:O	20:AU:73:HIS:CD2	2.74	0.41
22:Bb:452:C:C2	22:Bb:461:G:N2	2.89	0.41
22:Bb:606:A:C8	22:Bb:607:C:C6	3.09	0.41
22:Bb:1193:U:C5'	22:Bb:1194:U:OP1	2.69	0.41
2:BA:29:ALA:O	2:BA:32:ILE:HG22	2.21	0.41
12:BL:91:LYS:O	12:BL:91:LYS:HG3	2.20	0.41
20:BU:75:ASN:O	20:BU:79:ARG:N	2.51	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
31:CE:60:LEU:HD13	31:CE:60:LEU:C	2.46	0.41
31:CE:96:ARG:H	31:CE:99:MET:HE2	1.86	0.41
32:CF:54:ARG:HD2	32:CF:55:PRO:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:CF:167:GLU:CB	32:CF:168:PRO:HD2	2.50	0.41
37:CO:57:THR:HB	37:CO:58:THR:C	2.46	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:C1:88:U:C2'	58:C1:89:A:OP2	2.69	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
58:C1:2740:U:O2'	58:C1:2741:G:H5'	2.20	0.41
59:Cs:57:A:OP2	59:Cs:58:A:OP2	2.38	0.41
32:DF:62:LYS:HB3	32:DF:62:LYS:HE2	1.94	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
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
58:D1:2723:U:O2'	58:D1:2724:A:P	2.79	0.41
4:AD:11:LEU:O	4:AD:12:CYS:C	2.63	0.41
4:AD:24:GLU:O	4:AD:27:TYR:HB2	2.20	0.41
22:Ab:332:C:O2'	22:Ab:333:C:H5'	2.21	0.41
22:Ab:1189:G:C4	22:Ab:1190:C:C5	3.09	0.41
22:Ab:1433:C:O4'	22:Ab:1434:G:N2	2.54	0.41
22:Bb:312:G:H2'	22:Bb:313:G:H8	1.86	0.41
22:Bb:1269:A:N6	22:Bb:1270:A:N6	2.68	0.41
5:BE:27:ARG:HE	5:BE:27:ARG:HB2	1.78	0.41
26:C4:49:C:O2'	26:C4:60:A:O2'	2.37	0.41
29:CC:4:ILE:HG12	29:CC:5:LEU:O	2.21	0.41
29:CC:132:HIS:CD2	29:CC:135:HIS:NE2	2.89	0.41
37:CO:17:LYS:O	37:CO:18:ARG:C	2.63	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
54:C7:28:ARG:HA	54:C7:32:ASN:HB3	2.02	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
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)
29:DC:93:VAL:C	29:DC:95:ILE:N	2.79	0.41
30:DD:3:GLU:O	30:DD:19:GLU:CB	2.69	0.41
43:DU:2:PHE:HB2	43:DU:42:GLY:CA	2.51	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
51:DL:31:LEU:O	51:DL:32:GLN:HB2	2.21	0.41
58:D1:251:C:O2'	58:D1:455:A:N3	2.46	0.41
58:D1:448:A:C6	58:D1:449:A:C6	3.09	0.41
58:D1:1574:A:N7	58:D1:1575:G:H8	2.19	0.41
58:D1:1846:G:C8	58:D1:1846:G:C3'	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
3:AC:15:THR:HG21	3:AC:181:ASN:HA	2.02	0.41
4:AD:25:ARG:HG3	22:Ab:406:G:OP2	2.21	0.41
4:AD:150:GLU:CD	4:AD:151:LYS:H	2.29	0.41
8:AH:34:GLU:HA	8:AH:34:GLU:OE2	2.21	0.41
8:AH:97:VAL:HB	8:AH:129:VAL:C	2.45	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
14:AN:42:ILE:O	14:AN:43:CYS:C	2.63	0.41
17:AR:99:SER:C	17:AR:100:LYS:HG3	2.45	0.41
19:AT:44:MET:N	19:AT:44:MET:SD	2.94	0.41
20:AU:42:GLN:HE21	20:AU:42:GLN:HA	1.85	0.41
22:Ab:99:G:H2'	22:Ab:100:C:C6	2.56	0.41
22:Ab:588:G:H2'	22:Ab:589:U:O4'	2.21	0.41
22:Ab:1135:A:H2'	22:Ab:1136:C:H6	1.85	0.41
22:Ab:1145:C:H2'	22:Ab:1146:C:C6	2.56	0.41
22:Bb:487:C:OP1	12:BL:119:LYS:NZ	2.39	0.41
22:Bb:868:G:O2'	22:Bb:884:G:O6	2.35	0.41
22:Bb:1067:G:C5	22:Bb:1068:U:C4	3.09	0.41
22:Bb:1092:C:H2'	22:Bb:1093:A:O4'	2.21	0.41
22:Bb:1259:C:C6	22:Bb:1259:C:C3'	3.03	0.41
22:Bb:1305:G:H4'	22:Bb:1345:C:N3	2.35	0.41
22:Bb:1415:G:OP1	41:DS:107:ASP:HB2	2.21	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
9:BI:8:GLY:HA2	9:BI:79:LEU:HD12	2.03	0.41
11:BK:17:GLY:HA3	11:BK:77:MET:SD	2.61	0.41
11:BK:34:ASP:HB3	11:BK:40:ILE:HD11	2.02	0.41
13:BM:8:GLU:OE1	13:BM:22:ILE:HG23	2.21	0.41
13:BM:113:PRO:O	13:BM:115:LYS:HD3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:BR:9:VAL:O	17:BR:21:VAL:HA	2.21	0.41
18:BS:40:LEU:C	18:BS:42:ARG:N	2.76	0.41
19:BT:6:LYS:H	19:BT:6:LYS:HD2	1.85	0.41
26:C4:7:G:H8	26:C4:7:G:C5'	2.34	0.41
26:C4:50:G:C2	26:C4:51:U:H1'	2.55	0.41
26:C4:51:U:H2'	26:C4:51:U:O2	2.20	0.41
28:CB:30:GLU:HB2	28:CB:35:LYS:CE	2.49	0.41
28:CB:35:LYS:CG	28:CB:63:ARG:HG3	2.42	0.41
28:CB:232:PRO:HD2	28:CB:249:PRO:HA	2.03	0.41
29:CC:9:VAL:HG22	29:CC:25:VAL:HB	2.03	0.41
29:CC:61:ARG:HD3	58:C1:2799:C:H1'	2.02	0.41
30:CD:177:ALA:HB1	30:CD:178:PRO:CD	2.51	0.41
31:CE:77:ILE:HD13	31:CE:77:ILE:HG21	1.82	0.41
31:CE:130:ASN:HB3	31:CE:160:VAL:HA	2.03	0.41
32:CF:25:LYS:HB3	32:CF:32:GLU:OE2	2.20	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:17:LYS:C	37:CO:19:VAL:N	2.78	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:CD1	40:CR:36:TYR:N	2.88	0.41
42:CT:9:VAL:O	42:CT:13:LYS:HE3	2.21	0.41
43:CU:45:THR:O	43:CU:46:VAL:HG12	2.21	0.41
50:CK:47:ASN:ND2	58:C1:92:G:N3	2.69	0.41
56:C9:25:MET:HE3	56:C9:25:MET:HB3	1.92	0.41
56:C9:62:LEU:N	56:C9:63:PRO:HD2	2.36	0.41
58:C1:88:U:O2'	58:C1:89:A:OP2	2.33	0.41
58:C1:158:U:H4'	58:C1:159:G:C8	2.55	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
58:C1:1068:U:OP2	58:C1:1069:G:N7	2.54	0.41
58:C1:1670:C:H2'	58:C1:1671:G:O4'	2.21	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:C1:2220:A:H3'	58:C1:2221:C:H6	1.86	0.41
58:C1:2861:G:C2	58:C1:2862:C:C2	3.09	0.41
60:D2:57:G:N7	64:DV:18:G:N1	2.66	0.41
28:DB:58:HIS:CD2	58:D1:1613:A:H5'	2.56	0.41
29:DC:87:GLU:O	29:DC:87:GLU:HG3	2.20	0.41
29:DC:98:PRO:HD3	29:DC:175:VAL:CG1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:DC:101:ARG:NH1	29:DC:169:ASN:O	2.54	0.41
30:DD:65:TRP:HA	30:DD:66:PRO:HD2	1.80	0.41
31:DE:38:VAL:HG11	58:D1:2325:C:H5'	2.02	0.41
32:DF:86:GLU:OE1	32:DF:86:GLU:N	2.53	0.41
37:DO:23:PRO:HD2	37:DO:33:ARG:CZ	2.51	0.41
37:DO:25:SER:HA	58:D1:857:U:H3'	2.03	0.41
38:DP:135:ASP:C	38:DP:137:TYR:H	2.29	0.41
40:DR:53:SER:OG	40:DR:54:LEU:N	2.53	0.41
41:DS:6:LEU:O	41:DS:7:ILE:C	2.64	0.41
41:DS:10:VAL:O	41:DS:13:ARG:HG2	2.20	0.41
41:DS:83:ILE:HG13	41:DS:84:GLN:H	1.86	0.41
45:DX:24:GLY:O	45:DX:82:GLN:HA	2.21	0.41
45:DX:36:LYS:HB2	58:D1:1643:C:H5'	2.02	0.41
52:D5:60:GLU:O	52:D5:61:VAL:HB	2.20	0.41
58:D1:880:C:C2	58:D1:881:A:C8	3.09	0.41
58:D1:902:C:O2	58:D1:902:C:H2'	2.21	0.41
58:D1:1093:A:H4'	58:D1:1094:C:OP1	2.19	0.41
58:D1:1313:A:OP1	58:D1:2027:C:OP1	2.39	0.41
58:D1:1529:G:H2'	58:D1:1530:G:O5'	2.21	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:D1:2509:C:OP2	58:D1:2510:C:OP2	2.38	0.41
58:D1:2861:G:C2	58:D1:2862:C:C2	3.09	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
4:AD:72:GLU:HG2	22:Ab:529:C:H5'	2.03	0.41
7:AG:148:ASN:HD22	7:AG:148:ASN:N	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
22:Ab:1074:U:O2	22:Ab:1076:A:C8	2.74	0.41
22:Ab:1386:C:H2'	22:Ab:1386:C:O2	2.21	0.41
22:Ab:1387:C:O5'	22:Ab:1387:C:H6	2.04	0.41
22:Bb:67:G:C2	22:Bb:68:C:C6	3.09	0.41
22:Bb:90:U:O2'	22:Bb:91:G:H8	2.03	0.41
22:Bb:718:G:C6	22:Bb:719:C:C4	3.09	0.41
22:Bb:900:G:C6	22:Bb:901:A:C6	3.10	0.41
22:Bb:958:C:H5'	22:Bb:959:U:C5	2.56	0.41
22:Bb:1205:C:P	19:BT:78:ARG:HH21	2.44	0.41
22:Bb:1507:G:H4'	22:Bb:1508:G:OP2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BA:24:TRP:CH2	2:BA:26:PRO:HA	2.56	0.41
2:BA:239:VAL:O	2:BA:240:GLN:CB	2.68	0.41
8:BH:53:VAL:HG12	8:BH:54:ASP:OD2	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
40:CR:62:LYS:HB2	59:Cs:50:G:OP1	2.21	0.41
42:CT:34:LYS:HE3	42:CT:34:LYS:HA	2.03	0.41
43:CU:49:THR:HB	43:CU:50:PRO:CD	2.51	0.41
46:CY:7:VAL:HB	46:CY:8:LYS:CE	2.51	0.41
46:CY:47:LYS:CG	46:CY:60:PHE:HE2	2.34	0.41
56:C9:8:LYS:O	56:C9:12:LYS:HG3	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:OP1	58:C1:2801:C:H4'	2.21	0.41
61:D4:12:G:H1'	58:D1:1944:U:O2'	2.21	0.41
28:DB:264:LYS:HA	28:DB:265:PRO:HD2	1.89	0.41
28:DB:270:ILE:C	28:DB:271:ILE:CG1	2.94	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:89:GLY:HA3	58:D1:2323:U:O2'	2.21	0.41
31:DE:115:ARG:CG	31:DE:116:ASP:H	2.34	0.41
37:DO:51:PHE:O	37:DO:52:GLU:HB2	2.21	0.41
37:DO:125:VAL:CG1	37:DO:138:LEU:HD21	2.50	0.41
38:DP:39:PRO:O	38:DP:40:ALA:HB2	2.20	0.41
39:DQ:48:VAL:O	39:DQ:49:ASP:C	2.64	0.41
58:D1:151:G:H2'	58:D1:152:C:C6	2.56	0.41
58:D1:209:A:H4'	58:D1:210:A:O5'	2.20	0.41
58:D1:1042:G:O2'	58:D1:1043:C:H5'	2.21	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
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:19:MET:HB2	22:Ab:899:U:O2	2.20	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
12:AL:27:LEU:C	12:AL:29:GLY:N	2.77	0.40
22:Ab:1433:C:OP2	22:Ab:1434:G:C6	2.74	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:Bb:425:U:O2'	4:BD:22:LYS:NZ	2.53	0.40
22:Bb:485:C:H1'	22:Bb:533:C:H1'	2.03	0.40
22:Bb:749:G:H5''	22:Bb:750:A:OP1	2.21	0.40
22:Bb:811:U:O2'	22:Bb:837:A:N1	2.50	0.40
2:BA:212:GLN:HE22	2:BA:216:SER:HB2	1.86	0.40
24:BC:58:GLU:HB2	24:BC:65:ALA:HB3	2.03	0.40
24:BC:167:TRP:O	24:BC:168:ALA:CB	2.69	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
15:BO:9:GLN:O	15:BO:10:LYS:C	2.65	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
35:CM:67:LEU:C	35:CM:69:GLN:H	2.29	0.40
41:CS:65:LYS:HE3	41:CS:66:VAL:H	1.86	0.40
42:CT:31:SER:C	42:CT:33:ARG:H	2.27	0.40
42:CT:33:ARG:NH1	58:C1:1297:G:O4'	2.55	0.40
47:CZ:130:PRO:O	47:CZ:133:ILE:HG12	2.22	0.40
51:CL:13:ILE:HD11	58:C1:1034:G:C8	2.57	0.40
58:C1:338:G:H2'	58:C1:339:C:O4'	2.22	0.40
58:C1:635:G:H8	58:C1:635:G:C5'	2.33	0.40
58:C1:1967:U:H2'	58:C1:1968:C:H6	1.86	0.40
61:D4:10:G:H8	61:D4:10:G:O5'	2.05	0.40
40:DR:36:TYR:N	40:DR:36:TYR:HD1	2.19	0.40
41:DS:3:ARG:HD3	58:D1:2885:G:H4'	1.99	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
47:DZ:165:VAL:CG1	47:DZ:166:SER:N	2.84	0.40
49:DH:45:ASN:C	49:DH:45:ASN:ND2	2.79	0.40
58:D1:666:G:OP2	58:D1:2413:C:N4	2.54	0.40
58:D1:1574:A:N7	58:D1:1575:G:C8	2.89	0.40
58:D1:1589:C:H3'	58:D1:1589:C:C6	2.56	0.40
2:AA:182:ILE:O	2:AA:183:PRO:C	2.64	0.40
3:AC:27:LYS:HE3	3:AC:27:LYS:HB2	1.93	0.40
9:AI:12:GLU:O	9:AI:68:GLY:CA	2.69	0.40
12:AL:25:PRO:C	12:AL:27:LEU:H	2.26	0.40
22:Ab:345:A:O2'	22:Ab:346:G:H5'	2.20	0.40
22:Ab:658:G:H2'	22:Ab:659:A:C8	2.56	0.40
22:Ab:1082:G:C6	22:Ab:1083:C:C4	3.09	0.40
23:B2:20:U:H2'	23:B2:21:C:H6	1.81	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:Bb:1270:A:N1	22:Bb:1354:G:H1'	2.36	0.40
2:BA:18:GLY:HA2	2:BA:42:ILE:HG22	2.03	0.40
2:BA:168:THR:HG23	2:BA:192:SER:CB	2.52	0.40
11:BK:21:ILE:HG13	11:BK:30:VAL:HG12	2.04	0.40
16:BP:56:ALA:O	16:BP:60:LEU:HD12	2.21	0.40
28:CB:28:GLU:HB2	28:CB:29:PRO:CD	2.51	0.40
29:CC:81:ILE:O	29:CC:82:ARG:C	2.64	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:87:LEU:O	35:CM:88:GLU:C	2.64	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
58:C1:1088:C:H3'	58:C1:1088:C:H6	1.86	0.40
58:C1:1812:C:C4	58:C1:2598:A:C2	3.09	0.40
58:C1:1813:A:C2	58:C1:2598:A:C5	3.10	0.40
58:C1:2270:G:C6	58:C1:2271:C:C4	3.09	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
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
36:DN:23:ARG:HH11	58:D1:2573:U:HO2'	1.68	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
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
50:DK:16:LEU:O	50:DK:17:SER:CB	2.69	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
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
58:D1:1812:C:H1'	58:D1:2620:U:H5''	2.01	0.40
58:D1:1902:C:H5''	58:D1:1902:C:C6	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
1:A2:19:U:O2'	1:A2:20:U:H5'	2.20	0.40
2:AA:133:LYS:HE2	22:Ab:1141:C:H4'	2.03	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:70:LEU:O	13:AM:71:ARG:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:AM:84:ILE:HG13	19:AT:66:MET:SD	2.61	0.40
20:AU:13:LEU:O	20:AU:16:HIS:N	2.52	0.40
22:Ab:686:A:H3'	22:Ab:687:G:C5'	2.50	0.40
22:Bb:19:C:H2'	22:Bb:20:C:O4'	2.21	0.40
22:Bb:485:C:H2'	22:Bb:486:G:H8	1.86	0.40
22:Bb:942:A:N3	22:Bb:947:A:O2'	2.46	0.40
22:Bb:1360:A:P	7:BG:94:ARG:NH1	2.95	0.40
2:BA:19:HIS:CD2	2:BA:189:ASP:OD2	2.73	0.40
24:BC:23:TYR:CD2	24:BC:23:TYR:C	3.00	0.40
4:BD:155:LEU:O	4:BD:156:GLU:C	2.64	0.40
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
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
47:CZ:41:LEU:O	47:CZ:42:VAL:C	2.64	0.40
58:C1:66:G:H2'	58:C1:67:C:C6	2.57	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:C6	58:C1:1902:C:H5''	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
60:D2:53:G:N3	60:D2:53:G:H2'	2.36	0.40
60:D2:56:C:H5'	58:D1:942:C:H4'	2.02	0.40
28:DB:65:ILE:HD11	28:DB:67:PHE:CD2	2.56	0.40
28:DB:145:VAL:HG12	28:DB:146:GLU:O	2.21	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
37:DO:16:ARG:NH1	37:DO:16:ARG:HB2	2.36	0.40
37:DO:51:PHE:CE1	58:D1:184:A:OP2	2.75	0.40
51:DL:31:LEU:O	58:D1:1203:C:H4'	2.21	0.40
58:D1:538:A:H1'	58:D1:603:C:O2'	2.22	0.40
58:D1:2667:U:H3	58:D1:2676:A:H2	1.68	0.40
5:AE:12:LEU:HD22	5:AE:12:LEU:C	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:AI:69:GLY:HA3	22:Ab:1354:G:O3'	2.22	0.40
9:AI:104:ARG:CD	22:Ab:1100:G:O3'	2.70	0.40
13:AM:104:ARG:HB2	22:Ab:1208:C:C4	2.57	0.40
22:Ab:597:C:C6	22:Ab:597:C:H3'	2.56	0.40
22:Ab:1297:U:H2'	22:Ab:1298:G:O4'	2.22	0.40
22:Bb:1426:G:O2'	41:DS:118:ARG:NH1	2.55	0.40
2:BA:25:ASN:OD1	2:BA:25:ASN:C	2.64	0.40
15:BO:81:LEU:CD1	15:BO:85:LEU:HD13	2.49	0.40
37:CO:64:LYS:HE2	58:C1:655:A:OP1	2.21	0.40
39:CQ:85:PRO:C	39:CQ:87:TYR:N	2.79	0.40
41:CS:3:ARG:HE	58:C1:2885:G:H4'	1.83	0.40
45:CX:84:ALA:O	45:CX:85:PRO:C	2.64	0.40
46:CY:54:LYS:O	46:CY:55:TYR:C	2.64	0.40
58:C1:38:C:H2'	58:C1:39:C:C6	2.56	0.40
58:C1:282:G:H5''	58:C1:283:G:OP2	2.22	0.40
58:C1:781:A:C8	58:C1:782:C:C5	3.10	0.40
58:C1:894:G:C4	58:C1:977:A:H8	2.40	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
61:D4:6:G:O6	61:D4:68:C:N4	2.49	0.40
29:DC:61:ARG:HD3	58:D1:2799:C:H1'	2.01	0.40
33:DI:123:LEU:HD23	33:DI:142:VAL:HB	2.03	0.40
42:DT:76:TYR:CD2	42:DT:76:TYR:C	2.99	0.40
46:DY:101:LYS:HG2	46:DY:101:LYS:OXT	2.21	0.40
53:D6:55:ARG:C	53:D6:56:LYS:HD3	2.46	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
5:AE:6:PHE:CZ	5:AE:66:MET:HE1	2.56	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
22:Ab:783:G:C6	22:Ab:784:G:C4	3.10	0.40
22:Bb:61:A:H4'	22:Bb:62:G:O5'	2.21	0.40
22:Bb:99:G:H2'	22:Bb:100:C:C6	2.57	0.40
22:Bb:183:C:O4'	20:BU:89:ARG:NH2	2.54	0.40
22:Bb:251:G:P	17:BR:69:LYS:HZ3	2.45	0.40
22:Bb:714:G:C5	22:Bb:715:G:H1'	2.56	0.40
22:Bb:1053:U:H2'	22:Bb:1054:C:H6	1.86	0.40
2:BA:118:LEU:HB3	2:BA:142:LEU:HD12	2.03	0.40
4:BD:110:PHE:HD1	4:BD:110:PHE:H	1.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:BR:50:LYS:HE3	17:BR:51:TYR:CZ	2.56	0.40
26:C4:52:C:H2'	26:C4:53:G:H5'	2.04	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
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
30:CD:124:LEU:O	30:CD:193:VAL:HA	2.22	0.40
31:CE:139:LEU:HD12	31:CE:139:LEU:C	2.46	0.40
37:CO:15:ARG:HD2	58:C1:620:G:H5'	2.04	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
46:CY:13:VAL:HG21	46:CY:72:VAL:HB	2.03	0.40
56:C9:6:THR:HG22	56:C9:63:PRO:HD3	2.03	0.40
58:C1:554:G:C5	58:C1:2043:U:H5''	2.57	0.40
58:C1:874:U:O2	58:C1:874:U:C3'	2.70	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:H2'	58:C1:1865:G:N3	2.37	0.40
58:C1:1967:U:H2'	58:C1:1968:C:C6	2.56	0.40
28:DB:182:LEU:HB2	28:DB:271:ILE:O	2.20	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
54:D7:15:GLU:O	54:D7:16:CYS:C	2.64	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
58:D1:1862:C:H2'	58:D1:1863:U:O5'	2.22	0.40
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

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

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AA	232/234 (99%)	174 (75%)	47 (20%)	11 (5%)	2	12
2	BA	232/234 (99%)	180 (78%)	41 (18%)	11 (5%)	2	12
3	AC	204/238 (86%)	145 (71%)	42 (21%)	17 (8%)	0	4
4	AD	206/208 (99%)	161 (78%)	33 (16%)	12 (6%)	1	8
4	BD	206/208 (99%)	168 (82%)	27 (13%)	11 (5%)	1	10
5	AE	148/150 (99%)	130 (88%)	15 (10%)	3 (2%)	6	25
5	BE	148/150 (99%)	130 (88%)	14 (10%)	4 (3%)	4	20
6	AF	99/101 (98%)	92 (93%)	5 (5%)	2 (2%)	6	25
6	BF	99/101 (98%)	89 (90%)	9 (9%)	1 (1%)	12	40
7	AG	153/155 (99%)	124 (81%)	26 (17%)	3 (2%)	6	25
7	BG	153/155 (99%)	135 (88%)	17 (11%)	1 (1%)	18	47
8	AH	136/138 (99%)	110 (81%)	24 (18%)	2 (2%)	8	30
8	BH	136/138 (99%)	116 (85%)	19 (14%)	1 (1%)	18	47
9	AI	125/127 (98%)	97 (78%)	23 (18%)	5 (4%)	2	15
9	BI	125/127 (98%)	98 (78%)	22 (18%)	5 (4%)	2	15
10	AJ	96/98 (98%)	79 (82%)	13 (14%)	4 (4%)	2	14
10	BJ	96/98 (98%)	76 (79%)	15 (16%)	5 (5%)	1	10
11	AK	117/119 (98%)	102 (87%)	14 (12%)	1 (1%)	14	42
11	BK	117/119 (98%)	93 (80%)	20 (17%)	4 (3%)	3	17
12	AL	122/124 (98%)	92 (75%)	20 (16%)	10 (8%)	0	4
12	BL	122/124 (98%)	94 (77%)	16 (13%)	12 (10%)	0	3
13	AM	122/124 (98%)	83 (68%)	26 (21%)	13 (11%)	0	2
13	BM	122/124 (98%)	83 (68%)	26 (21%)	13 (11%)	0	2
14	AN	58/60 (97%)	43 (74%)	12 (21%)	3 (5%)	1	10
14	BN	58/60 (97%)	41 (71%)	14 (24%)	3 (5%)	1	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	AO	86/88 (98%)	73 (85%)	9 (10%)	4 (5%)	2	12
15	BO	86/88 (98%)	72 (84%)	13 (15%)	1 (1%)	10	35
16	AP	81/83 (98%)	63 (78%)	15 (18%)	3 (4%)	2	16
16	BP	81/83 (98%)	67 (83%)	14 (17%)	0	100	100
17	AR	97/99 (98%)	89 (92%)	5 (5%)	3 (3%)	3	18
17	BR	97/99 (98%)	84 (87%)	10 (10%)	3 (3%)	3	18
18	AS	68/70 (97%)	57 (84%)	5 (7%)	6 (9%)	0	3
18	BS	68/70 (97%)	54 (79%)	10 (15%)	4 (6%)	1	8
19	AT	76/78 (97%)	61 (80%)	7 (9%)	8 (10%)	0	2
19	BT	76/78 (97%)	55 (72%)	13 (17%)	8 (10%)	0	2
20	AU	97/99 (98%)	77 (79%)	14 (14%)	6 (6%)	1	7
20	BU	97/99 (98%)	75 (77%)	19 (20%)	3 (3%)	3	18
21	AW	22/24 (92%)	19 (86%)	2 (9%)	1 (4%)	2	12
21	BW	22/24 (92%)	17 (77%)	3 (14%)	2 (9%)	0	3
24	BC	204/206 (99%)	153 (75%)	41 (20%)	10 (5%)	1	11
27	CA	83/206 (40%)	56 (68%)	22 (26%)	5 (6%)	1	7
28	CB	269/271 (99%)	210 (78%)	39 (14%)	20 (7%)	1	5
28	DB	269/271 (99%)	209 (78%)	38 (14%)	22 (8%)	0	4
29	CC	202/204 (99%)	143 (71%)	43 (21%)	16 (8%)	1	4
29	DC	202/204 (99%)	145 (72%)	32 (16%)	25 (12%)	0	1
30	CD	205/207 (99%)	162 (79%)	30 (15%)	13 (6%)	1	7
30	DD	205/207 (99%)	166 (81%)	24 (12%)	15 (7%)	1	5
31	CE	179/181 (99%)	132 (74%)	32 (18%)	15 (8%)	0	4
31	DE	179/181 (99%)	139 (78%)	28 (16%)	12 (7%)	1	6
32	CF	157/159 (99%)	112 (71%)	25 (16%)	20 (13%)	0	1
32	DF	157/159 (99%)	113 (72%)	26 (17%)	18 (12%)	0	2
33	CI	143/145 (99%)	112 (78%)	22 (15%)	9 (6%)	1	7
33	DI	143/145 (99%)	104 (73%)	29 (20%)	10 (7%)	1	6
35	CM	136/138 (99%)	103 (76%)	24 (18%)	9 (7%)	1	6
35	DM	136/138 (99%)	96 (71%)	30 (22%)	10 (7%)	1	5
36	CN	120/122 (98%)	106 (88%)	10 (8%)	4 (3%)	3	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	DN	120/122 (98%)	110 (92%)	8 (7%)	2 (2%)	7	28
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%)	3	19
38	DP	139/141 (99%)	117 (84%)	17 (12%)	5 (4%)	2	16
39	CQ	115/117 (98%)	93 (81%)	14 (12%)	8 (7%)	1	6
39	DQ	115/117 (98%)	98 (85%)	11 (10%)	6 (5%)	1	10
40	CR	96/98 (98%)	62 (65%)	23 (24%)	11 (12%)	0	2
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	0
41	DS	135/137 (98%)	89 (66%)	28 (21%)	18 (13%)	0	1
42	CT	115/117 (98%)	103 (90%)	10 (9%)	2 (2%)	7	28
42	DT	115/117 (98%)	93 (81%)	15 (13%)	7 (6%)	1	7
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	0
44	CW	111/113 (98%)	92 (83%)	12 (11%)	7 (6%)	1	7
45	CX	90/92 (98%)	77 (86%)	7 (8%)	6 (7%)	1	6
45	DX	90/92 (98%)	79 (88%)	9 (10%)	2 (2%)	5	24
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	7
47	DZ	174/176 (99%)	136 (78%)	28 (16%)	10 (6%)	1	9
48	Ca	82/84 (98%)	72 (88%)	9 (11%)	1 (1%)	10	35
48	Da	82/84 (98%)	74 (90%)	7 (8%)	1 (1%)	10	35
49	CH	91/93 (98%)	73 (80%)	10 (11%)	8 (9%)	0	3
49	DH	91/93 (98%)	73 (80%)	12 (13%)	6 (7%)	1	6
50	CK	69/71 (97%)	50 (72%)	12 (17%)	7 (10%)	0	3
50	DK	69/71 (97%)	54 (78%)	11 (16%)	4 (6%)	1	8
51	CL	57/59 (97%)	51 (90%)	5 (9%)	1 (2%)	6	26
51	DL	57/59 (97%)	52 (91%)	3 (5%)	2 (4%)	3	16
52	C5	28/30 (93%)	20 (71%)	5 (18%)	3 (11%)	0	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	D5	28/30 (93%)	18 (64%)	7 (25%)	3 (11%)	0	2
53	C6	57/59 (97%)	48 (84%)	5 (9%)	4 (7%)	1	6
53	D6	57/59 (97%)	46 (81%)	7 (12%)	4 (7%)	1	6
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%)	1	11
56	D9	61/63 (97%)	41 (67%)	15 (25%)	5 (8%)	0	4
57	C0	34/36 (94%)	32 (94%)	2 (6%)	0	100	100
57	D0	34/36 (94%)	32 (94%)	2 (6%)	0	100	100
62	DA	83/206 (40%)	52 (63%)	28 (34%)	3 (4%)	2	16
63	DW	111/113 (98%)	94 (85%)	11 (10%)	6 (5%)	1	10
All	All	11440/11918 (96%)	8901 (78%)	1752 (15%)	787 (7%)	1	6

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	AA	202/202 (100%)	180 (89%)	22 (11%)	6 22
2	BA	202/202 (100%)	182 (90%)	20 (10%)	7 26
3	AC	160/187 (86%)	144 (90%)	16 (10%)	7 26
4	AD	180/180 (100%)	160 (89%)	20 (11%)	6 21
4	BD	180/180 (100%)	161 (89%)	19 (11%)	6 23
5	AE	115/115 (100%)	103 (90%)	12 (10%)	7 24
5	BE	115/115 (100%)	99 (86%)	16 (14%)	3 14
6	AF	90/90 (100%)	85 (94%)	5 (6%)	19 46
6	BF	90/90 (100%)	85 (94%)	5 (6%)	19 46
7	AG	126/126 (100%)	111 (88%)	15 (12%)	5 19
7	BG	126/126 (100%)	114 (90%)	12 (10%)	8 29
8	AH	119/119 (100%)	108 (91%)	11 (9%)	8 29
8	BH	119/119 (100%)	106 (89%)	13 (11%)	6 22
9	AI	98/98 (100%)	83 (85%)	15 (15%)	3 10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	BI	98/98 (100%)	89 (91%)	9 (9%)	8	29
10	AJ	88/88 (100%)	77 (88%)	11 (12%)	4	18
10	BJ	88/88 (100%)	76 (86%)	12 (14%)	3	15
11	AK	90/90 (100%)	80 (89%)	10 (11%)	6	21
11	BK	90/90 (100%)	82 (91%)	8 (9%)	9	31
12	AL	104/104 (100%)	87 (84%)	17 (16%)	2	10
12	BL	104/104 (100%)	87 (84%)	17 (16%)	2	10
13	AM	99/99 (100%)	84 (85%)	15 (15%)	3	10
13	BM	99/99 (100%)	81 (82%)	18 (18%)	2	7
14	AN	49/49 (100%)	46 (94%)	3 (6%)	17	43
14	BN	49/49 (100%)	45 (92%)	4 (8%)	10	35
15	AO	79/79 (100%)	76 (96%)	3 (4%)	29	54
15	BO	79/79 (100%)	74 (94%)	5 (6%)	16	42
16	AP	72/72 (100%)	65 (90%)	7 (10%)	8	28
16	BP	72/72 (100%)	61 (85%)	11 (15%)	3	10
17	AR	94/94 (100%)	90 (96%)	4 (4%)	26	51
17	BR	94/94 (100%)	84 (89%)	10 (11%)	6	23
18	AS	61/61 (100%)	54 (88%)	7 (12%)	5	20
18	BS	61/61 (100%)	52 (85%)	9 (15%)	3	12
19	AT	69/69 (100%)	54 (78%)	15 (22%)	1	3
19	BT	69/69 (100%)	54 (78%)	15 (22%)	1	3
20	AU	76/76 (100%)	67 (88%)	9 (12%)	5	20
20	BU	76/76 (100%)	63 (83%)	13 (17%)	2	9
21	AW	19/19 (100%)	18 (95%)	1 (5%)	20	47
21	BW	19/19 (100%)	17 (90%)	2 (10%)	6	23
24	BC	160/160 (100%)	142 (89%)	18 (11%)	5	21
27	CA	61/74 (82%)	53 (87%)	8 (13%)	4	16
28	CB	213/213 (100%)	176 (83%)	37 (17%)	2	8
28	DB	213/213 (100%)	174 (82%)	39 (18%)	2	7
29	CC	165/165 (100%)	133 (81%)	32 (19%)	1	5
29	DC	165/165 (100%)	137 (83%)	28 (17%)	2	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	CD	165/165 (100%)	140 (85%)	25 (15%)	3	10
30	DD	165/165 (100%)	139 (84%)	26 (16%)	2	10
31	CE	155/155 (100%)	135 (87%)	20 (13%)	4	16
31	DE	155/155 (100%)	125 (81%)	30 (19%)	1	5
32	CF	132/132 (100%)	113 (86%)	19 (14%)	3	13
32	DF	132/132 (100%)	105 (80%)	27 (20%)	1	4
33	CI	122/122 (100%)	102 (84%)	20 (16%)	2	10
33	DI	122/122 (100%)	103 (84%)	19 (16%)	2	10
35	CM	117/117 (100%)	93 (80%)	24 (20%)	1	4
35	DM	117/117 (100%)	93 (80%)	24 (20%)	1	4
36	CN	100/100 (100%)	81 (81%)	19 (19%)	1	6
36	DN	100/100 (100%)	86 (86%)	14 (14%)	3	13
37	CO	112/112 (100%)	81 (72%)	31 (28%)	0	1
37	DO	112/112 (100%)	84 (75%)	28 (25%)	0	1
38	CP	111/111 (100%)	97 (87%)	14 (13%)	4	18
38	DP	111/111 (100%)	96 (86%)	15 (14%)	4	15
39	CQ	100/100 (100%)	81 (81%)	19 (19%)	1	6
39	DQ	100/100 (100%)	83 (83%)	17 (17%)	2	9
40	CR	77/77 (100%)	63 (82%)	14 (18%)	2	7
40	DR	77/77 (100%)	58 (75%)	19 (25%)	1	2
41	CS	120/120 (100%)	92 (77%)	28 (23%)	1	2
41	DS	120/120 (100%)	98 (82%)	22 (18%)	2	7
42	CT	92/92 (100%)	76 (83%)	16 (17%)	2	8
42	DT	92/92 (100%)	80 (87%)	12 (13%)	4	16
43	CU	82/82 (100%)	61 (74%)	21 (26%)	0	1
43	DU	82/82 (100%)	65 (79%)	17 (21%)	1	4
44	CW	91/92 (99%)	79 (87%)	12 (13%)	4	16
45	CX	74/74 (100%)	60 (81%)	14 (19%)	1	6
45	DX	74/74 (100%)	60 (81%)	14 (19%)	1	6
46	CY	84/84 (100%)	65 (77%)	19 (23%)	1	3
46	DY	84/84 (100%)	65 (77%)	19 (23%)	1	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
47	CZ	155/155 (100%)	142 (92%)	13 (8%)	10	34
47	DZ	155/155 (100%)	134 (86%)	21 (14%)	4	15
48	Ca	66/66 (100%)	57 (86%)	9 (14%)	3	15
48	Da	66/66 (100%)	57 (86%)	9 (14%)	3	15
49	CH	78/78 (100%)	57 (73%)	21 (27%)	0	1
49	DH	78/78 (100%)	64 (82%)	14 (18%)	2	7
50	CK	66/66 (100%)	55 (83%)	11 (17%)	2	9
50	DK	66/66 (100%)	53 (80%)	13 (20%)	1	5
51	CL	51/51 (100%)	48 (94%)	3 (6%)	18	44
51	DL	51/51 (100%)	48 (94%)	3 (6%)	18	44
52	C5	27/27 (100%)	23 (85%)	4 (15%)	3	12
52	D5	27/27 (100%)	24 (89%)	3 (11%)	6	21
53	C6	51/51 (100%)	44 (86%)	7 (14%)	3	14
53	D6	51/51 (100%)	42 (82%)	9 (18%)	2	8
54	C7	43/43 (100%)	33 (77%)	10 (23%)	1	2
54	D7	43/43 (100%)	35 (81%)	8 (19%)	1	6
55	C8	41/41 (100%)	36 (88%)	5 (12%)	5	19
55	D8	41/41 (100%)	32 (78%)	9 (22%)	1	3
56	C9	53/53 (100%)	40 (76%)	13 (24%)	1	2
56	D9	53/53 (100%)	42 (79%)	11 (21%)	1	4
57	C0	33/33 (100%)	30 (91%)	3 (9%)	9	30
57	D0	33/33 (100%)	29 (88%)	4 (12%)	5	19
62	DA	61/74 (82%)	54 (88%)	7 (12%)	5	20
63	DW	91/91 (100%)	82 (90%)	9 (10%)	7	26
All	All	9654/9708 (99%)	8219 (85%)	1435 (15%)	3	12

All (1435) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	AA	7	VAL
2	AA	11	LEU
2	AA	20	GLU
2	AA	36	ARG
2	AA	42	ILE

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Mol	Chain	Res	Type
2	AA	46	LYS
2	AA	63	MET
2	AA	87	ARG
2	AA	98	LEU
2	AA	101	MET
2	AA	107	THR
2	AA	119	GLU
2	AA	130	ARG
2	AA	136	VAL
2	AA	145	LEU
2	AA	172	ILE
2	AA	187	LEU
2	AA	206	ASP
2	AA	221	LEU
2	AA	226	ARG
2	AA	236	TYR
2	AA	238	LEU
3	AC	5	ILE
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	151	VAL
3	AC	170	GLN
3	AC	178	LEU
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	13	ARG
4	AD	15	GLU
4	AD	19	LEU
4	AD	31	CYS
4	AD	36	ARG

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Mol	Chain	Res	Type
4	AD	47	ARG
4	AD	50	ARG
4	AD	58	LEU
4	AD	86	LYS
4	AD	108	LEU
4	AD	110	PHE
4	AD	132	ARG
4	AD	135	LEU
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	27	ARG
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
6	AF	23	LYS
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	49	ILE
7	AG	54	THR
7	AG	60	LYS
7	AG	63	LYS
7	AG	86	GLN
7	AG	104	LEU
7	AG	113	GLU
7	AG	114	ARG
7	AG	136	LYS
7	AG	137	LYS

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Mol	Chain	Res	Type
7	AG	146	GLU
8	AH	1	MET
8	AH	2	LEU
8	AH	30	ARG
8	AH	39	LEU
8	AH	52	ASP
8	AH	60	ARG
8	AH	83	ILE
8	AH	91	ARG
8	AH	98	LYS
8	AH	112	LEU
8	AH	119	LEU
9	AI	4	TYR
9	AI	10	ARG
9	AI	40	LEU
9	AI	79	LEU
9	AI	89	ASN
9	AI	95	LYS
9	AI	102	LEU
9	AI	103	THR
9	AI	109	VAL
9	AI	110	GLU
9	AI	112	LYS
9	AI	114	TYR
9	AI	118	LYS
9	AI	126	SER
9	AI	128	ARG
10	AJ	19	SER
10	AJ	49	VAL
10	AJ	50	ILE
10	AJ	55	LYS
10	AJ	59	SER
10	AJ	69	ASN
10	AJ	78	ASN
10	AJ	79	ARG
10	AJ	80	LYS
10	AJ	96	ILE
10	AJ	98	ILE
11	AK	28	THR
11	AK	30	VAL
11	AK	51	LYS
11	AK	87	THR

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Mol	Chain	Res	Type
11	AK	95	ILE
11	AK	109	VAL
11	AK	119	CYS
11	AK	124	LYS
11	AK	125	PHE
11	AK	126	ARG
12	AL	7	ILE
12	AL	16	GLU
12	AL	17	LYS
12	AL	20	LYS
12	AL	40	VAL
12	AL	41	ARG
12	AL	42	THR
12	AL	43	VAL
12	AL	47	LYS
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	116	SER
12	AL	126	LYS
13	AM	4	ILE
13	AM	32	GLU
13	AM	35	GLU
13	AM	46	LYS
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	101	GLN
13	AM	108	ARG
13	AM	111	LYS
13	AM	115	LYS
14	AN	33	VAL
14	AN	35	ARG
14	AN	44	LEU
15	AO	65	ARG

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Mol	Chain	Res	Type
15	AO	82	ILE
15	AO	88	ARG
16	AP	2	VAL
16	AP	16	HIS
16	AP	21	VAL
16	AP	55	ARG
16	AP	67	THR
16	AP	69	THR
16	AP	72	ARG
17	AR	9	VAL
17	AR	38	ARG
17	AR	52	LYS
17	AR	74	LEU
18	AS	31	LEU
18	AS	32	ARG
18	AS	47	THR
18	AS	61	LYS
18	AS	65	ILE
18	AS	82	THR
18	AS	83	GLU
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	64	GLU
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

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Mol	Chain	Res	Type
20	AU	88	VAL
20	AU	93	GLU
21	AW	24	ARG
2	BA	36	ARG
2	BA	69	LEU
2	BA	71	VAL
2	BA	87	ARG
2	BA	90	MET
2	BA	98	LEU
2	BA	107	THR
2	BA	133	LYS
2	BA	140	HIS
2	BA	145	LEU
2	BA	172	ILE
2	BA	178	ARG
2	BA	179	LYS
2	BA	187	LEU
2	BA	195	ASP
2	BA	196	LEU
2	BA	198	ASP
2	BA	206	ASP
2	BA	221	LEU
2	BA	231	GLU
24	BC	5	ILE
24	BC	14	ILE
24	BC	17	ASP
24	BC	26	LYS
24	BC	27	LYS
24	BC	34	LEU
24	BC	37	GLN
24	BC	44	GLU
24	BC	62	ASP
24	BC	76	VAL
24	BC	98	ASN
24	BC	167	TRP
24	BC	178	LEU
24	BC	190	ARG
24	BC	196	LEU
24	BC	198	VAL
24	BC	202	ILE
24	BC	207	VAL
4	BD	9	CYS

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Mol	Chain	Res	Type
4	BD	10	ARG
4	BD	11	LEU
4	BD	13	ARG
4	BD	33	MET
4	BD	36	ARG
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	132	ARG
4	BD	135	LEU
4	BD	137	SER
4	BD	168	ARG
4	BD	188	LEU
4	BD	200	GLU
5	BE	10	MET
5	BE	12	LEU
5	BE	20	GLN
5	BE	24	ARG
5	BE	31	LEU
5	BE	41	VAL
5	BE	47	LYS
5	BE	51	VAL
5	BE	53	LEU
5	BE	64	ARG
5	BE	68	GLU
5	BE	72	GLN
5	BE	79	GLU
5	BE	91	LEU
5	BE	100	VAL
5	BE	101	ILE
6	BF	1	MET
6	BF	40	VAL
6	BF	70	ASP
6	BF	94	GLN
6	BF	98	LEU
7	BG	5	ARG
7	BG	30	ILE
7	BG	37	ASN

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Mol	Chain	Res	Type
7	BG	66	VAL
7	BG	75	VAL
7	BG	104	LEU
7	BG	113	GLU
7	BG	114	ARG
7	BG	118	VAL
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	45	ILE
8	BH	52	ASP
8	BH	60	ARG
8	BH	63	LEU
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	47	LEU
9	BI	79	LEU
9	BI	95	LYS
9	BI	112	LYS
9	BI	114	TYR
9	BI	118	LYS
9	BI	128	ARG
10	BJ	16	LEU
10	BJ	49	VAL
10	BJ	50	ILE
10	BJ	55	LYS
10	BJ	62	HIS
10	BJ	74	ILE
10	BJ	81	THR
10	BJ	86	MET
10	BJ	90	LEU
10	BJ	96	ILE
10	BJ	97	GLU

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Mol	Chain	Res	Type
10	BJ	98	ILE
11	BK	29	ILE
11	BK	48	ILE
11	BK	87	THR
11	BK	109	VAL
11	BK	117	ASN
11	BK	124	LYS
11	BK	126	ARG
11	BK	129	SER
12	BL	7	ILE
12	BL	13	LYS
12	BL	18	VAL
12	BL	19	ARG
12	BL	20	LYS
12	BL	21	LYS
12	BL	24	VAL
12	BL	36	VAL
12	BL	41	ARG
12	BL	44	THR
12	BL	47	LYS
12	BL	53	ARG
12	BL	62	SER
12	BL	83	VAL
12	BL	85	ILE
12	BL	89	ARG
12	BL	92	ASP
13	BM	17	VAL
13	BM	32	GLU
13	BM	47	ASP
13	BM	50	GLU
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	98	VAL
13	BM	101	GLN
13	BM	108	ARG
13	BM	115	LYS
13	BM	117	VAL
13	BM	120	LYS

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Mol	Chain	Res	Type
13	BM	121	LYS
13	BM	122	LYS
14	BN	13	THR
14	BN	27	CYS
14	BN	42	ILE
14	BN	44	LEU
15	BO	39	LEU
15	BO	41	GLU
15	BO	48	LYS
15	BO	65	ARG
15	BO	82	ILE
16	BP	2	VAL
16	BP	4	ILE
16	BP	12	LYS
16	BP	27	LYS
16	BP	28	ARG
16	BP	47	ASP
16	BP	54	GLU
16	BP	55	ARG
16	BP	67	THR
16	BP	69	THR
16	BP	82	GLN
17	BR	7	THR
17	BR	9	VAL
17	BR	11	VAL
17	BR	35	VAL
17	BR	38	ARG
17	BR	49	GLU
17	BR	52	LYS
17	BR	60	ILE
17	BR	74	LEU
17	BR	89	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	70	ILE
18	BS	82	THR
18	BS	87	ARG
19	BT	5	LEU

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Mol	Chain	Res	Type
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	36	LEU
20	BU	38	LYS
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	53	ARG
27	CA	56	GLN
27	CA	58	VAL
27	CA	63	SER
27	CA	64	LEU
27	CA	99	ILE
28	CB	10	THR
28	CB	13	ARG
28	CB	20	ASP
28	CB	23	GLU
28	CB	24	ILE

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Mol	Chain	Res	Type
28	CB	25	THR
28	CB	26	LYS
28	CB	28	GLU
28	CB	33	LEU
28	CB	35	LYS
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	106	ILE
28	CB	111	LEU
28	CB	116	GLN
28	CB	127	VAL
28	CB	138	VAL
28	CB	147	LEU
28	CB	157	ARG
28	CB	166	GLN
28	CB	173	VAL
28	CB	192	THR
28	CB	211	ARG
28	CB	212	SER
28	CB	218	ARG
28	CB	221	VAL
28	CB	229	VAL
28	CB	257	LEU
28	CB	259	THR
28	CB	260	ARG
28	CB	271	ILE
29	CC	9	VAL
29	CC	16	ARG
29	CC	17	ASP
29	CC	18	ASP
29	CC	33	VAL
29	CC	34	VAL
29	CC	49	LEU
29	CC	52	LEU
29	CC	54	GLN
29	CC	55	ASN

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Mol	Chain	Res	Type
29	CC	57	LYS
29	CC	58	ARG
29	CC	63	LEU
29	CC	64	LYS
29	CC	75	VAL
29	CC	76	ARG
29	CC	78	LEU
29	CC	79	ARG
29	CC	82	ARG
29	CC	107	THR
29	CC	111	ARG
29	CC	117	MET
29	CC	119	ARG
29	CC	128	SER
29	CC	144	ARG
29	CC	145	LYS
29	CC	152	LYS
29	CC	175	VAL
29	CC	181	LEU
29	CC	196	VAL
29	CC	197	ILE
29	CC	202	LYS
30	CD	4	VAL
30	CD	11	VAL
30	CD	20	LEU
30	CD	23	ASP
30	CD	24	LEU
30	CD	28	ILE
30	CD	33	LEU
30	CD	65	TRP
30	CD	66	PRO
30	CD	74	ARG
30	CD	83	PHE
30	CD	110	LEU
30	CD	124	LEU
30	CD	125	LEU
30	CD	126	VAL
30	CD	137	LYS
30	CD	140	LEU
30	CD	165	ARG
30	CD	170	LEU
30	CD	179	GLU

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Mol	Chain	Res	Type
30	CD	183	VAL
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	60	LEU
31	CE	71	THR
31	CE	80	PHE
31	CE	81	LYS
31	CE	82	LEU
31	CE	96	ARG
31	CE	116	ASP
31	CE	137	GLU
31	CE	139	LEU
31	CE	143	GLU
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	71	LEU
32	CF	85	LYS
32	CF	86	GLU
32	CF	88	LEU
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

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Mol	Chain	Res	Type
32	CF	162	ILE
32	CF	170	ARG
33	CI	4	ILE
33	CI	12	LEU
33	CI	20	ASP
33	CI	35	LEU
33	CI	41	GLU
33	CI	47	LEU
33	CI	77	LEU
33	CI	86	THR
33	CI	87	LYS
33	CI	92	VAL
33	CI	99	GLU
33	CI	109	ILE
33	CI	114	LEU
33	CI	118	LYS
33	CI	122	GLU
33	CI	123	LEU
33	CI	125	GLU
33	CI	128	LEU
33	CI	129	THR
33	CI	144	VAL
35	CM	2	LYS
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	71	ILE
35	CM	87	LEU
35	CM	97	ARG
35	CM	99	LEU
35	CM	106	MET
35	CM	109	LYS

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Mol	Chain	Res	Type
35	CM	120	LEU
35	CM	121	LYS
35	CM	131	GLN
35	CM	134	ARG
36	CN	5	GLN
36	CN	8	LEU
36	CN	10	VAL
36	CN	20	MET
36	CN	24	VAL
36	CN	28	SER
36	CN	32	TYR
36	CN	38	VAL
36	CN	47	ILE
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	107	ARG
36	CN	108	GLU
36	CN	117	LEU
37	CO	13	ASN
37	CO	16	ARG
37	CO	21	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	75	ILE

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Mol	Chain	Res	Type
37	CO	81	GLN
37	CO	83	VAL
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
37	CO	135	LEU
38	CP	5	ARG
38	CP	16	ARG
38	CP	18	LYS
38	CP	21	THR
38	CP	45	GLN
38	CP	55	VAL
38	CP	58	PHE
38	CP	75	THR
38	CP	76	LYS
38	CP	79	LEU
38	CP	105	GLU
38	CP	110	THR
38	CP	127	ILE
38	CP	131	ILE
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	48	VAL
39	CQ	54	LEU
39	CQ	66	VAL
39	CQ	67	LEU
39	CQ	71	GLN
39	CQ	75	LEU
39	CQ	79	LEU
39	CQ	83	ILE
39	CQ	95	THR
39	CQ	97	VAL

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Mol	Chain	Res	Type
39	CQ	99	LYS
39	CQ	100	LEU
39	CQ	105	ARG
40	CR	11	LYS
40	CR	18	ILE
40	CR	20	ARG
40	CR	21	THR
40	CR	36	TYR
40	CR	44	LYS
40	CR	54	LEU
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	58	ASN
41	CS	59	THR
41	CS	63	VAL
41	CS	65	LYS
41	CS	67	SER
41	CS	78	LEU
41	CS	82	LEU
41	CS	83	ILE
41	CS	85	LYS
41	CS	89	VAL
41	CS	93	ARG
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	133	GLU
41	CS	137	LYS
42	CT	8	VAL
42	CT	11	ARG
42	CT	13	LYS
42	CT	16	LYS
42	CT	17	ILE
42	CT	33	ARG
42	CT	34	LYS
42	CT	52	ARG
42	CT	60	LEU
42	CT	74	LEU
42	CT	77	SER
42	CT	83	LEU
42	CT	95	LEU
42	CT	101	ARG
42	CT	102	GLU
42	CT	108	GLU
43	CU	2	PHE
43	CU	5	VAL
43	CU	13	ARG
43	CU	16	PRO
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	52	VAL
43	CU	53	GLU
43	CU	57	VAL
43	CU	61	VAL
43	CU	68	LYS
43	CU	79	VAL
43	CU	91	TYR
43	CU	95	LEU
43	CU	99	ILE
44	CW	4	LYS
44	CW	11	ARG

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Mol	Chain	Res	Type
44	CW	19	LEU
44	CW	20	VAL
44	CW	23	LEU
44	CW	36	LEU
44	CW	39	THR
44	CW	51	LEU
44	CW	52	GLU
44	CW	67	ASP
44	CW	76	VAL
44	CW	107	LEU
45	CX	15	GLU
45	CX	23	GLU
45	CX	27	THR
45	CX	48	LYS
45	CX	52	VAL
45	CX	57	LEU
45	CX	68	ARG
45	CX	70	LEU
45	CX	72	LYS
45	CX	73	ARG
45	CX	76	ARG
45	CX	80	ILE
45	CX	81	VAL
45	CX	83	VAL
46	CY	2	ARG
46	CY	3	VAL
46	CY	7	VAL
46	CY	14	LEU
46	CY	30	VAL
46	CY	34	LYS
46	CY	38	ILE
46	CY	39	VAL
46	CY	46	LYS
46	CY	50	ARG
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	91	GLU
46	CY	96	ILE

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Mol	Chain	Res	Type
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	81	ARG
47	CZ	139	VAL
47	CZ	146	ILE
47	CZ	156	LYS
47	CZ	166	SER
48	Ca	5	LYS
48	Ca	12	ASN
48	Ca	14	ARG
48	Ca	19	LYS
48	Ca	20	ARG
48	Ca	36	ILE
48	Ca	41	ARG
48	Ca	74	ARG
48	Ca	84	LEU
49	CH	3	LYS
49	CH	4	VAL
49	CH	17	SER
49	CH	39	LYS
49	CH	40	ARG
49	CH	41	ARG
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	72	GLU
49	CH	75	GLU
49	CH	80	LEU
49	CH	82	LEU
49	CH	83	GLU
49	CH	88	LYS
49	CH	89	GLU

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Mol	Chain	Res	Type
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
51	CL	47	VAL
52	C5	39	ARG
52	C5	48	ILE
52	C5	51	TYR
52	C5	53	THR
53	C6	6	VAL
53	C6	29	THR
53	C6	44	THR
53	C6	46	CYS
53	C6	48	GLU
53	C6	56	LYS
53	C6	57	VAL
54	C7	9	LEU
54	C7	10	LEU
54	C7	17	LYS
54	C7	18	ARG
54	C7	30	THR
54	C7	33	LYS
54	C7	42	TRP
54	C7	44	ARG
54	C7	46	HIS
54	C7	52	VAL
55	C8	8	ASN
55	C8	15	THR
55	C8	24	THR
55	C8	43	THR
55	C8	48	LYS

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Mol	Chain	Res	Type
56	C9	4	MET
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	35	GLN
56	C9	44	LYS
56	C9	46	ARG
56	C9	49	VAL
56	C9	56	GLU
56	C9	61	LEU
57	C0	2	LYS
57	C0	26	ILE
57	C0	28	GLU
62	DA	23	ASP
62	DA	36	LYS
62	DA	47	LEU
62	DA	53	ARG
62	DA	56	GLN
62	DA	64	LEU
62	DA	75	LEU
28	DB	10	THR
28	DB	20	ASP
28	DB	24	ILE
28	DB	25	THR
28	DB	26	LYS
28	DB	28	GLU
28	DB	35	LYS
28	DB	49	ILE
28	DB	61	LEU
28	DB	65	ILE
28	DB	69	ARG
28	DB	78	LYS
28	DB	83	GLU
28	DB	92	ILE
28	DB	94	LEU
28	DB	99	ASP
28	DB	103	ARG
28	DB	106	ILE
28	DB	127	VAL

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Mol	Chain	Res	Type
28	DB	141	VAL
28	DB	142	VAL
28	DB	147	LEU
28	DB	154	LYS
28	DB	155	LEU
28	DB	157	ARG
28	DB	165	ILE
28	DB	166	GLN
28	DB	173	VAL
28	DB	174	ILE
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	270	ILE
28	DB	271	ILE
29	DC	1	MET
29	DC	9	VAL
29	DC	11	MET
29	DC	14	ILE
29	DC	17	ASP
29	DC	18	ASP
29	DC	33	VAL
29	DC	34	VAL
29	DC	55	ASN
29	DC	60	ASN
29	DC	63	LEU
29	DC	64	LYS
29	DC	72	VAL
29	DC	78	LEU
29	DC	79	ARG
29	DC	82	ARG
29	DC	92	THR
29	DC	95	ILE
29	DC	107	THR
29	DC	111	ARG
29	DC	119	ARG
29	DC	145	LYS

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Mol	Chain	Res	Type
29	DC	169	ASN
29	DC	175	VAL
29	DC	181	LEU
29	DC	188	VAL
29	DC	202	LYS
29	DC	203	LYS
30	DD	11	VAL
30	DD	12	LEU
30	DD	17	ARG
30	DD	19	GLU
30	DD	20	LEU
30	DD	23	ASP
30	DD	27	GLU
30	DD	28	ILE
30	DD	33	LEU
30	DD	38	ARG
30	DD	50	SER
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	126	VAL
30	DD	127	GLU
30	DD	149	ASP
30	DD	165	ARG
30	DD	170	LEU
30	DD	175	THR
30	DD	192	LEU
30	DD	199	TRP
30	DD	200	GLU
31	DE	4	ASP
31	DE	5	VAL
31	DE	10	LYS
31	DE	18	GLU
31	DE	21	ARG
31	DE	26	GLN
31	DE	34	LEU
31	DE	35	GLU
31	DE	39	ILE
31	DE	43	LEU

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Mol	Chain	Res	Type
31	DE	45	GLU
31	DE	53	LEU
31	DE	63	ILE
31	DE	67	LYS
31	DE	70	VAL
31	DE	79	ASN
31	DE	80	PHE
31	DE	82	LEU
31	DE	83	ARG
31	DE	84	LYS
31	DE	88	ILE
31	DE	96	ARG
31	DE	108	ASN
31	DE	113	ARG
31	DE	115	ARG
31	DE	118	ARG
31	DE	128	ARG
31	DE	130	ASN
31	DE	147	ASP
31	DE	159	VAL
32	DF	23	ARG
32	DF	24	VAL
32	DF	34	GLU
32	DF	45	VAL
32	DF	46	GLU
32	DF	53	GLU
32	DF	76	VAL
32	DF	77	LYS
32	DF	85	LYS
32	DF	86	GLU
32	DF	88	LEU
32	DF	89	ILE
32	DF	98	LEU
32	DF	105	LEU
32	DF	111	HIS
32	DF	119	GLU
32	DF	122	THR
32	DF	127	GLU
32	DF	134	SER
32	DF	140	LYS
32	DF	143	GLN
32	DF	144	VAL

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Mol	Chain	Res	Type
32	DF	151	ILE
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	9	LEU
33	DI	12	LEU
33	DI	37	VAL
33	DI	41	GLU
33	DI	52	ARG
33	DI	77	LEU
33	DI	82	ARG
33	DI	86	THR
33	DI	87	LYS
33	DI	110	ASP
33	DI	118	LYS
33	DI	122	GLU
33	DI	123	LEU
33	DI	129	THR
33	DI	138	ILE
33	DI	140	LEU
33	DI	144	VAL
35	DM	2	LYS
35	DM	3	THR
35	DM	4	TYR
35	DM	12	ARG
35	DM	15	LEU
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	54	VAL
35	DM	55	VAL
35	DM	56	ASN
35	DM	60	ILE
35	DM	63	THR
35	DM	65	LYS

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Mol	Chain	Res	Type
35	DM	73	THR
35	DM	87	LEU
35	DM	99	LEU
35	DM	109	LYS
35	DM	119	ARG
35	DM	131	GLN
36	DN	8	LEU
36	DN	10	VAL
36	DN	20	MET
36	DN	23	ARG
36	DN	24	VAL
36	DN	40	VAL
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	108	GLU
36	DN	117	LEU
37	DO	6	LEU
37	DO	13	ASN
37	DO	16	ARG
37	DO	32	THR
37	DO	36	LYS
37	DO	39	LYS
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	76	LYS
37	DO	81	GLN
37	DO	83	VAL
37	DO	85	LEU
37	DO	95	VAL
37	DO	98	GLU
37	DO	105	LEU
37	DO	108	LYS

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Mol	Chain	Res	Type
37	DO	112	LEU
37	DO	114	ILE
37	DO	123	LEU
37	DO	125	VAL
37	DO	135	LEU
37	DO	139	LYS
38	DP	5	ARG
38	DP	18	LYS
38	DP	45	GLN
38	DP	47	ILE
38	DP	55	VAL
38	DP	59	ARG
38	DP	67	ARG
38	DP	75	THR
38	DP	79	LEU
38	DP	81	VAL
38	DP	96	VAL
38	DP	110	THR
38	DP	115	MET
38	DP	131	ILE
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	54	LEU
39	DQ	65	LEU
39	DQ	67	LEU
39	DQ	71	GLN
39	DQ	74	LYS
39	DQ	76	VAL
39	DQ	79	LEU
39	DQ	104	ARG
39	DQ	113	LEU
39	DQ	117	VAL
39	DQ	118	GLU
40	DR	11	LYS
40	DR	18	ILE
40	DR	23	ARG
40	DR	26	LEU

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Mol	Chain	Res	Type
40	DR	32	LEU
40	DR	35	ILE
40	DR	36	TYR
40	DR	50	SER
40	DR	52	SER
40	DR	56	LEU
40	DR	78	LEU
40	DR	82	ILE
40	DR	84	GLN
40	DR	89	ARG
40	DR	92	TYR
40	DR	97	ARG
40	DR	98	VAL
40	DR	101	LEU
40	DR	107	GLU
41	DS	6	LEU
41	DS	11	GLU
41	DS	13	ARG
41	DS	18	ASP
41	DS	30	VAL
41	DS	32	TYR
41	DS	38	ASN
41	DS	41	ARG
41	DS	50	ILE
41	DS	51	ARG
41	DS	58	ASN
41	DS	59	THR
41	DS	62	THR
41	DS	65	LYS
41	DS	78	LEU
41	DS	82	LEU
41	DS	85	LYS
41	DS	87	ASP
41	DS	89	VAL
41	DS	93	ARG
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	66	ASN

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Mol	Chain	Res	Type
42	DT	71	GLN
42	DT	74	LEU
42	DT	83	LEU
42	DT	84	LYS
42	DT	95	LEU
42	DT	100	VAL
42	DT	112	ARG
43	DU	18	LEU
43	DU	19	LYS
43	DU	20	LEU
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	68	LYS
43	DU	82	ARG
43	DU	89	GLN
43	DU	95	LEU
43	DU	99	ILE
63	DW	11	ARG
63	DW	41	LYS
63	DW	47	VAL
63	DW	51	LEU
63	DW	52	GLU
63	DW	82	LEU
63	DW	85	VAL
63	DW	95	ILE
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	70	LEU

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Mol	Chain	Res	Type
45	DX	76	ARG
45	DX	80	ILE
45	DX	81	VAL
45	DX	88	LYS
45	DX	90	GLU
46	DY	7	VAL
46	DY	9	LYS
46	DY	14	LEU
46	DY	31	LEU
46	DY	33	LYS
46	DY	34	LYS
46	DY	39	VAL
46	DY	45	VAL
46	DY	49	VAL
46	DY	55	TYR
46	DY	62	GLU
46	DY	66	PRO
46	DY	67	LEU
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	19	ARG
47	DZ	20	ARG
47	DZ	34	ASN
47	DZ	37	VAL
47	DZ	39	VAL
47	DZ	53	ILE
47	DZ	63	ASP
47	DZ	76	LEU
47	DZ	79	ARG
47	DZ	81	ARG
47	DZ	82	ARG
47	DZ	92	SER
47	DZ	116	VAL
47	DZ	121	HIS
47	DZ	123	ASP
47	DZ	125	LEU

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Mol	Chain	Res	Type
47	DZ	145	GLU
47	DZ	162	GLU
47	DZ	163	LEU
48	Da	5	LYS
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	36	ILE
49	DH	3	LYS
49	DH	4	VAL
49	DH	25	LYS
49	DH	39	LYS
49	DH	46	LEU
49	DH	56	GLN
49	DH	58	ILE
49	DH	59	THR
49	DH	62	VAL
49	DH	75	GLU
49	DH	80	LEU
49	DH	82	LEU
49	DH	92	LYS
49	DH	94	LEU
50	DK	2	LYS
50	DK	3	LEU
50	DK	10	LEU
50	DK	14	ARG
50	DK	15	LYS
50	DK	32	LEU
50	DK	51	ARG
50	DK	53	LEU
50	DK	56	GLN
50	DK	59	ARG
50	DK	61	LEU
50	DK	69	ARG
50	DK	70	GLN
51	DL	8	LEU
51	DL	18	ASP
51	DL	58	VAL

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Mol	Chain	Res	Type
52	D5	39	ARG
52	D5	49	GLU
52	D5	53	THR
53	D6	6	VAL
53	D6	11	THR
53	D6	29	THR
53	D6	36	CYS
53	D6	44	THR
53	D6	49	CYS
53	D6	51	TYR
53	D6	57	VAL
53	D6	60	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	14	VAL
56	D9	30	ARG
56	D9	31	HIS
56	D9	32	LEU
56	D9	33	ASN
56	D9	34	TRP
56	D9	36	LYS
56	D9	44	LYS
56	D9	58	ILE
56	D9	61	LEU
57	D0	2	LYS
57	D0	12	ASP

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Mol	Chain	Res	Type
57	D0	26	ILE
57	D0	27	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (233) such sidechains are listed below:

Mol	Chain	Res	Type
2	AA	40	HIS
2	AA	76	GLN
2	AA	78	GLN
2	AA	212	GLN
3	AC	69	HIS
3	AC	107	GLN
3	AC	162	GLN
4	AD	42	GLN
4	AD	62	GLN
4	AD	74	GLN
4	AD	123	HIS
4	AD	129	ASN
5	AE	20	GLN
6	AF	18	GLN
6	AF	32	ASN
6	AF	73	ASN
6	AF	100	ASN
7	AG	86	GLN
7	AG	96	GLN
7	AG	106	GLN
7	AG	148	ASN
9	AI	34	ASN
9	AI	117	HIS
10	AJ	56	HIS
10	AJ	78	ASN
11	AK	38	ASN
11	AK	116	HIS
12	AL	8	ASN
12	AL	9	GLN
12	AL	49	ASN
13	AM	12	ASN
15	AO	37	ASN
15	AO	46	HIS
16	AP	16	HIS
16	AP	76	GLN
18	AS	36	ASN

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Mol	Chain	Res	Type
19	AT	57	HIS
20	AU	26	ASN
20	AU	42	GLN
20	AU	45	GLN
20	AU	75	ASN
2	BA	19	HIS
2	BA	78	GLN
2	BA	94	ASN
2	BA	146	GLN
2	BA	212	GLN
24	BC	118	GLN
24	BC	170	GLN
4	BD	123	HIS
4	BD	129	ASN
4	BD	160	GLN
5	BE	20	GLN
5	BE	65	ASN
6	BF	16	GLN
6	BF	32	ASN
6	BF	100	ASN
7	BG	37	ASN
7	BG	148	ASN
9	BI	3	GLN
9	BI	87	GLN
9	BI	89	ASN
9	BI	124	GLN
10	BJ	33	GLN
10	BJ	68	HIS
10	BJ	78	ASN
11	BK	22	HIS
11	BK	26	ASN
11	BK	117	ASN
12	BL	49	ASN
12	BL	75	HIS
13	BM	62	ASN
13	BM	92	HIS
14	BN	49	HIS
15	BO	37	ASN
15	BO	46	HIS
16	BP	76	GLN
18	BS	36	ASN
19	BT	23	ASN

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Mol	Chain	Res	Type
19	BT	69	HIS
20	BU	26	ASN
27	CA	56	GLN
28	CB	58	HIS
28	CB	96	HIS
28	CB	126	GLN
28	CB	143	HIS
28	CB	186	HIS
28	CB	198	ASN
28	CB	227	ASN
29	CC	48	GLN
29	CC	55	ASN
29	CC	129	HIS
29	CC	169	ASN
29	CC	192	ASN
30	CD	8	GLN
30	CD	75	HIS
30	CD	169	ASN
31	CE	41	GLN
32	CF	65	HIS
32	CF	139	GLN
32	CF	147	ASN
33	CI	43	ASN
33	CI	139	GLN
35	CM	45	ASN
35	CM	56	ASN
36	CN	82	ASN
36	CN	88	ASN
37	CO	13	ASN
37	CO	38	GLN
37	CO	68	GLN
37	CO	70	GLN
37	CO	81	GLN
37	CO	128	HIS
38	CP	45	GLN
38	CP	89	ASN
38	CP	123	HIS
39	CQ	3	HIS
39	CQ	13	HIS
39	CQ	23	ASN
39	CQ	24	GLN
39	CQ	31	HIS

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Mol	Chain	Res	Type
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
42	CT	94	ASN
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
46	CY	92	ASN
47	CZ	65	GLN
47	CZ	73	GLN
47	CZ	75	ASN
47	CZ	118	GLN
47	CZ	121	HIS
47	CZ	132	ASN
48	Ca	70	GLN
49	CH	19	GLN
49	CH	45	ASN
50	CK	70	GLN
51	CL	19	GLN
51	CL	32	GLN
51	CL	33	GLN
51	CL	46	ASN
51	CL	52	HIS
52	C5	46	ASN
53	C6	23	HIS
53	C6	43	HIS
54	C7	49	HIS
55	C8	8	ASN
56	C9	31	HIS
57	C0	29	ASN
62	DA	56	GLN

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Mol	Chain	Res	Type
62	DA	66	HIS
28	DB	96	HIS
28	DB	116	GLN
28	DB	143	HIS
28	DB	166	GLN
28	DB	186	HIS
28	DB	198	ASN
29	DC	48	GLN
29	DC	55	ASN
29	DC	129	HIS
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	105	HIS
35	DM	56	ASN
35	DM	94	HIS
35	DM	101	HIS
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
38	DP	45	GLN
39	DQ	13	HIS
39	DQ	16	HIS
39	DQ	23	ASN
39	DQ	31	HIS
39	DQ	53	HIS
39	DQ	71	GLN
40	DR	84	GLN
41	DS	38	ASN
41	DS	43	GLN
41	DS	58	ASN

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Mol	Chain	Res	Type
41	DS	123	GLN
42	DT	14	HIS
42	DT	49	HIS
42	DT	66	ASN
42	DT	117	GLN
63	DW	57	ASN
63	DW	61	ASN
45	DX	41	ASN
45	DX	55	ASN
47	DZ	32	HIS
47	DZ	50	GLN
47	DZ	54	HIS
47	DZ	132	ASN
48	Da	12	ASN
48	Da	29	GLN
49	DH	45	ASN
49	DH	56	GLN
50	DK	65	ASN
50	DK	70	GLN
50	DK	71	ASN
51	DL	19	GLN
51	DL	33	GLN
51	DL	46	ASN
52	D5	46	ASN
53	D6	23	HIS
53	D6	43	HIS
55	D8	8	ASN
56	D9	31	HIS
57	D0	34	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A2	8/9 (88%)	4 (50%)	2 (25%)
22	Ab	1503/1504 (99%)	333 (22%)	0
22	Bb	1503/1504 (99%)	345 (22%)	0
23	B2	7/10 (70%)	4 (57%)	1 (14%)
25	C2	74/76 (97%)	25 (33%)	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%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
58	C1	2802/2899 (96%)	818 (29%)	155 (5%)
58	D1	2802/2899 (96%)	829 (29%)	149 (5%)
59	Cs	118/119 (99%)	35 (29%)	0
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	9296/9519 (97%)	2564 (27%)	326 (3%)

All (2564) 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

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Mol	Chain	Res	Type
22	Ab	99	G
22	Ab	109	G
22	Ab	110	A
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	302	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

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Mol	Chain	Res	Type
22	Ab	348	C
22	Ab	349	A
22	Ab	350	G
22	Ab	352	A
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

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Mol	Chain	Res	Type
22	Ab	496	U
22	Ab	502	C
22	Ab	503	C
22	Ab	505	G
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	717	A
22	Ab	718	G
22	Ab	732	C
22	Ab	733	C
22	Ab	737	A
22	Ab	739	G
22	Ab	744	G

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Mol	Chain	Res	Type
22	Ab	758	G
22	Ab	761	A
22	Ab	770	G
22	Ab	777	U
22	Ab	778	A
22	Ab	780	C
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	862	U
22	Ab	863	G
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
22	Ab	1152	A
22	Ab	1153	G
22	Ab	1165	A
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	1267	A
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

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Mol	Chain	Res	Type
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
22	Ab	1313	G
22	Ab	1317	C
22	Ab	1318	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	1471	A
22	Ab	1475	G
22	Ab	1476	U
22	Ab	1477	A

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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	323	A
22	Bb	324	C
22	Bb	325	A
22	Bb	328	G
22	Bb	341	C
22	Bb	348	C

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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	561	G
22	Bb	568	G
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	707	U
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

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Mol	Chain	Res	Type
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
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	891	A
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	923	G
22	Bb	924	A
22	Bb	938	U

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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	22	G
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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	157	U
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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	554	G
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
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

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Mol	Chain	Res	Type
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	733	C
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
58	C1	792	A
58	C1	793	U
58	C1	799	C
58	C1	804	C
58	C1	810	A
58	C1	811	G
58	C1	821	G
58	C1	822	G
58	C1	823	A
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

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Mol	Chain	Res	Type
58	C1	859	U
58	C1	865	A
58	C1	873	U
58	C1	874	U
58	C1	875	A
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
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

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Mol	Chain	Res	Type
58	C1	1019	C
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	1151	A
58	C1	1152	G
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

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Mol	Chain	Res	Type
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
58	C1	1295	G
58	C1	1298	A
58	C1	1299	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	1333	U
58	C1	1334	C
58	C1	1345	U

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Mol	Chain	Res	Type
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	1411	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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
58	C1	1578	C
58	C1	1579	G
58	C1	1589	C
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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	1920	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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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	2693	U
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
58	C1	2725	A
58	C1	2732	U
58	C1	2738	U
58	C1	2739	G
58	C1	2742	C
58	C1	2745	A
58	C1	2746	A
58	C1	2760	A

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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	157	U
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
58	D1	233	G
58	D1	234	C
58	D1	236	G
58	D1	237	C
58	D1	240	G
58	D1	248	G

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Mol	Chain	Res	Type
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
58	D1	386	G
58	D1	388	G
58	D1	391	U
58	D1	392	A
58	D1	395	C
58	D1	396	G

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Mol	Chain	Res	Type
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
58	D1	552	A
58	D1	553	A
58	D1	554	G
58	D1	555	C
58	D1	556	A
58	D1	557	G

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Mol	Chain	Res	Type
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
58	D1	733	C
58	D1	747	G
58	D1	750	G
58	D1	753	G
58	D1	754	C
58	D1	763	G

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Mol	Chain	Res	Type
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	820	A
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	906	U
58	D1	912	A
58	D1	913	C
58	D1	915	G
58	D1	917	U
58	D1	924	A

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Mol	Chain	Res	Type
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
58	D1	1072	A
58	D1	1076	G
58	D1	1079	G

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Mol	Chain	Res	Type
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	1151	A
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
58	D1	1223	C
58	D1	1224	C

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Mol	Chain	Res	Type
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
58	D1	1390	C
58	D1	1392	G

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Mol	Chain	Res	Type
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
58	D1	1513	C
58	D1	1515	A

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Mol	Chain	Res	Type
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	1589	C
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
58	D1	1624	U

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Mol	Chain	Res	Type
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
58	D1	1769	A

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Mol	Chain	Res	Type
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	1814	A
58	D1	1815	A
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

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Mol	Chain	Res	Type
58	D1	1896	C
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	1920	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

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Mol	Chain	Res	Type
58	D1	2012	U
58	D1	2013	G
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

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Mol	Chain	Res	Type
58	D1	2152	G
58	D1	2154	G
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

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Mol	Chain	Res	Type
58	D1	2297	A
58	D1	2298	A
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

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Mol	Chain	Res	Type
58	D1	2449	U
58	D1	2450	A
58	D1	2451	C
58	D1	2452	C
58	D1	2453	C
58	D1	2458	G
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

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Mol	Chain	Res	Type
58	D1	2565	U
58	D1	2568	G
58	D1	2577	A
58	D1	2578	G
58	D1	2592	G
58	D1	2593	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

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Mol	Chain	Res	Type
58	D1	2739	G
58	D1	2742	C
58	D1	2745	A
58	D1	2746	A
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

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Mol	Chain	Res	Type
64	DV	2	C
64	DV	3	C
64	DV	12	U
64	DV	16	U
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

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Mol	Chain	Res	Type
58	C1	216	A
58	C1	267	G
58	C1	284	U
58	C1	296	C
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

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Mol	Chain	Res	Type
58	C1	1331	A
58	C1	1333	U
58	C1	1345	U
58	C1	1346	A
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

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Mol	Chain	Res	Type
58	C1	1933	A
58	C1	1955	C
58	C1	1960	U
58	C1	1983	C
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

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Mol	Chain	Res	Type
58	C1	2620	U
58	C1	2622	U
58	C1	2666	G
58	C1	2673	A
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

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Mol	Chain	Res	Type
58	D1	209	A
58	D1	284	U
58	D1	296	C
58	D1	306	A
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

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Mol	Chain	Res	Type
58	D1	1331	A
58	D1	1345	U
58	D1	1346	A
58	D1	1351	C
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

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Mol	Chain	Res	Type
58	D1	1987	A
58	D1	1991	A
58	D1	2005	G
58	D1	2013	G
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

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Mol	Chain	Res	Type
58	D1	2808	U
58	D1	2809	C
58	D1	2812	G
58	D1	2829	A
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 oligosaccharides 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	Ab	1601	-	44,45,45	1.42	5 (11%)	63,67,67	1.87	14 (22%)
66	3V6	D1	3001	67	22,25,25	2.29	8 (36%)	24,39,39	2.97	9 (37%)
66	3V6	C1	3001	67	22,25,25	2.03	8 (36%)	24,39,39	2.03	8 (33%)
65	PAR	Bb	1601	-	44,45,45	1.53	7 (15%)	63,67,67	2.19	19 (30%)

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	Ab	1601	-	-	6/18/94/94	2/4/4/4
66	3V6	D1	3001	67	-	3/12/53/53	0/2/2/2
66	3V6	C1	3001	67	-	1/12/53/53	0/2/2/2
65	PAR	Bb	1601	-	-	9/18/94/94	0/4/4/4

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
65	Bb	1601	PAR	C41-C51	5.90	1.65	1.53
66	D1	3001	3V6	CAK-CAN	-5.55	1.42	1.49
65	Ab	1601	PAR	C34-C24	-5.17	1.47	1.53
66	C1	3001	3V6	CAK-CAS	4.33	1.64	1.53
66	D1	3001	3V6	CAS-CAU	4.00	1.59	1.53
66	C1	3001	3V6	CAV-NAL	3.67	1.50	1.45
66	C1	3001	3V6	CAK-CAN	-3.56	1.44	1.49
66	D1	3001	3V6	OAE-CAO	3.43	1.28	1.21
66	D1	3001	3V6	CAV-NAL	3.35	1.50	1.45
65	Ab	1601	PAR	O33-C33	-3.33	1.35	1.43
65	Bb	1601	PAR	C22-C32	-3.28	1.46	1.53
65	Ab	1601	PAR	C11-C21	2.84	1.57	1.52
66	C1	3001	3V6	CAQ-CAN	2.81	1.42	1.37
66	D1	3001	3V6	CAW-CAQ	-2.80	1.45	1.50
66	C1	3001	3V6	OAG-CAN	2.80	1.40	1.32
65	Bb	1601	PAR	C62-C12	-2.75	1.48	1.53
66	D1	3001	3V6	CAT-CLJ	-2.61	1.73	1.78
66	C1	3001	3V6	CAT-CLJ	-2.54	1.73	1.78
66	D1	3001	3V6	OAM-CAX	2.53	1.53	1.47
66	D1	3001	3V6	CAQ-CAN	2.49	1.42	1.37
65	Ab	1601	PAR	C33-C43	-2.17	1.47	1.52
65	Ab	1601	PAR	O23-C23	2.16	1.48	1.43
66	C1	3001	3V6	CAO-CAQ	-2.14	1.40	1.44
66	C1	3001	3V6	CAT-CLI	-2.07	1.74	1.78
65	Bb	1601	PAR	C44-C34	2.06	1.57	1.52
65	Bb	1601	PAR	O11-C42	2.05	1.49	1.43
65	Bb	1601	PAR	O62-C62	2.03	1.48	1.43
65	Bb	1601	PAR	C11-C21	2.03	1.56	1.52

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
65	Ab	1601	PAR	O52-C13-O43	-8.88	102.30	111.37
66	D1	3001	3V6	OAM-CAO-OAE	8.12	127.88	117.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
65	Bb	1601	PAR	O54-C54-C64	-7.95	90.80	106.07
65	Bb	1601	PAR	O52-C13-O43	-5.65	105.59	111.37
66	D1	3001	3V6	OAG-CAN-CAQ	-5.59	114.56	123.15
66	D1	3001	3V6	OAE-CAO-CAQ	-4.96	118.86	125.56
66	D1	3001	3V6	CLJ-CAT-CLI	-4.79	100.97	108.87
65	Bb	1601	PAR	O51-C51-C41	4.69	118.16	109.70
65	Bb	1601	PAR	C32-C22-C12	-4.38	103.52	111.02
65	Ab	1601	PAR	C13-O52-C52	-4.37	107.62	117.98
66	C1	3001	3V6	OAE-CAO-CAQ	-4.26	119.80	125.56
66	C1	3001	3V6	CAB-CAS-CAK	4.25	116.78	110.75
66	C1	3001	3V6	OAG-CAN-CAK	3.90	119.71	113.29
66	D1	3001	3V6	CAS-CAK-CAN	-3.86	109.50	114.39
65	Bb	1601	PAR	C53-C43-C33	-3.61	103.46	114.84
65	Bb	1601	PAR	C14-O54-C54	3.57	120.68	113.72
65	Bb	1601	PAR	O33-C14-O54	-3.43	101.66	110.69
66	C1	3001	3V6	OAG-CAN-CAQ	-3.38	117.97	123.15
66	C1	3001	3V6	CLJ-CAT-CLI	-3.28	103.45	108.87
65	Bb	1601	PAR	C13-O52-C52	-3.24	110.29	117.98
65	Ab	1601	PAR	C11-C21-N21	3.23	116.03	110.20
65	Bb	1601	PAR	C44-C34-C24	3.21	116.32	110.99
65	Ab	1601	PAR	C14-O33-C33	-3.19	110.42	117.98
66	D1	3001	3V6	OAG-CAN-CAK	3.11	118.41	113.29
66	C1	3001	3V6	OAM-CAO-OAE	2.93	121.28	117.56
65	Bb	1601	PAR	O41-C41-C31	-2.85	103.66	110.38
65	Bb	1601	PAR	O54-C54-C44	2.84	114.81	109.70
65	Bb	1601	PAR	O53-C53-C43	-2.70	102.14	111.33
66	D1	3001	3V6	OAM-CAX-CAC	2.64	111.43	105.93
65	Ab	1601	PAR	C41-C31-C21	-2.64	106.61	110.99
65	Bb	1601	PAR	O43-C43-C53	2.59	114.70	109.22
65	Bb	1601	PAR	C11-O11-C42	2.54	124.00	117.98
66	D1	3001	3V6	CAK-CAN-CAQ	2.51	126.99	123.53
65	Ab	1601	PAR	C44-C34-C24	-2.48	106.88	110.99
66	D1	3001	3V6	CAB-CAS-CAU	2.47	115.65	112.35
65	Bb	1601	PAR	C31-C41-C51	2.38	114.54	110.23
65	Ab	1601	PAR	O51-C51-C61	2.33	112.22	106.44
65	Ab	1601	PAR	C23-C33-C43	2.32	107.30	103.24
65	Ab	1601	PAR	C53-C43-C33	-2.30	107.59	114.84
66	C1	3001	3V6	CAS-CAK-CAN	-2.27	111.52	114.39
65	Bb	1601	PAR	C34-C44-C54	2.23	114.28	110.23
66	C1	3001	3V6	CAW-CAU-CAS	-2.19	106.81	111.31
65	Bb	1601	PAR	O41-C41-C51	2.16	114.64	109.32
65	Bb	1601	PAR	C11-C21-C31	2.14	115.66	110.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
65	Ab	1601	PAR	O62-C62-C12	2.12	113.87	109.90
65	Ab	1601	PAR	O43-C13-C23	2.09	107.64	104.98
65	Bb	1601	PAR	O54-C14-C24	2.07	114.66	110.08
65	Ab	1601	PAR	C32-C22-C12	-2.06	107.48	111.02
65	Ab	1601	PAR	C13-C23-C33	-2.03	99.66	102.10
65	Ab	1601	PAR	C64-C54-C44	-2.03	108.06	112.80

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
65	Ab	1601	PAR	C23-C13-O52-C52
65	Ab	1601	PAR	O43-C13-O52-C52
65	Bb	1601	PAR	C21-C11-O11-C42
66	C1	3001	3V6	NAL-C-CA-CB
66	D1	3001	3V6	O-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	Ab	1601	PAR	C52-C42-O11-C11
65	Bb	1601	PAR	O51-C11-O11-C42
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
65	Bb	1601	PAR	C24-C14-O33-C33
65	Ab	1601	PAR	C32-C42-O11-C11
65	Bb	1601	PAR	C43-C33-O33-C14

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

4 monomers are involved in 23 short contacts:

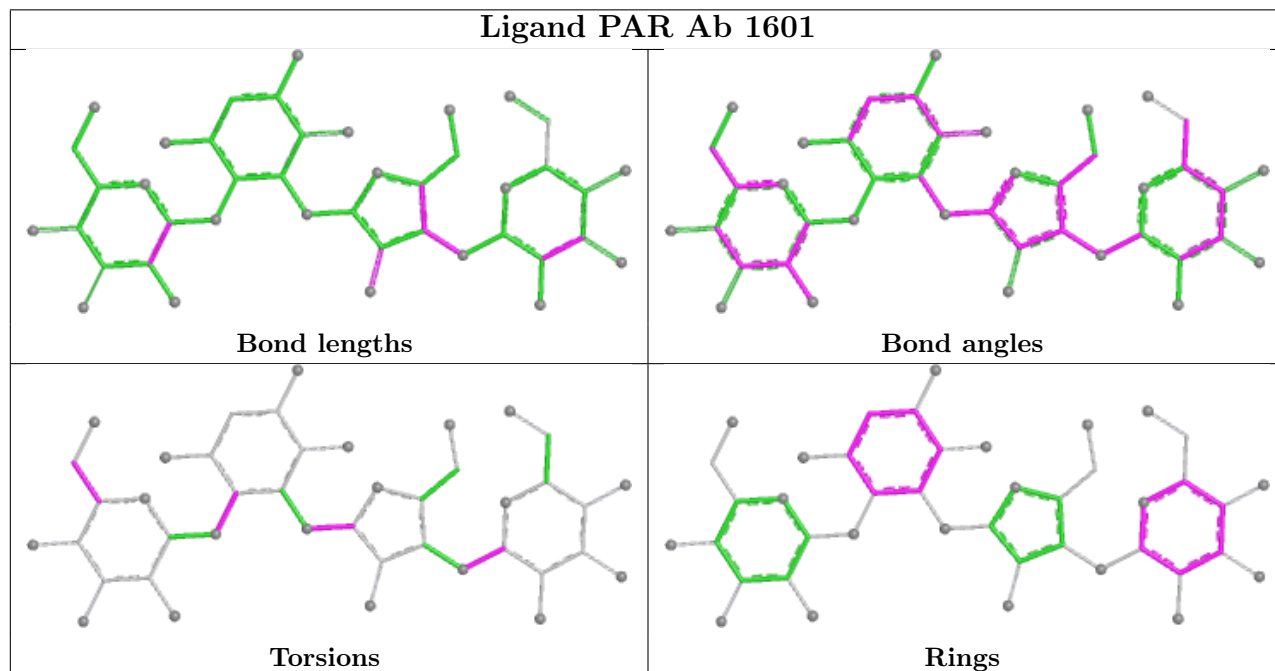
Mol	Chain	Res	Type	Clashes	Symm-Clashes
65	Ab	1601	PAR	4	0

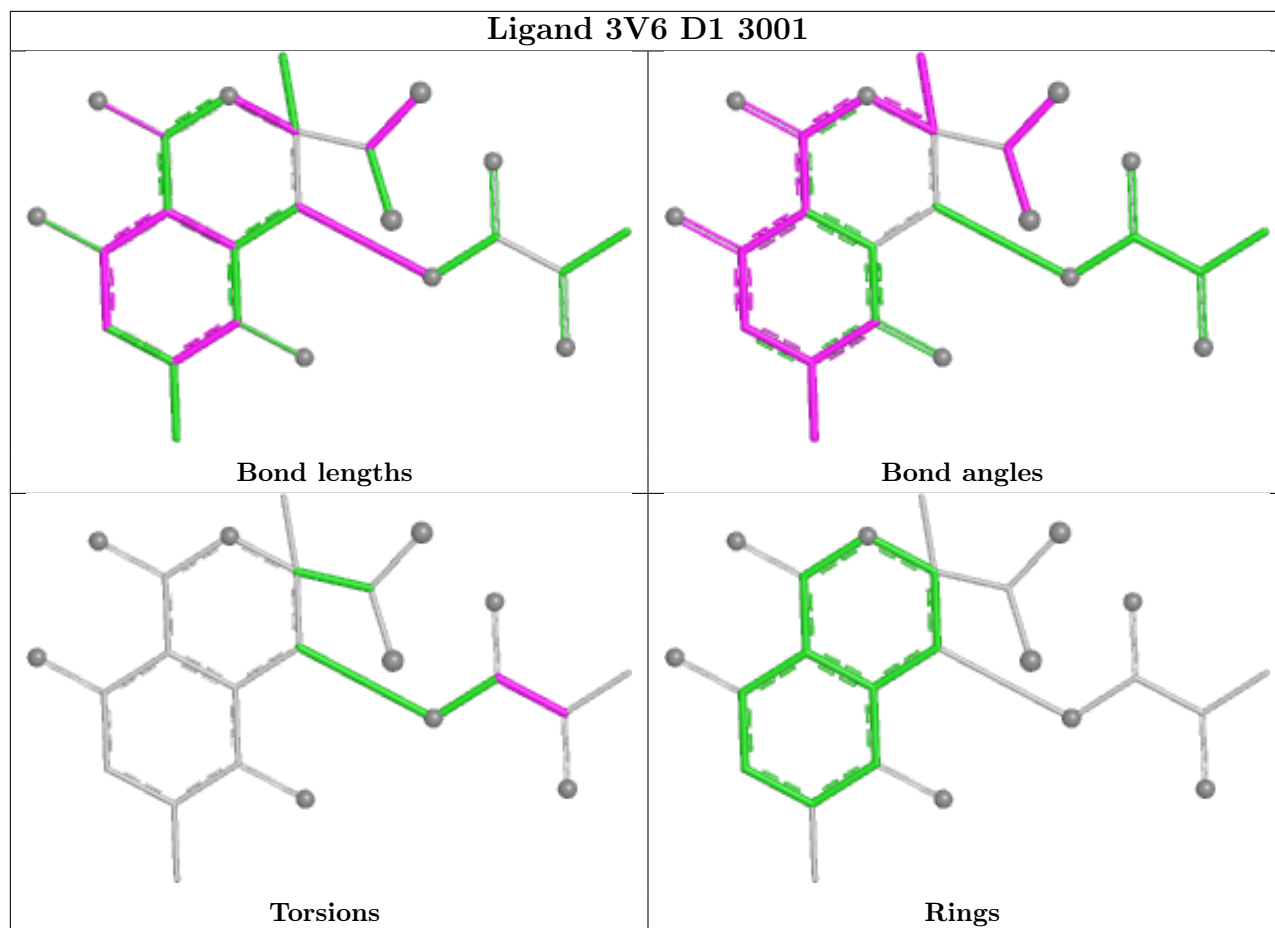
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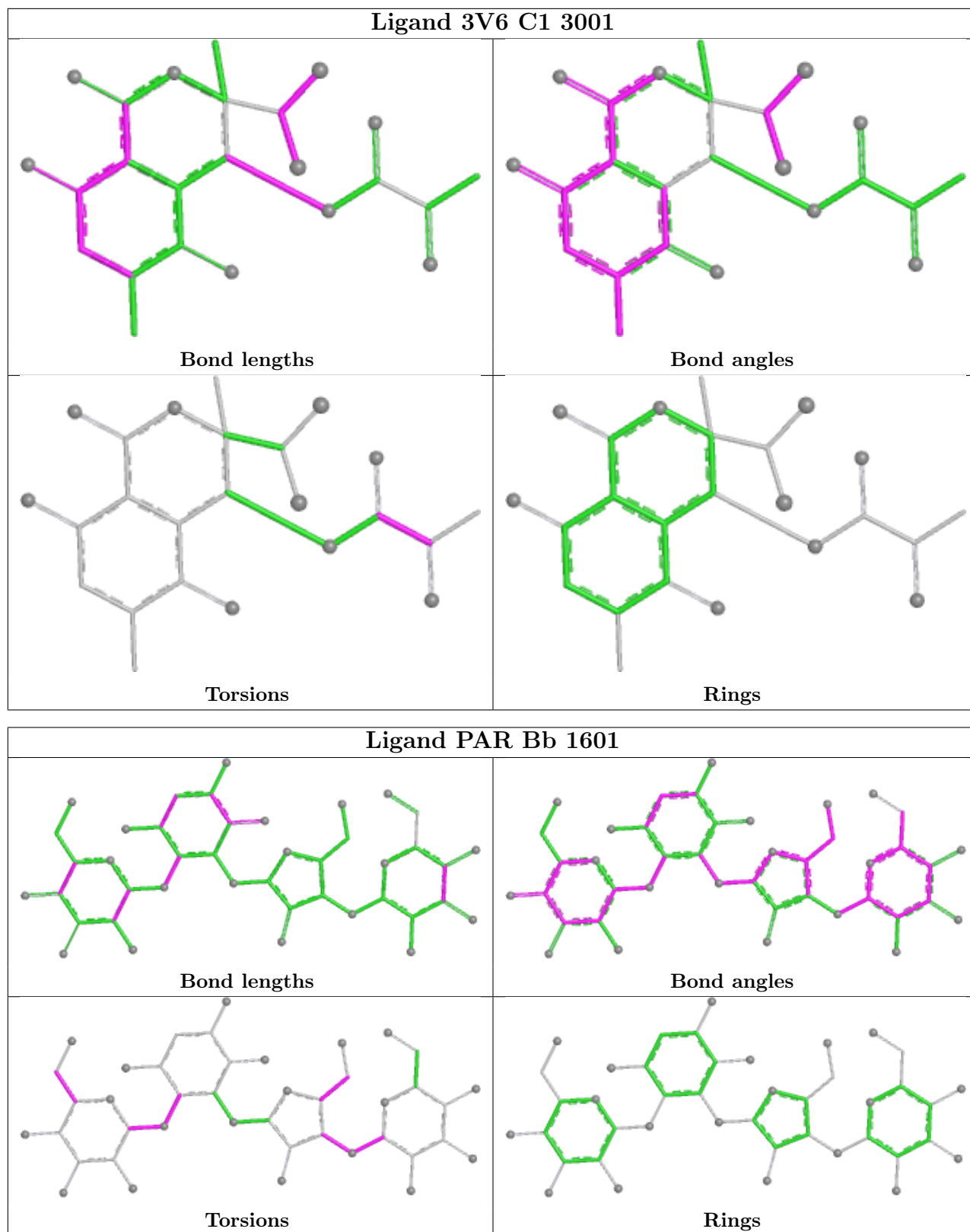
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
66	D1	3001	3V6	11	0
66	C1	3001	3V6	5	0
65	Bb	1601	PAR	3	0

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







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

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

6.1 Protein, DNA and RNA chains i

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A2	9/9 (100%)	0.48	0 100 100	50, 89, 110, 114	0
2	AA	234/234 (100%)	0.53	6 (2%) 57 42	78, 124, 168, 197	0
2	BA	234/234 (100%)	0.75	12 (5%) 33 25	80, 130, 179, 209	0
3	AC	206/238 (86%)	0.69	19 (9%) 14 14	65, 108, 148, 173	0
4	AD	208/208 (100%)	0.54	15 (7%) 21 18	51, 86, 123, 147	0
4	BD	208/208 (100%)	0.42	13 (6%) 26 20	48, 78, 117, 144	0
5	AE	150/150 (100%)	0.27	5 (3%) 49 36	66, 91, 124, 144	0
5	BE	150/150 (100%)	0.05	0 100 100	57, 83, 122, 141	0
6	AF	101/101 (100%)	-0.09	2 (1%) 65 49	55, 85, 109, 170	0
6	BF	101/101 (100%)	0.18	0 100 100	52, 96, 130, 158	0
7	AG	155/155 (100%)	0.24	13 (8%) 17 15	58, 86, 125, 181	0
7	BG	155/155 (100%)	0.82	16 (10%) 12 12	78, 112, 154, 184	0
8	AH	138/138 (100%)	0.29	2 (1%) 73 59	60, 90, 117, 184	0
8	BH	138/138 (100%)	0.46	4 (2%) 53 39	63, 95, 123, 145	0
9	AI	127/127 (100%)	0.99	18 (14%) 6 8	62, 108, 150, 175	0
9	BI	127/127 (100%)	1.20	27 (21%) 2 4	77, 131, 179, 215	0
10	AJ	98/98 (100%)	1.12	13 (13%) 7 8	77, 121, 176, 188	0
10	BJ	98/98 (100%)	1.31	23 (23%) 2 3	65, 134, 173, 202	0
11	AK	119/119 (100%)	0.20	5 (4%) 40 29	39, 76, 110, 158	0
11	BK	119/119 (100%)	0.47	5 (4%) 40 29	47, 94, 141, 193	0
12	AL	124/124 (100%)	0.62	11 (8%) 15 14	49, 82, 125, 180	0
12	BL	124/124 (100%)	0.21	9 (7%) 21 18	41, 60, 104, 158	0
13	AM	124/124 (100%)	0.71	13 (10%) 11 12	66, 98, 144, 197	0
13	BM	124/124 (100%)	1.10	19 (15%) 5 7	66, 113, 164, 204	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
14	AN	60/60 (100%)	1.26	13 (21%) 2 4	65, 103, 130, 142	0
14	BN	60/60 (100%)	1.13	8 (13%) 7 8	59, 94, 119, 134	0
15	AO	88/88 (100%)	0.16	1 (1%) 78 65	46, 76, 112, 123	0
15	BO	88/88 (100%)	0.57	3 (3%) 48 35	55, 94, 120, 132	0
16	AP	83/83 (100%)	0.34	0 100 100	52, 73, 101, 136	0
16	BP	83/83 (100%)	0.72	4 (4%) 35 26	59, 89, 135, 152	0
17	AR	99/99 (100%)	0.30	1 (1%) 79 66	59, 80, 108, 115	0
17	BR	99/99 (100%)	0.62	3 (3%) 52 39	65, 94, 126, 135	0
18	AS	70/70 (100%)	0.08	1 (1%) 73 59	56, 88, 119, 156	0
18	BS	70/70 (100%)	0.41	1 (1%) 73 59	66, 94, 142, 180	0
19	AT	78/78 (100%)	0.78	9 (11%) 9 10	67, 110, 164, 180	0
19	BT	78/78 (100%)	1.25	14 (17%) 3 5	79, 118, 161, 184	0
20	AU	99/99 (100%)	0.76	12 (12%) 8 9	62, 86, 125, 146	0
20	BU	99/99 (100%)	1.00	15 (15%) 5 7	64, 107, 146, 154	0
21	AW	24/24 (100%)	1.10	2 (8%) 17 15	63, 80, 112, 138	0
21	BW	24/24 (100%)	2.01	9 (37%) 1 1	64, 91, 132, 163	0
22	Ab	1504/1504 (100%)	-0.24	22 (1%) 72 57	30, 75, 154, 300	0
22	Bb	1504/1504 (100%)	-0.13	22 (1%) 72 57	31, 81, 165, 318	0
23	B2	10/10 (100%)	0.98	2 (20%) 3 4	60, 107, 138, 172	0
24	BC	206/206 (100%)	0.58	14 (6%) 23 19	64, 105, 149, 169	0
25	C2	75/76 (98%)	1.08	8 (10%) 11 11	99, 250, 345, 377	0
25	C3	76/76 (100%)	0.14	3 (3%) 43 31	60, 130, 198, 227	0
25	D3	76/76 (100%)	0.16	0 100 100	59, 147, 212, 228	0
26	C4	77/77 (100%)	-0.29	1 (1%) 75 61	44, 79, 132, 159	0
27	CA	87/206 (42%)	1.59	29 (33%) 1 1	98, 186, 221, 241	0
28	CB	271/271 (100%)	-0.10	4 (1%) 72 57	23, 48, 83, 150	0
28	DB	271/271 (100%)	0.04	6 (2%) 62 47	20, 52, 86, 158	0
29	CC	204/204 (100%)	0.28	10 (4%) 35 26	31, 68, 123, 150	0
29	DC	204/204 (100%)	0.16	10 (4%) 35 26	24, 61, 124, 169	0
30	CD	207/207 (100%)	-0.02	3 (1%) 73 59	29, 64, 133, 194	0
30	DD	207/207 (100%)	0.05	7 (3%) 48 35	20, 65, 146, 223	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
31	CE	181/181 (100%)	0.51	12 (6%) 24 19	59, 92, 137, 213	0
31	DE	181/181 (100%)	0.99	20 (11%) 10 11	76, 117, 154, 198	0
32	CF	159/159 (100%)	0.93	19 (11%) 9 10	82, 134, 175, 219	0
32	DF	159/159 (100%)	0.52	14 (8%) 15 14	45, 85, 126, 178	0
33	CI	145/145 (100%)	0.27	6 (4%) 41 29	40, 88, 128, 150	0
33	DI	145/145 (100%)	0.53	6 (4%) 41 29	60, 108, 139, 165	0
34	CJ	0/130	-	-	-	-
34	DJ	0/130	-	-	-	-
35	CM	138/138 (100%)	0.43	7 (5%) 33 25	47, 78, 118, 130	0
35	DM	138/138 (100%)	0.48	9 (6%) 25 20	36, 73, 121, 151	0
36	CN	122/122 (100%)	0.14	2 (1%) 70 56	35, 66, 89, 111	0
36	DN	122/122 (100%)	-0.32	0 100 100	27, 51, 75, 107	0
37	CO	146/146 (100%)	0.69	16 (10%) 10 11	34, 77, 127, 168	0
37	DO	146/146 (100%)	0.89	20 (13%) 6 8	31, 87, 123, 165	0
38	CP	141/141 (100%)	0.43	8 (5%) 29 22	44, 75, 111, 192	0
38	DP	141/141 (100%)	0.50	8 (5%) 29 22	42, 71, 106, 219	0
39	CQ	117/117 (100%)	0.23	7 (5%) 27 21	38, 63, 94, 127	0
39	DQ	117/117 (100%)	0.23	5 (4%) 40 29	27, 61, 99, 130	0
40	CR	98/98 (100%)	0.79	13 (13%) 7 8	47, 89, 130, 176	0
40	DR	98/98 (100%)	1.76	36 (36%) 1 1	68, 113, 143, 163	0
41	CS	137/137 (100%)	0.68	13 (9%) 14 13	45, 79, 142, 200	0
41	DS	137/137 (100%)	0.50	11 (8%) 18 16	43, 71, 148, 192	0
42	CT	117/117 (100%)	0.21	4 (3%) 48 35	37, 66, 116, 138	0
42	DT	117/117 (100%)	0.25	3 (2%) 57 42	31, 68, 111, 153	0
43	CU	101/101 (100%)	0.17	1 (0%) 79 66	35, 92, 122, 134	0
43	DU	101/101 (100%)	0.43	4 (3%) 42 30	26, 86, 123, 196	0
44	CW	113/113 (100%)	0.00	1 (0%) 81 68	38, 54, 90, 182	0
45	CX	92/92 (100%)	0.25	0 100 100	39, 65, 89, 109	0
45	DX	92/92 (100%)	0.02	1 (1%) 78 65	33, 55, 88, 115	0
46	CY	100/100 (100%)	1.57	24 (24%) 2 3	58, 94, 168, 214	0
46	DY	100/100 (100%)	1.13	22 (22%) 2 4	48, 81, 193, 251	0
47	CZ	176/176 (100%)	0.74	10 (5%) 29 22	76, 118, 157, 233	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
47	DZ	176/176 (100%)	0.90	18 (10%) 12 12	69, 119, 173, 203	0
48	Ca	84/84 (100%)	0.68	10 (11%) 9 10	44, 67, 127, 170	0
48	Da	84/84 (100%)	1.11	16 (19%) 3 4	49, 82, 137, 167	0
49	CH	93/93 (100%)	-0.00	2 (2%) 62 47	30, 54, 102, 140	0
49	DH	93/93 (100%)	0.28	1 (1%) 78 65	29, 66, 121, 179	0
50	CK	71/71 (100%)	0.46	6 (8%) 16 15	42, 85, 125, 180	0
50	DK	71/71 (100%)	0.31	5 (7%) 22 18	37, 68, 124, 179	0
51	CL	59/59 (100%)	0.30	1 (1%) 69 54	45, 72, 111, 223	0
51	DL	59/59 (100%)	0.53	1 (1%) 69 54	48, 79, 120, 213	0
52	C5	30/30 (100%)	0.22	0 100 100	76, 99, 130, 155	0
52	D5	30/30 (100%)	0.97	2 (6%) 24 19	99, 128, 155, 167	0
53	C6	59/59 (100%)	0.50	5 (8%) 16 15	34, 63, 160, 206	0
53	D6	59/59 (100%)	0.37	5 (8%) 16 15	28, 65, 172, 205	0
54	C7	44/44 (100%)	1.22	9 (20%) 2 4	54, 101, 146, 183	0
54	D7	44/44 (100%)	1.62	14 (31%) 1 1	84, 125, 165, 181	0
55	C8	48/48 (100%)	0.04	3 (6%) 26 20	26, 40, 79, 139	0
55	D8	48/48 (100%)	-0.14	2 (4%) 40 29	21, 34, 77, 135	0
56	C9	63/63 (100%)	0.68	8 (12%) 8 9	34, 54, 90, 123	0
56	D9	63/63 (100%)	0.83	8 (12%) 8 9	39, 66, 102, 136	0
57	C0	36/36 (100%)	1.60	12 (33%) 1 1	93, 125, 175, 177	0
57	D0	36/36 (100%)	1.66	10 (27%) 1 2	73, 106, 141, 145	0
58	C1	2807/2899 (96%)	-0.56	21 (0%) 84 73	21, 54, 148, 279	0
58	D1	2807/2899 (96%)	-0.49	33 (1%) 76 63	16, 52, 155, 267	0
59	Cs	119/119 (100%)	-0.13	3 (2%) 58 43	58, 83, 138, 197	0
59	Ds	119/119 (100%)	0.48	4 (3%) 48 35	62, 104, 147, 172	0
60	D2	20/20 (100%)	0.90	1 (5%) 34 25	133, 235, 281, 283	0
61	D4	76/76 (100%)	-0.16	1 (1%) 75 61	37, 79, 120, 201	0
62	DA	87/206 (42%)	1.41	17 (19%) 3 4	118, 190, 257, 309	0
63	DW	113/113 (100%)	-0.02	1 (0%) 81 68	33, 51, 100, 159	0
64	DV	55/55 (100%)	1.22	9 (16%) 4 6	110, 248, 297, 345	0
All	All	20982/21697 (96%)	0.13	1017 (4%) 35 26	16, 77, 159, 377	0

All (1017) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
31	CE	2	PRO	10.5
40	CR	54	LEU	8.2
13	AM	124	PRO	7.8
22	Bb	85	C	7.8
4	AD	49	ARG	7.6
48	Ca	6	GLY	7.4
40	DR	14	VAL	7.4
53	C6	2	ALA	7.2
13	BM	124	PRO	7.1
11	BK	128	ALA	7.1
9	AI	66	ARG	6.7
48	Da	4	LYS	6.6
46	CY	61	ILE	6.6
13	AM	123	ALA	6.4
48	Ca	8	GLY	6.3
48	Da	8	GLY	6.3
32	DF	42	ARG	6.2
38	DP	141	GLN	6.1
4	BD	26	CYS	6.1
2	BA	96	ARG	6.0
46	DY	2	ARG	6.0
13	AM	84	ILE	5.9
8	AH	1	MET	5.8
46	CY	44	ILE	5.8
62	DA	47	LEU	5.7
62	DA	43	VAL	5.7
32	DF	44	VAL	5.7
50	DK	72	ALA	5.6
38	CP	141	GLN	5.6
46	DY	28	LYS	5.6
22	Ab	1268	A	5.6
22	Ab	82	U	5.6
35	CM	68	GLU	5.3
22	Ab	81	U	5.3
40	DR	12	PHE	5.2
13	BM	122	LYS	5.2
48	Ca	7	LEU	5.2
48	Ca	4	LYS	5.2
43	DU	36	PRO	5.2
56	C9	63	PRO	5.2
47	DZ	169	GLU	5.2
22	Bb	1268	A	5.1

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Mol	Chain	Res	Type	RSRZ
46	CY	49	VAL	5.1
56	C9	48	PHE	5.0
41	CS	92	GLY	5.0
14	BN	2	ALA	5.0
57	D0	12	ASP	5.0
13	BM	84	ILE	5.0
14	AN	2	ALA	5.0
48	Ca	5	LYS	5.0
53	D6	60	VAL	5.0
62	DA	51	PRO	5.0
28	DB	35	LYS	5.0
32	DF	12	PRO	4.9
62	DA	45	ALA	4.9
46	CY	48	ALA	4.9
40	CR	14	VAL	4.9
27	CA	57	ASN	4.8
46	DY	3	VAL	4.8
21	BW	9	ARG	4.7
46	CY	3	VAL	4.6
47	DZ	166	SER	4.6
13	AM	122	LYS	4.6
4	BD	9	CYS	4.6
40	DR	11	LYS	4.6
4	BD	31	CYS	4.6
22	Bb	84	A	4.6
7	AG	8	GLU	4.6
55	D8	48	LYS	4.6
19	BT	81	ARG	4.6
24	BC	13	GLY	4.6
32	CF	158	HIS	4.6
4	BD	12	CYS	4.5
27	CA	56	GLN	4.5
46	CY	45	VAL	4.5
11	AK	129	SER	4.5
19	AT	5	LEU	4.5
27	CA	90	GLY	4.5
22	Ab	85	C	4.4
58	C1	297	G	4.4
37	DO	27	HIS	4.4
21	BW	6	ARG	4.4
38	DP	140	ALA	4.4
12	AL	27	LEU	4.4

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Mol	Chain	Res	Type	RSRZ
31	DE	35	GLU	4.3
62	DA	49	ILE	4.3
27	CA	58	VAL	4.3
40	DR	82	ILE	4.3
64	DV	55	C	4.3
12	AL	28	LYS	4.3
30	CD	24	LEU	4.3
21	BW	15	ARG	4.3
38	CP	140	ALA	4.3
46	CY	28	LYS	4.2
57	D0	29	ASN	4.2
31	CE	28	VAL	4.2
37	CO	51	PHE	4.2
48	Da	3	HIS	4.2
48	Da	6	GLY	4.2
13	BM	125	ARG	4.2
40	DR	87	PHE	4.2
31	DE	86	MET	4.1
58	C1	298	G	4.1
21	BW	5	ASP	4.1
33	CI	20	ASP	4.1
40	DR	53	SER	4.1
31	CE	98	ARG	4.1
30	DD	24	LEU	4.1
27	CA	46	LYS	4.1
46	CY	63	LYS	4.1
29	CC	75	VAL	4.0
37	DO	28	GLY	4.0
20	AU	9	ASN	4.0
32	CF	170	ARG	4.0
8	BH	1	MET	4.0
11	AK	127	LYS	4.0
62	DA	107	TRP	4.0
58	D1	2200	C	4.0
2	BA	152	PHE	4.0
14	BN	30	ALA	4.0
56	C9	64	TYR	4.0
48	Da	7	LEU	4.0
25	C3	17	C	4.0
32	DF	43	VAL	3.9
57	C0	17	ILE	3.9
4	AD	161	ASN	3.9

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Mol	Chain	Res	Type	RSRZ
10	BJ	36	GLY	3.9
4	AD	31	CYS	3.9
39	CQ	2	ARG	3.9
9	BI	115	GLY	3.9
42	CT	118	GLY	3.9
50	DK	70	GLN	3.9
56	D9	48	PHE	3.9
9	AI	102	LEU	3.9
29	CC	66	HIS	3.9
10	BJ	59	SER	3.9
55	C8	48	LYS	3.9
12	AL	26	ALA	3.9
58	C1	2200	C	3.8
24	BC	207	VAL	3.8
7	BG	84	ASN	3.8
25	C2	75	C	3.8
58	D1	1578	C	3.8
37	DO	51	PHE	3.8
29	CC	76	ARG	3.8
48	Da	5	LYS	3.8
47	DZ	167	PRO	3.8
52	D5	51	TYR	3.8
13	AM	125	ARG	3.8
46	CY	60	PHE	3.8
58	C1	2812	G	3.8
11	BK	129	SER	3.8
19	BT	38	SER	3.8
3	AC	155	GLY	3.8
37	CO	62	LEU	3.8
40	CR	11	LYS	3.7
47	DZ	163	LEU	3.7
12	AL	64	TYR	3.7
19	AT	10	PHE	3.7
57	D0	26	ILE	3.7
11	BK	127	LYS	3.7
37	CO	27	HIS	3.7
22	Bb	86	U	3.7
48	Ca	2	ALA	3.7
9	AI	29	ASN	3.7
28	CB	35	LYS	3.7
56	D9	63	PRO	3.7
32	CF	83	TYR	3.7

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Mol	Chain	Res	Type	RSRZ
32	CF	157	TYR	3.7
13	BM	98	VAL	3.7
41	DS	29	ARG	3.7
20	BU	10	LEU	3.7
28	DB	26	LYS	3.7
41	CS	25	GLY	3.7
12	BL	91	LYS	3.6
14	AN	14	PRO	3.6
12	AL	20	LYS	3.6
58	D1	2330	G	3.6
3	AC	160	ALA	3.6
3	AC	196	LEU	3.6
20	BU	14	LYS	3.6
20	BU	101	GLY	3.6
33	DI	117	GLU	3.6
31	CE	129	GLY	3.6
47	DZ	96	VAL	3.6
58	D1	1590	A	3.5
11	AK	117	ASN	3.5
41	CS	11	GLU	3.5
37	CO	110	TYR	3.5
7	BG	80	VAL	3.5
56	D9	51	ALA	3.5
58	D1	532	G	3.5
35	DM	68	GLU	3.5
40	DR	94	TYR	3.5
32	DF	156	ALA	3.5
33	DI	138	ILE	3.5
24	BC	166	GLU	3.5
50	DK	11	GLU	3.5
55	C8	46	VAL	3.5
10	AJ	55	LYS	3.5
39	DQ	11	ASN	3.5
13	BM	123	ALA	3.5
48	Da	2	ALA	3.5
29	DC	17	ASP	3.5
29	DC	76	ARG	3.5
31	DE	105	LYS	3.4
40	DR	100	ALA	3.4
10	BJ	64	GLU	3.4
20	BU	18	GLN	3.4
21	AW	25	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
37	CO	64	LYS	3.4
5	AE	15	ARG	3.4
13	BM	117	VAL	3.4
27	CA	105	ASP	3.4
53	C6	59	GLU	3.4
54	D7	12	GLU	3.4
41	DS	39	ARG	3.4
56	D9	50	LEU	3.4
40	DR	90	GLY	3.4
14	AN	13	THR	3.4
48	Ca	3	HIS	3.4
57	C0	30	PRO	3.4
22	Ab	84	A	3.3
4	AD	19	LEU	3.3
13	BM	121	LYS	3.3
41	DS	92	GLY	3.3
32	CF	136	ILE	3.3
40	DR	16	ASN	3.3
53	C6	60	VAL	3.3
12	BL	28	LYS	3.3
37	DO	64	LYS	3.3
6	AF	55	ASP	3.3
37	DO	104	GLY	3.3
47	CZ	112	ARG	3.3
32	DF	85	LYS	3.3
13	AM	85	GLY	3.3
3	AC	177	THR	3.3
10	BJ	66	ARG	3.3
27	CA	52	ARG	3.3
55	C8	47	ARG	3.3
25	C2	74	C	3.3
59	Cs	88	C	3.3
9	BI	11	LYS	3.3
32	DF	86	GLU	3.3
62	DA	52	ARG	3.3
20	AU	14	LYS	3.3
29	CC	69	LYS	3.3
62	DA	41	VAL	3.3
11	AK	128	ALA	3.3
54	C7	12	GLU	3.3
46	CY	59	GLY	3.3
41	CS	106	SER	3.2

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Mol	Chain	Res	Type	RSRZ
57	D0	2	LYS	3.2
9	AI	115	GLY	3.2
64	DV	1	G	3.2
4	AD	3	ARG	3.2
58	D1	571	A	3.2
46	CY	46	LYS	3.2
3	AC	10	PHE	3.2
7	AG	80	VAL	3.2
57	C0	12	ASP	3.2
10	BJ	47	PHE	3.2
46	DY	61	ILE	3.2
15	BO	38	ARG	3.2
27	CA	91	ALA	3.2
38	DP	10	ARG	3.2
42	CT	58	ARG	3.2
10	BJ	40	LEU	3.2
2	BA	136	VAL	3.2
13	AM	7	VAL	3.2
40	DR	69	VAL	3.2
48	Ca	9	SER	3.2
9	BI	64	THR	3.2
14	BN	29	ARG	3.2
4	AD	12	CYS	3.2
38	DP	136	ALA	3.2
19	BT	68	GLY	3.2
41	DS	91	ARG	3.2
53	D6	2	ALA	3.2
22	Bb	83	U	3.1
4	AD	9	CYS	3.1
24	BC	161	GLU	3.1
27	CA	110	PHE	3.1
22	Ab	980	G	3.1
42	CT	59	ARG	3.1
46	CY	2	ARG	3.1
20	BU	106	ALA	3.1
54	D7	23	THR	3.1
9	BI	85	LEU	3.1
12	BL	29	GLY	3.1
19	BT	5	LEU	3.1
40	CR	104	GLY	3.1
27	CA	51	PRO	3.1
46	CY	47	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
47	DZ	114	GLY	3.1
4	AD	26	CYS	3.1
27	CA	41	VAL	3.1
35	DM	1	MET	3.1
20	AU	12	ALA	3.1
40	DR	54	LEU	3.1
43	DU	101	GLY	3.1
41	CS	91	ARG	3.1
46	DY	51	VAL	3.1
58	D1	1098	C	3.1
32	CF	12	PRO	3.1
25	C2	1	G	3.1
3	AC	154	SER	3.1
32	CF	169	VAL	3.1
50	CK	4	SER	3.1
39	DQ	72	ASP	3.1
21	BW	23	PRO	3.1
58	D1	2306	C	3.0
2	BA	144	ARG	3.0
37	DO	15	ARG	3.0
43	DU	37	VAL	3.0
20	BU	11	SER	3.0
47	CZ	114	GLY	3.0
54	D7	42	TRP	3.0
46	CY	53	PRO	3.0
58	C1	532	G	3.0
37	DO	110	TYR	3.0
29	CC	57	LYS	3.0
46	DY	60	PHE	3.0
33	CI	12	LEU	3.0
49	CH	95	LEU	3.0
10	BJ	26	ALA	3.0
37	DO	7	ARG	3.0
11	BK	117	ASN	3.0
40	DR	35	ILE	3.0
31	DE	3	LEU	3.0
46	CY	64	GLU	3.0
57	C0	13	LYS	3.0
51	DL	9	VAL	3.0
57	C0	20	HIS	3.0
4	AD	21	LEU	2.9
14	AN	39	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
39	CQ	10	LEU	2.9
7	BG	5	ARG	2.9
47	CZ	80	ARG	2.9
9	BI	61	ALA	2.9
31	DE	67	LYS	2.9
62	DA	44	HIS	2.9
22	Bb	87	C	2.9
32	DF	170	ARG	2.9
54	C7	14	THR	2.9
32	DF	167	GLU	2.9
47	DZ	168	GLU	2.9
21	BW	2	GLY	2.9
46	DY	59	GLY	2.9
3	AC	6	HIS	2.9
31	DE	94	LEU	2.9
53	D6	58	LEU	2.9
13	AM	121	LYS	2.9
35	DM	129	PRO	2.9
7	AG	83	ALA	2.9
10	BJ	63	PHE	2.9
27	CA	54	SER	2.9
32	DF	158	HIS	2.9
14	AN	3	ARG	2.9
27	CA	49	ILE	2.9
20	BU	24	LEU	2.9
39	DQ	105	ARG	2.9
10	BJ	58	ASP	2.9
62	DA	23	ASP	2.9
22	Ab	981	G	2.9
7	BG	85	TYR	2.9
27	CA	60	GLY	2.9
41	CS	39	ARG	2.9
9	BI	13	ALA	2.9
47	CZ	113	ALA	2.9
56	C9	51	ALA	2.9
9	BI	29	ASN	2.9
31	DE	28	VAL	2.9
46	DY	49	VAL	2.9
57	C0	23	VAL	2.9
37	CO	28	GLY	2.9
40	CR	57	LYS	2.9
58	C1	1590	A	2.9

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Mol	Chain	Res	Type	RSRZ
58	D1	2812	G	2.9
64	DV	31	A	2.9
56	C9	50	LEU	2.9
7	AG	86	GLN	2.8
32	CF	155	SER	2.8
28	CB	40	THR	2.8
56	C9	56	GLU	2.8
29	DC	75	VAL	2.8
52	D5	36	VAL	2.8
54	D7	26	ASN	2.8
39	DQ	2	ARG	2.8
13	AM	100	GLY	2.8
24	BC	10	PHE	2.8
56	D9	32	LEU	2.8
57	D0	30	PRO	2.8
19	AT	81	ARG	2.8
58	C1	2813	C	2.8
2	BA	133	LYS	2.8
9	BI	37	PHE	2.8
32	CF	71	LEU	2.8
41	DS	105	LEU	2.8
51	CL	1	MET	2.8
46	DY	50	ARG	2.8
47	DZ	141	VAL	2.8
9	AI	96	LEU	2.8
4	BD	23	GLY	2.8
31	CE	86	MET	2.8
57	D0	10	ILE	2.8
54	C7	39	TYR	2.8
7	AG	2	ALA	2.8
12	AL	19	ARG	2.8
63	DW	92	ARG	2.8
13	BM	7	VAL	2.8
57	D0	31	LYS	2.8
3	AC	165	THR	2.8
9	BI	110	GLU	2.8
18	AS	85	LEU	2.8
31	DE	103	LEU	2.8
53	D6	59	GLU	2.8
62	DA	48	GLY	2.8
58	D1	2900	A	2.8
29	CC	132	HIS	2.8

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Mol	Chain	Res	Type	RSRZ
54	D7	49	HIS	2.8
22	Bb	1112	C	2.8
27	CA	45	ALA	2.8
50	CK	72	ALA	2.8
13	BM	27	LYS	2.8
59	Cs	17	C	2.8
3	AC	207	VAL	2.8
9	AI	109	VAL	2.8
60	D2	53	G	2.8
31	DE	82	LEU	2.8
13	BM	105	THR	2.8
31	CE	88	ILE	2.8
37	CO	26	GLY	2.7
42	DT	58	ARG	2.7
40	DR	37	ALA	2.7
44	CW	113	LYS	2.7
19	BT	67	VAL	2.7
25	C2	73	A	2.7
10	BJ	88	LEU	2.7
33	CI	114	LEU	2.7
41	DS	88	ILE	2.7
9	AI	30	GLY	2.7
7	BG	33	ASP	2.7
58	D1	1579	G	2.7
37	DO	39	LYS	2.7
46	CY	27	VAL	2.7
24	BC	12	LEU	2.7
32	DF	168	PRO	2.7
41	DS	1	MET	2.7
47	CZ	28	MET	2.7
11	BK	49	GLY	2.7
13	BM	100	GLY	2.7
25	C2	58	A	2.7
27	CA	50	ASP	2.7
27	CA	106	ALA	2.7
9	AI	87	GLN	2.7
31	DE	68	PRO	2.7
9	BI	101	PHE	2.7
4	AD	23	GLY	2.7
40	DR	107	GLU	2.7
14	AN	12	ARG	2.7
22	Ab	1108	U	2.7

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Mol	Chain	Res	Type	RSRZ
2	BA	165	VAL	2.7
7	AG	84	ASN	2.7
37	CO	147	LEU	2.7
20	AU	8	ARG	2.7
41	CS	3	ARG	2.7
41	CS	115	ARG	2.7
7	BG	81	GLY	2.7
20	AU	74	LYS	2.7
35	DM	36	GLY	2.7
9	AI	64	THR	2.7
35	CM	67	LEU	2.7
9	BI	31	GLN	2.6
31	DE	63	ILE	2.6
4	AD	209	ARG	2.6
9	BI	66	ARG	2.6
40	DR	13	ARG	2.6
47	DZ	80	ARG	2.6
27	CA	70	LYS	2.6
22	Ab	1112	C	2.6
32	DF	53	GLU	2.6
47	DZ	113	ALA	2.6
3	AC	172	ARG	2.6
22	Bb	981	G	2.6
30	CD	133	ASN	2.6
48	Da	46	LYS	2.6
7	BG	82	GLY	2.6
9	BI	12	GLU	2.6
12	BL	16	GLU	2.6
22	Ab	1113	A	2.6
37	DO	149	GLU	2.6
56	D9	56	GLU	2.6
6	AF	101	ALA	2.6
19	BT	41	VAL	2.6
27	CA	47	LEU	2.6
30	DD	26	ALA	2.6
32	CF	141	VAL	2.6
50	CK	44	LEU	2.6
54	D7	10	LEU	2.6
33	DI	118	LYS	2.6
2	AA	195	ASP	2.6
22	Ab	80	U	2.6
22	Ab	79	G	2.6

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Mol	Chain	Res	Type	RSRZ
58	C1	1579	G	2.6
3	AC	153	VAL	2.6
3	AC	189	ALA	2.6
5	AE	16	THR	2.6
35	CM	3	THR	2.6
37	DO	30	THR	2.6
14	AN	35	ARG	2.6
46	DY	4	LYS	2.6
58	D1	33	C	2.6
64	DV	17	C	2.6
39	CQ	11	ASN	2.6
46	CY	62	GLU	2.6
53	C6	58	LEU	2.6
27	CA	43	VAL	2.6
13	AM	120	LYS	2.6
20	BU	74	LYS	2.6
22	Ab	1109	U	2.6
50	CK	8	LYS	2.6
2	BA	148	TYR	2.6
64	DV	50	G	2.6
32	CF	168	PRO	2.6
23	B2	14	A	2.6
38	CP	12	GLN	2.6
9	BI	100	GLY	2.6
30	CD	131	GLY	2.6
31	DE	85	GLY	2.6
57	C0	37	GLY	2.6
2	BA	155	LEU	2.6
10	BJ	71	LEU	2.6
31	DE	34	LEU	2.6
17	BR	24	GLU	2.6
13	BM	94	ARG	2.6
27	CA	53	ARG	2.6
37	CO	65	ARG	2.6
37	DO	65	ARG	2.6
39	DQ	8	ARG	2.6
40	CR	98	VAL	2.6
21	BW	14	TRP	2.5
10	AJ	59	SER	2.5
24	BC	2	GLY	2.5
12	BL	27	LEU	2.5
2	BA	22	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
10	AJ	22	LYS	2.5
13	BM	99	ARG	2.5
28	CB	34	VAL	2.5
46	CY	43	ASN	2.5
12	BL	26	ALA	2.5
32	CF	156	ALA	2.5
58	C1	570	A	2.5
57	D0	20	HIS	2.5
33	DI	114	LEU	2.5
53	C6	54	GLY	2.5
37	CO	7	ARG	2.5
17	BR	58	GLU	2.5
29	CC	73	GLU	2.5
41	CS	130	ALA	2.5
41	DS	36	GLU	2.5
14	BN	13	THR	2.5
58	D1	2815	G	2.5
9	BI	36	TYR	2.5
7	BG	59	LEU	2.5
21	BW	25	LYS	2.5
64	DV	54	C	2.5
48	Da	9	SER	2.5
56	D9	35	GLN	2.5
24	BC	5	ILE	2.5
31	CE	77	ILE	2.5
47	CZ	104	PHE	2.5
46	DY	53	PRO	2.5
4	BD	22	LYS	2.5
13	BM	31	LYS	2.5
29	CC	61	ARG	2.5
40	DR	97	ARG	2.5
42	CT	36	ARG	2.5
46	CY	4	LYS	2.5
32	DF	45	VAL	2.5
54	C7	13	CYS	2.5
62	DA	85	GLU	2.5
27	CA	55	ASP	2.5
40	CR	61	ASN	2.5
9	AI	19	LEU	2.5
24	BC	16	ARG	2.5
38	CP	18	LYS	2.5
33	CI	9	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
40	CR	15	ARG	2.5
41	CS	105	LEU	2.5
48	Da	74	ARG	2.5
31	DE	2	PRO	2.5
9	BI	117	HIS	2.5
20	AU	73	HIS	2.5
24	BC	193	TYR	2.5
54	D7	39	TYR	2.5
7	AG	82	GLY	2.5
40	DR	28	VAL	2.5
40	DR	84	GLN	2.5
39	CQ	6	SER	2.4
50	CK	5	GLU	2.4
56	C9	40	GLU	2.4
58	D1	2138	A	2.4
2	AA	70	PHE	2.4
10	AJ	46	ARG	2.4
12	AL	21	LYS	2.4
37	DO	41	ARG	2.4
32	CF	88	LEU	2.4
58	D1	2814	C	2.4
47	CZ	95	PRO	2.4
9	AI	4	TYR	2.4
9	BI	114	TYR	2.4
19	BT	80	TYR	2.4
37	DO	26	GLY	2.4
40	DR	98	VAL	2.4
50	DK	13	ALA	2.4
62	DA	108	MET	2.4
38	CP	112	GLU	2.4
27	CA	59	ARG	2.4
28	DB	262	ARG	2.4
40	DR	89	ARG	2.4
46	CY	50	ARG	2.4
57	C0	31	LYS	2.4
8	BH	2	LEU	2.4
41	DS	6	LEU	2.4
27	CA	40	THR	2.4
13	AM	10	PRO	2.4
16	BP	46	PRO	2.4
46	CY	77	PRO	2.4
58	C1	571	A	2.4

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Mol	Chain	Res	Type	RSRZ
4	BD	2	GLY	2.4
10	AJ	62	HIS	2.4
12	BL	64	TYR	2.4
13	BM	92	HIS	2.4
32	DF	157	TYR	2.4
10	BJ	38	ILE	2.4
37	DO	70	GLN	2.4
46	DY	44	ILE	2.4
58	D1	2413	C	2.4
13	BM	101	GLN	2.4
22	Ab	86	U	2.4
22	Ab	1184	G	2.4
22	Ab	1434	G	2.4
22	Bb	1169	G	2.4
9	AI	110	GLU	2.4
13	AM	102	ARG	2.4
16	BP	35	LYS	2.4
17	BR	100	LYS	2.4
31	DE	30	GLU	2.4
40	DR	30	ARG	2.4
48	Da	57	PHE	2.4
46	DY	17	SER	2.4
41	CS	24	PRO	2.4
49	CH	84	GLY	2.4
57	D0	37	GLY	2.4
31	CE	52	ILE	2.4
57	D0	17	ILE	2.4
4	AD	22	LYS	2.4
20	AU	45	GLN	2.4
31	DE	74	LYS	2.4
40	DR	33	LYS	2.4
46	CY	101	LYS	2.4
2	AA	154	LEU	2.4
4	BD	24	GLU	2.4
10	AJ	88	LEU	2.4
13	BM	8	GLU	2.4
15	BO	7	GLU	2.4
19	BT	73	GLU	2.4
58	C1	1578	C	2.4
19	AT	4	SER	2.4
58	C1	2815	G	2.4
9	AI	65	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
32	CF	44	VAL	2.4
46	DY	45	VAL	2.4
54	D7	20	ASN	2.4
7	AG	7	ALA	2.4
8	BH	62	TYR	2.4
27	CA	18	LYS	2.4
57	C0	15	LYS	2.4
7	AG	146	GLU	2.4
12	AL	127	GLU	2.4
22	Bb	1170	A	2.4
20	AU	70	SER	2.4
22	Bb	1108	U	2.4
3	AC	194	GLY	2.3
9	BI	27	THR	2.3
10	BJ	48	THR	2.3
58	C1	2413	C	2.3
9	AI	117	HIS	2.3
35	CM	1	MET	2.3
22	Bb	79	G	2.3
58	D1	2807	G	2.3
12	AL	60	LEU	2.3
16	BP	66	PRO	2.3
46	DY	52	SER	2.3
9	AI	95	LYS	2.3
56	C9	34	TRP	2.3
12	BL	14	GLY	2.3
58	C1	217	A	2.3
10	BJ	98	ILE	2.3
21	AW	6	ARG	2.3
40	CR	105	ALA	2.3
7	BG	101	LEU	2.3
20	AU	10	LEU	2.3
40	CR	12	PHE	2.3
14	AN	8	GLU	2.3
29	DC	73	GLU	2.3
30	DD	190	GLU	2.3
14	AN	18	VAL	2.3
37	DO	71	VAL	2.3
10	BJ	55	LYS	2.3
11	AK	11	LYS	2.3
29	DC	69	LYS	2.3
43	DU	19	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
7	AG	6	ARG	2.3
19	BT	76	PRO	2.3
54	D7	31	PRO	2.3
13	AM	78	ILE	2.3
24	BC	167	TRP	2.3
33	DI	84	GLY	2.3
40	DR	108	GLY	2.3
31	DE	99	MET	2.3
12	AL	69	TYR	2.3
10	AJ	90	LEU	2.3
10	BJ	69	ASN	2.3
40	DR	26	LEU	2.3
4	BD	110	PHE	2.3
42	DT	97	ASP	2.3
58	D1	2307	U	2.3
25	C2	17	C	2.3
33	CI	118	LYS	2.3
39	CQ	9	LYS	2.3
41	DS	28	VAL	2.3
12	AL	44	THR	2.3
19	AT	80	TYR	2.3
2	AA	152	PHE	2.3
58	C1	2672	G	2.3
57	C0	14	CYS	2.3
14	AN	17	LYS	2.3
4	AD	47	ARG	2.3
7	AG	5	ARG	2.3
28	DB	271	ILE	2.3
29	CC	56	PRO	2.3
29	DC	77	ILE	2.3
46	DY	56	PRO	2.3
35	DM	77	GLY	2.3
40	DR	60	GLY	2.3
22	Ab	1231	C	2.3
25	C2	61	C	2.3
58	C1	33	C	2.3
27	CA	68	LEU	2.3
2	AA	140	HIS	2.3
7	BG	26	PHE	2.3
47	DZ	149	SER	2.3
14	BN	34	TYR	2.3
54	C7	21	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
10	BJ	70	ARG	2.3
47	DZ	165	VAL	2.3
62	DA	50	ASP	2.3
25	C2	53	G	2.2
58	D1	2142	G	2.2
58	D1	2345	G	2.2
28	DB	270	ILE	2.2
36	CN	51	ALA	2.2
38	DP	107	ALA	2.2
40	DR	104	GLY	2.2
62	DA	89	ALA	2.2
25	C3	16	U	2.2
58	C1	1071	U	2.2
58	D1	570	A	2.2
4	BD	20	TYR	2.2
9	AI	127	LYS	2.2
18	BS	88	LYS	2.2
35	DM	137	LYS	2.2
46	DY	47	LYS	2.2
22	Ab	1095	C	2.2
39	CQ	68	ARG	2.2
48	Da	41	ARG	2.2
19	AT	9	VAL	2.2
20	AU	75	ASN	2.2
32	CF	43	VAL	2.2
56	D9	40	GLU	2.2
2	AA	122	PHE	2.2
9	BI	116	LYS	2.2
22	Ab	1016	G	2.2
31	CE	67	LYS	2.2
10	BJ	46	ARG	2.2
31	DE	115	ARG	2.2
9	BI	108	VAL	2.2
50	CK	12	GLU	2.2
31	DE	106	LEU	2.2
38	DP	7	MET	2.2
40	DR	101	LEU	2.2
46	CY	58	GLY	2.2
62	DA	68	LEU	2.2
20	BU	68	LYS	2.2
40	CR	99	LYS	2.2
45	DX	72	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
62	DA	84	LYS	2.2
10	AJ	47	PHE	2.2
4	BD	209	ARG	2.2
14	BN	12	ARG	2.2
28	CB	262	ARG	2.2
54	C7	42	TRP	2.2
30	DD	7	TYR	2.2
35	CM	4	TYR	2.2
38	DP	32	TYR	2.2
22	Bb	6	U	2.2
3	AC	157	ILE	2.2
29	CC	77	ILE	2.2
4	AD	24	GLU	2.2
10	BJ	85	LEU	2.2
22	Ab	1509	A	2.2
30	DD	27	GLU	2.2
33	CI	7	GLU	2.2
59	Ds	87	G	2.2
54	D7	9	LEU	2.2
19	AT	42	PRO	2.2
20	BU	28	ALA	2.2
46	CY	66	PRO	2.2
31	CE	126	ASP	2.2
35	DM	109	LYS	2.2
37	DO	61	ARG	2.2
7	AG	156	TRP	2.2
22	Ab	1011	C	2.2
58	D1	676	C	2.2
54	D7	46	HIS	2.2
47	DZ	126	VAL	2.2
14	AN	32	SER	2.2
46	DY	57	GLN	2.2
3	AC	101	LEU	2.2
47	DZ	125	LEU	2.2
9	BI	43	ALA	2.2
10	AJ	32	ALA	2.2
38	CP	136	ALA	2.2
47	DZ	97	GLU	2.2
10	AJ	10	GLY	2.2
20	BU	58	LYS	2.2
35	CM	44	PRO	2.2
37	DO	20	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
46	DY	82	PRO	2.2
25	C3	18	G	2.2
58	D1	1152	G	2.2
64	DV	49	G	2.2
19	AT	41	VAL	2.1
47	DZ	139	VAL	2.1
22	Bb	1380	C	2.1
26	C4	1	C	2.1
27	CA	103	ILE	2.1
36	CN	22	ILE	2.1
58	C1	296	C	2.1
2	BA	142	LEU	2.1
20	BU	29	LYS	2.1
29	DC	64	LYS	2.1
35	DM	18	ALA	2.1
10	BJ	39	PRO	2.1
14	AN	57	ARG	2.1
37	CO	8	PRO	2.1
19	AT	13	ASP	2.1
58	D1	1071	U	2.1
19	BT	9	VAL	2.1
19	BT	47	HIS	2.1
35	DM	9	VAL	2.1
15	AO	3	ILE	2.1
27	CA	100	ILE	2.1
32	CF	77	LYS	2.1
40	DR	32	LEU	2.1
22	Bb	1016	G	2.1
38	DP	12	GLN	2.1
46	DY	5	MET	2.1
55	D8	47	ARG	2.1
57	C0	18	ARG	2.1
58	C1	2141	G	2.1
7	BG	7	ALA	2.1
9	AI	106	ALA	2.1
16	BP	64	ALA	2.1
40	CR	100	ALA	2.1
24	BC	174	PRO	2.1
37	CO	149	GLU	2.1
46	DY	77	PRO	2.1
47	CZ	162	GLU	2.1
58	D1	2161	C	2.1

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Mol	Chain	Res	Type	RSRZ
20	BU	9	ASN	2.1
27	CA	37	PHE	2.1
28	DB	44	ASN	2.1
37	CO	91	PHE	2.1
7	BG	91	VAL	2.1
32	CF	111	HIS	2.1
14	BN	50	LYS	2.1
33	DI	140	LEU	2.1
37	DO	108	LYS	2.1
47	DZ	120	ILE	2.1
49	DH	95	LEU	2.1
4	AD	32	ALA	2.1
5	AE	20	GLN	2.1
19	BT	75	ALA	2.1
29	DC	204	ALA	2.1
8	AH	99	GLU	2.1
12	BL	127	GLU	2.1
14	BN	51	GLY	2.1
43	CU	36	PRO	2.1
47	CZ	84	GLU	2.1
48	Ca	13	GLY	2.1
48	Da	48	GLY	2.1
58	D1	89	A	2.1
64	DV	53	A	2.1
20	AU	11	SER	2.1
47	DZ	88	PHE	2.1
24	BC	3	ASN	2.1
2	BA	197	VAL	2.1
10	BJ	34	VAL	2.1
29	DC	72	VAL	2.1
32	CF	113	VAL	2.1
58	D1	1589	C	2.1
10	AJ	99	LYS	2.1
7	AG	16	LEU	2.1
10	BJ	50	ILE	2.1
29	DC	89	ASP	2.1
42	DT	16	LYS	2.1
48	Da	75	LEU	2.1
53	D6	4	HIS	2.1
54	D7	45	LYS	2.1
54	C7	34	LEU	2.1
54	C7	43	CYS	2.1

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Mol	Chain	Res	Type	RSRZ
7	BG	4	ARG	2.1
9	BI	128	ARG	2.1
10	AJ	5	ARG	2.1
37	CO	33	ARG	2.1
40	DR	15	ARG	2.1
41	CS	32	TYR	2.1
13	BM	67	GLU	2.1
9	BI	28	VAL	2.1
41	DS	89	VAL	2.1
46	DY	7	VAL	2.1
20	AU	54	LYS	2.1
23	B2	15	A	2.1
2	BA	196	LEU	2.1
3	AC	178	LEU	2.1
19	BT	40	ILE	2.1
3	AC	176	HIS	2.1
31	DE	100	TRP	2.1
54	D7	13	CYS	2.1
9	AI	119	ALA	2.1
40	CR	55	ALA	2.1
58	C1	676	C	2.1
59	Ds	6	C	2.1
22	Bb	980	G	2.1
59	Cs	89	G	2.1
4	BD	167	GLY	2.1
7	BG	34	GLY	2.1
38	CP	15	GLY	2.1
40	DR	22	GLY	2.1
3	AC	161	GLU	2.1
31	CE	13	GLU	2.1
54	C7	51	GLU	2.1
35	CM	5	VAL	2.0
58	C1	158	U	2.0
59	Ds	40	U	2.0
61	D4	48	U	2.0
7	BG	32	ARG	2.0
9	BI	99	LEU	2.0
20	BU	26	ASN	2.0
21	BW	24	ARG	2.0
30	DD	133	ASN	2.0
30	DD	205	ARG	2.0
15	BO	50	HIS	2.0

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Mol	Chain	Res	Type	RSRZ
17	AR	13	ASP	2.0
22	Bb	1165	A	2.0
40	DR	21	THR	2.0
40	DR	88	ASP	2.0
41	CS	27	THR	2.0
57	C0	21	GLY	2.0
31	CE	48	GLU	2.0
37	DO	107	LYS	2.0
38	CP	22	LYS	2.0
50	DK	20	GLU	2.0
58	D1	2305	C	2.0
58	D1	2813	C	2.0
59	Ds	49	C	2.0
4	BD	132	ARG	2.0
9	BI	19	LEU	2.0
9	BI	111	ARG	2.0
22	Ab	1172	G	2.0
22	Bb	1010	G	2.0
22	Bb	1015	G	2.0
39	CQ	105	ARG	2.0
40	DR	106	ARG	2.0
48	Ca	84	LEU	2.0
58	D1	298	G	2.0
58	D1	2672	G	2.0
9	BI	81	ILE	2.0
7	BG	2	ALA	2.0
19	BT	77	THR	2.0
24	BC	189	ALA	2.0
48	Da	85	ALA	2.0
3	AC	184	TYR	2.0
40	DR	36	TYR	2.0
54	D7	30	THR	2.0
32	CF	82	GLY	2.0
10	AJ	39	PRO	2.0
14	AN	15	LYS	2.0
47	CZ	50	GLN	2.0
48	Da	47	PRO	2.0
5	AE	27	ARG	2.0
8	BH	93	VAL	2.0
22	Bb	1432	A	2.0
37	CO	21	ARG	2.0
40	DR	85	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
58	D1	2331	A	2.0
64	DV	21	A	2.0
10	BJ	65	LEU	2.0
20	BU	13	LEU	2.0
37	CO	6	LEU	2.0
5	AE	13	ILE	2.0
22	Bb	88	C	2.0
22	Bb	341	C	2.0
58	D1	2308	C	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

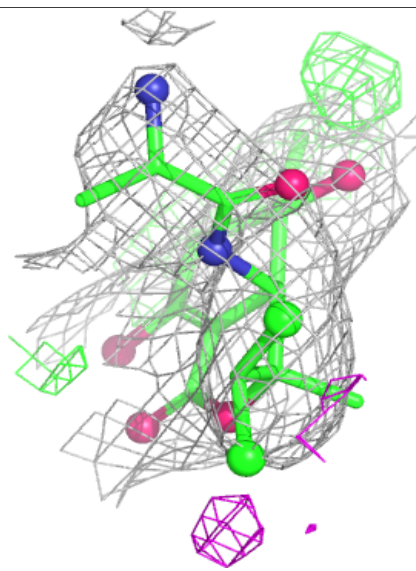
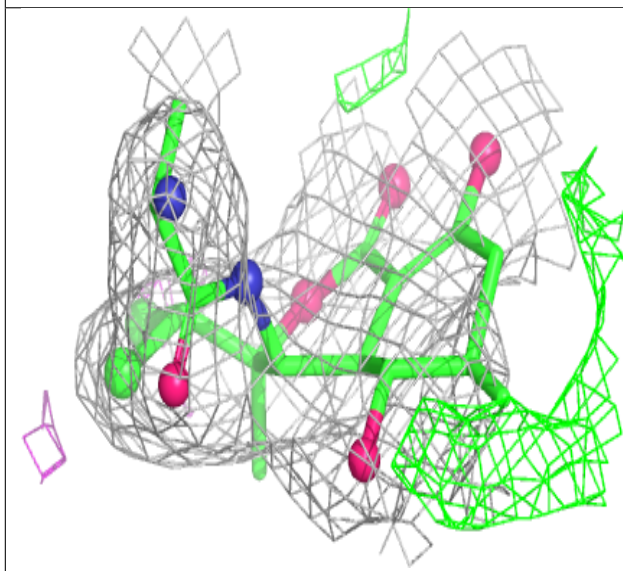
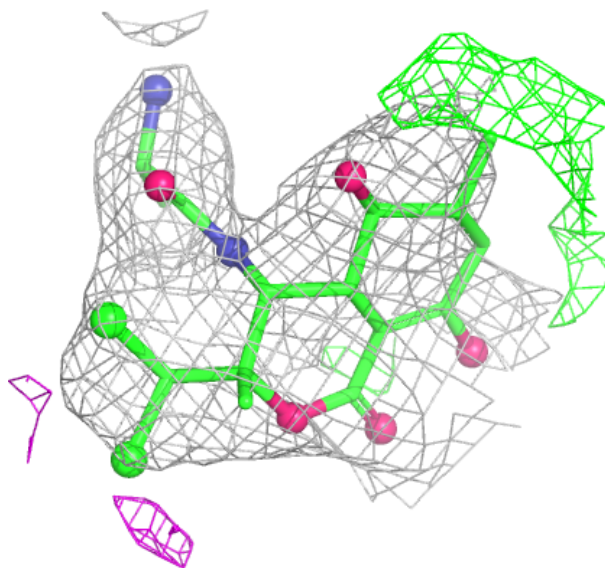
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
66	3V6	C1	3001	24/24	0.87	0.17	46,63,76,91	0
67	MG	D1	3002	1/1	0.89	0.13	40,40,40,40	0
65	PAR	Ab	1601	42/42	0.91	0.14	51,65,75,91	0
66	3V6	D1	3001	24/24	0.92	0.13	32,55,75,86	0
67	MG	C1	3002	1/1	0.93	0.13	41,41,41,41	0
65	PAR	Bb	1601	42/42	0.95	0.10	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.

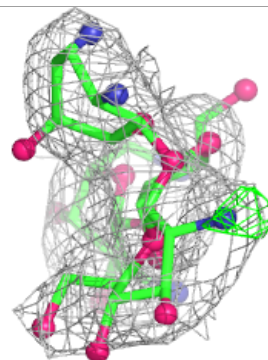
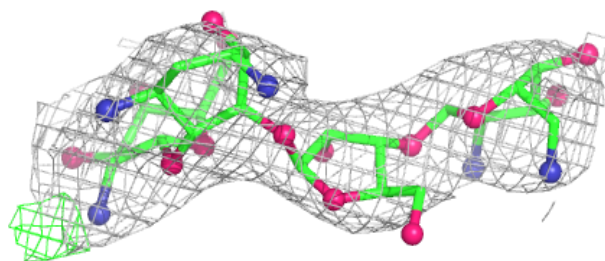
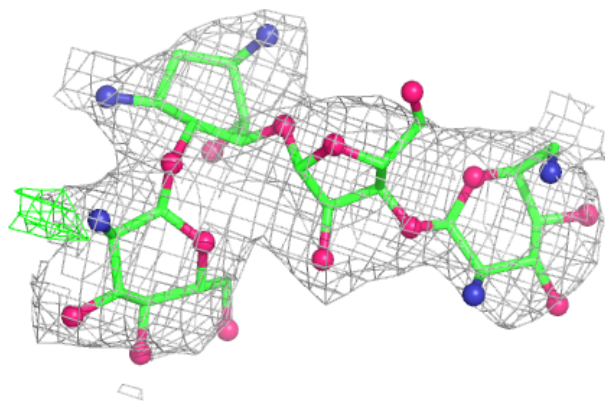
Electron density around 3V6 C1 3001:

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



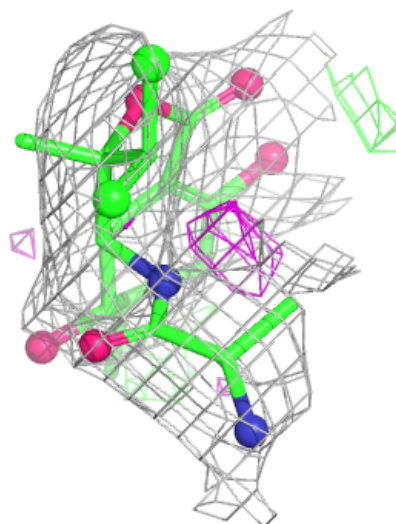
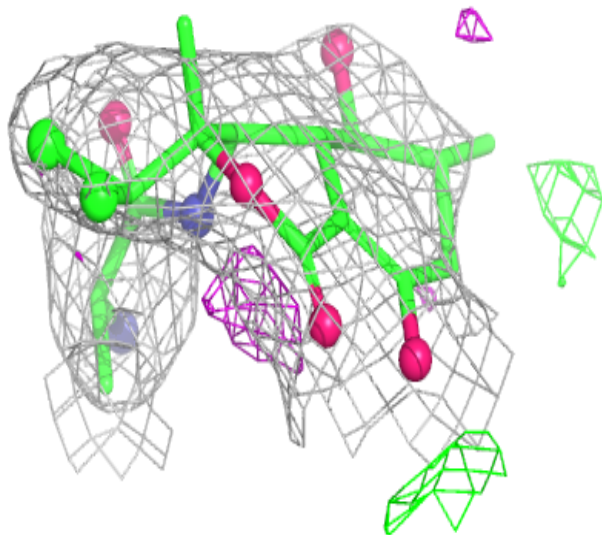
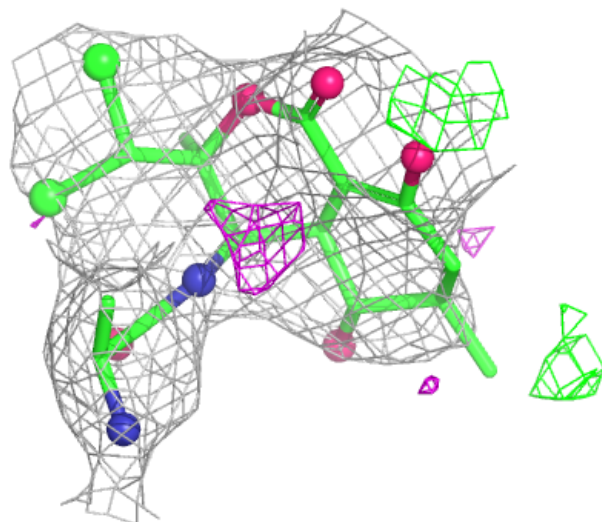
Electron density around PAR Ab 1601:

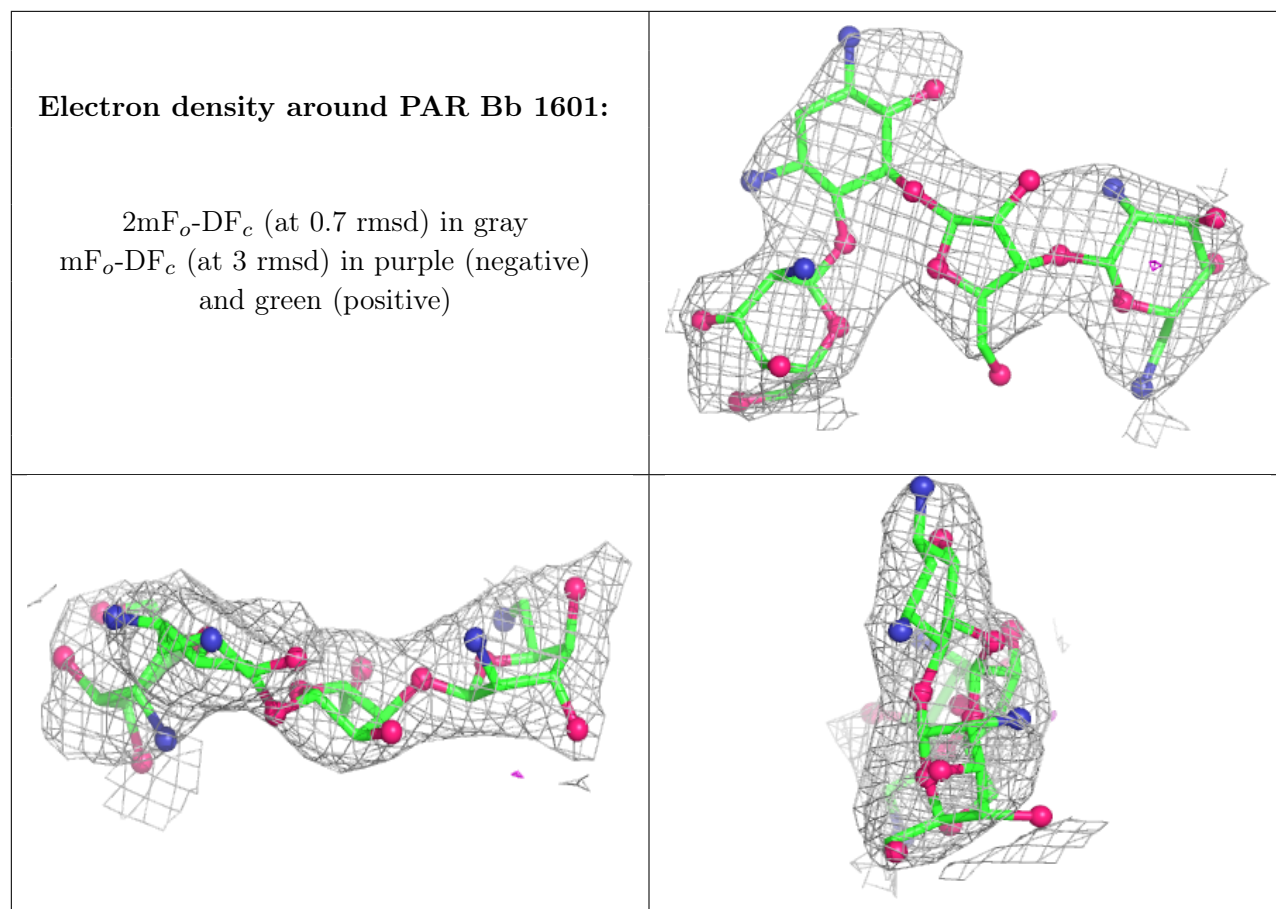
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.5 Other polymers [i](#)

There are no such residues in this entry.