



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 12:34 am BST

PDB ID : 1VY5
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome in the post-catalysis state of peptide bond formation containing dipeptidyl-tRNA in the A site and deacylated tRNA in the P site.
Authors : Polikanov, Y.S.; Steitz, T.A.; Innis, C.A.
Deposited on : 2014-05-13
Resolution : 2.55 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

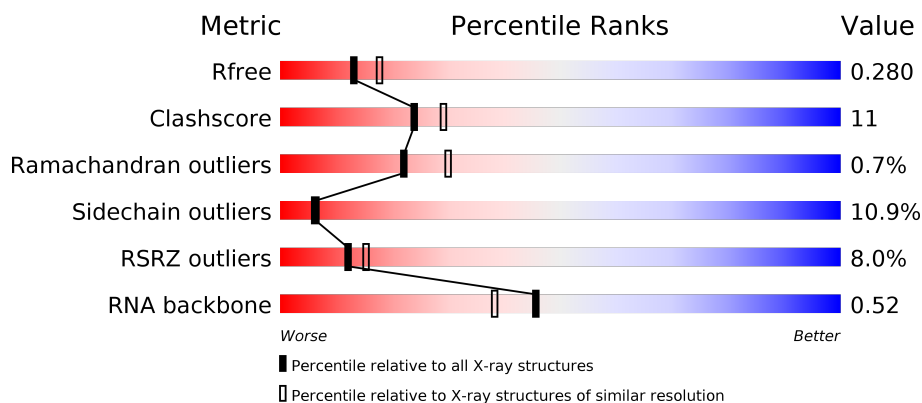
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)
RNA backbone	3102	1026 (2.88-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	AA	1521	<div> <div>2%</div> <div>52% 37% 9%</div> </div>
1	CA	1521	<div> <div>4%</div> <div>45% 42% 10%</div> </div>
2	AB	256	<div> <div>12%</div> <div>42% 41% 6% 10%</div> </div>
2	CB	256	<div> <div>20%</div> <div>36% 43% 11% 10%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	AC	239	
3	CC	239	
4	AD	209	
4	CD	209	
5	AE	162	
5	CE	162	
6	AF	101	
6	CF	101	
7	AG	156	
7	CG	156	
8	AH	138	
8	CH	138	
9	AI	128	
9	CI	128	
10	AJ	105	
10	CJ	105	
11	AK	129	
11	CK	129	
12	AL	132	
12	CL	132	
13	AM	126	
13	CM	126	
14	AN	61	
14	CN	61	
15	AO	89	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
15	CO	89	
16	AP	88	
16	CP	88	
17	AQ	105	
17	CQ	105	
18	AR	88	
18	CR	88	
19	AS	93	
19	CS	93	
20	AT	106	
20	CT	106	
21	AU	27	
21	CU	27	
22	AV	24	
22	CV	24	
23	AW	76	
23	CW	76	
24	AX	77	
24	CX	77	
25	AY	76	
25	CY	76	
26	BA	2915	
26	DA	2915	
27	BB	121	
27	DB	121	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
28	BD	276	
28	DD	276	
29	BE	206	
29	DE	206	
30	BF	210	
30	DF	210	
31	BG	182	
31	DG	182	
32	BH	180	
32	DH	180	
33	BI	148	
33	DI	148	
34	BN	140	
34	DN	140	
35	BO	122	
35	DO	122	
36	BP	150	
36	DP	150	
37	BQ	141	
37	DQ	141	
38	BR	118	
38	DR	118	
39	BS	112	
39	DS	112	
40	BT	146	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
40	DT	146	
41	BU	118	
41	DU	118	
42	BV	101	
42	DV	101	
43	BW	113	
43	DW	113	
44	BX	96	
44	DX	96	
45	BY	110	
45	DY	110	
46	BZ	206	
46	DZ	206	
47	B0	85	
47	D0	85	
48	B1	98	
48	D1	98	
49	B2	72	
49	D2	72	
50	B3	60	
50	D3	60	
51	B4	71	
51	D4	71	
52	B5	60	
52	D5	60	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
53	B6	54	
53	D6	54	
54	B7	49	
54	D7	49	
55	B8	65	
55	D8	65	
56	B9	37	
56	D9	37	

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
25	5MU	CY	54	-	-	-	X
25	PSU	CY	55	-	-	-	X
57	MG	DA	3651	-	-	-	X
57	MG	DD	303	-	-	-	X

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 297141 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 16S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1498	Total	C	N	O	P	0	0	0
			32205	14333	5970	10404	1498			
1	CA	1503	Total	C	N	O	P	0	0	0
			32312	14381	5990	10438	1503			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	231	Total	C	N	O	S	0	0	0
			1846	1179	331	331	5			
2	CB	231	Total	C	N	O	S	0	0	0
			1825	1167	326	327	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	206	Total	C	N	O	S	0	0	0
			1552	976	302	273	1			
3	CC	206	Total	C	N	O	S	0	0	0
			1542	968	300	273	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AD	208	Total	C	N	O	S	0	0	0
			1659	1040	326	286	7			
4	CD	208	Total	C	N	O	S	0	0	0
			1674	1050	333	284	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AE	148	Total	C	N	O	S	0	0	0
			1129	714	213	198	4			
5	CE	148	Total	C	N	O	S	0	0	0
			1133	716	214	199	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AF	100	Total	C	N	O	S	0	0	0
			806	511	143	149	3			
6	CF	100	Total	C	N	O	S	0	0	0
			816	516	146	151	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AG	155	Total	C	N	O	S	0	0	0
			1231	766	243	216	6			
7	CG	155	Total	C	N	O	S	0	0	0
			1235	769	244	216	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AH	137	Total	C	N	O	S	0	0	0
			1088	689	206	191	2			
8	CH	137	Total	C	N	O	S	0	0	0
			1088	689	206	191	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AI	127	Total	C	N	O		0	0	0
			983	623	193	167				
9	CI	127	Total	C	N	O		0	0	0
			978	619	190	169				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AJ	97	Total	C	N	O		0	0	0
			709	440	138	131				

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	CJ	96	Total	C	N	O			
			714	445	138	131	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	AK	114	Total	C	N	O	S		
			829	516	155	155	3	0	0
11	CK	114	Total	C	N	O	S		
			833	519	156	155	3	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	AL	122	Total	C	N	O	S		
			930	585	185	159	1	0	0
12	CL	122	Total	C	N	O	S		
			930	585	185	159	1	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	AM	123	Total	C	N	O	S		
			958	592	198	166	2	0	0
13	CM	122	Total	C	N	O	S		
			950	586	197	165	2	0	0

- 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		
			492	312	104	72	4	0	0
14	CN	60	Total	C	N	O	S		
			492	312	104	72	4	0	0

- 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		
			728	456	144	126	2	0	0
15	CO	88	Total	C	N	O	S		
			728	456	144	126	2	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AP	82	Total	C	N	O	S	0	0	0
			681	433	134	113	1			
16	CP	82	Total	C	N	O	S	0	0	0
			677	430	133	113	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			
17	CQ	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	AR	68	Total	C	N	O	0	0	0
			555	355	108	92			
18	CR	68	Total	C	N	O	0	0	0
			555	355	108	92			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AS	83	Total	C	N	O	S	0	0	0
			652	417	120	113	2			
19	CS	83	Total	C	N	O	S	0	0	0
			646	412	119	113	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AT	96	Total	C	N	O	S	0	0	0
			728	446	156	124	2			
20	CT	96	Total	C	N	O	S	0	0	0
			727	446	155	124	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	AU	23	Total	C	N	O	0	0	0
			199	122	48	29			
21	CU	23	Total	C	N	O	0	0	0
			199	122	48	29			

- Molecule 22 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	13	Total	C	N	O	P	0	0	0
			277	125	51	88	13			
22	CV	12	Total	C	N	O	P	0	0	0
			252	115	46	80	11			

- Molecule 23 is a RNA chain called A-site tRNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
23	AW	74	Total	C	N	O	P	S	0	0	0
			1607	727	288	516	73	3			
23	CW	72	Total	C	N	O	P	S	0	0	0
			1560	702	281	503	72	2			

- Molecule 24 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
24	AX	76	Total	C	N	O	P	S	0	0	0
			1625	725	294	529	76	1			
24	CX	76	Total	C	N	O	P	S	0	0	0
			1625	725	294	529	76	1			

- Molecule 25 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
25	AY	74	Total	C	N	O	P	S	0	0	0
			1581	707	285	515	73	1			
25	CY	73	Total	C	N	O	P	S	0	0	0
			1561	698	283	507	72	1			

- Molecule 26 is a RNA chain called 23S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	BA	2819	Total	C	N	O	P	0	0	0
			60729	27026	11370	19515	2818			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	DA	2800	Total	C	N	O	P	0	0	0
			60311	26840	11284	19388	2799			

- Molecule 27 is a RNA chain called 5S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BB	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			
27	DB	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	BD	275	Total	C	N	O	S	0	0	0
			2136	1349	423	361	3			
28	DD	275	Total	C	N	O	S	0	0	0
			2136	1349	423	361	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	BE	204	Total	C	N	O	S	0	0	0
			1559	985	298	270	6			
29	DE	204	Total	C	N	O	S	0	0	0
			1559	985	298	270	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	BF	203	Total	C	N	O	S	0	0	1
			1584	1009	298	275	2			
30	DF	203	Total	C	N	O	S	0	0	1
			1580	1007	297	274	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	BG	181	Total	C	N	O	S	0	0	0
			1425	914	256	251	4			
31	DG	181	Total	C	N	O	S	0	0	0
			1424	911	258	251	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BH	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			
32	DH	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BI	146	Total	C	N	O	S	0	0	0
			1085	693	189	202	1			
33	DI	146	Total	C	N	O	S	0	0	0
			1061	680	186	194	1			

- Molecule 34 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BN	140	Total	C	N	O	S	0	0	0
			1117	719	207	187	4			
34	DN	140	Total	C	N	O	S	0	0	0
			1117	719	207	187	4			

- Molecule 35 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			
35	DO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

- Molecule 36 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BP	149	Total	C	N	O	S	0	0	0
			1135	706	230	196	3			
36	DP	149	Total	C	N	O	S	0	0	0
			1135	706	230	196	3			

- Molecule 37 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			
37	DQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

- Molecule 38 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BR	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			
38	DR	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			

- Molecule 39 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BS	110	Total	C	N	O		0	0	0
			877	553	175	149				
39	DS	110	Total	C	N	O		0	0	0
			870	549	173	148				

- Molecule 40 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BT	131	Total	C	N	O	S	0	0	0
			1091	680	225	185	1			
40	DT	131	Total	C	N	O	S	0	0	0
			1083	675	224	183	1			

- Molecule 41 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BU	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			
41	DU	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			

- Molecule 42 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BV	101	Total	C	N	O	S	0	0	0
			771	495	140	135	1			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	DV	101	Total	C	N	O	S	0	0	0
			771	495	140	135	1			

- Molecule 43 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BW	112	Total	C	N	O	S	0	0	0
			886	557	174	153	2			
43	DW	112	Total	C	N	O	S	0	0	0
			886	557	174	153	2			

- Molecule 44 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BX	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			
44	DX	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			

- Molecule 45 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BY	107	Total	C	N	O	S	0	0	0
			806	517	152	131	6			
45	DY	107	Total	C	N	O	S	0	0	0
			806	517	152	131	6			

- Molecule 46 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BZ	171	Total	C	N	O	S	0	0	0
			1349	862	243	242	2			
46	DZ	174	Total	C	N	O	S	0	0	0
			1360	870	243	245	2			

- Molecule 47 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	B0	83	Total	C	N	O	S	0	0	0
			653	404	139	109	1			
47	D0	83	Total	C	N	O	S	0	0	0
			653	404	139	109	1			

- Molecule 48 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	B1	97	Total	C	N	O	S	0	0	0
			755	475	148	131	1			
48	D1	97	Total	C	N	O	S	0	0	0
			755	475	148	131	1			

- Molecule 49 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	B2	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			
49	D2	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
50	B3	59	Total	C	N	O	0	0	0
			469	298	90	81			
50	D3	59	Total	C	N	O	0	0	0
			464	296	90	78			

- Molecule 51 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	B4	69	Total	C	N	O	S	0	0	0
			558	352	102	99	5			
51	D4	69	Total	C	N	O	S	0	0	0
			532	339	97	91	5			

- Molecule 52 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	B5	59	Total	C	N	O	S	0	0	0
			455	285	89	76	5			
52	D5	59	Total	C	N	O	S	0	0	0
			455	285	89	76	5			

- Molecule 53 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	B6	53	Total	C	N	O	S	0	0	0
			453	281	91	77	4			
53	D6	53	Total	C	N	O	S	0	0	0
			449	279	91	75	4			

- Molecule 54 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	B7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			
54	D7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			

- Molecule 55 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	B8	64	Total	C	N	O	S	0	0	0
			511	328	99	82	2			
55	D8	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			

- Molecule 56 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	B9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			
56	D9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

- Molecule 57 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	B4	1	Total	Mg	0	0
			1	1		
57	BA	812	Total	Mg	0	0
			812	812		
57	AK	1	Total	Mg	0	0
			1	1		
57	DQ	4	Total	Mg	0	0
			4	4		
57	D3	1	Total	Mg	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	DF	4	Total 4	Mg 4	0	0
57	CV	1	Total 1	Mg 1	0	0
57	B8	1	Total 1	Mg 1	0	0
57	BE	8	Total 8	Mg 8	0	0
57	AW	4	Total 4	Mg 4	0	0
57	DU	2	Total 2	Mg 2	0	0
57	B1	1	Total 1	Mg 1	0	0
57	AN	2	Total 2	Mg 2	0	0
57	BP	5	Total 5	Mg 5	0	0
57	AX	15	Total 15	Mg 15	0	0
57	DN	1	Total 1	Mg 1	0	0
57	CA	170	Total 170	Mg 170	0	0
57	B5	1	Total 1	Mg 1	0	0
57	BB	20	Total 20	Mg 20	0	0
57	D8	1	Total 1	Mg 1	0	0
57	AE	3	Total 3	Mg 3	0	0
57	DG	1	Total 1	Mg 1	0	0
57	B9	1	Total 1	Mg 1	0	0
57	BF	9	Total 9	Mg 9	0	0
57	BX	3	Total 3	Mg 3	0	0
57	B2	1	Total 1	Mg 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	AA	214	Total 214	Mg 214	0	0
57	BQ	5	Total 5	Mg 5	0	0
57	CX	3	Total 3	Mg 3	0	0
57	DV	3	Total 3	Mg 3	0	0
57	B6	2	Total 2	Mg 2	0	0
57	AM	1	Total 1	Mg 1	0	0
57	BU	8	Total 8	Mg 8	0	0
57	DR	1	Total 1	Mg 1	0	0
57	BN	6	Total 6	Mg 6	0	0
57	CT	1	Total 1	Mg 1	0	0
57	D0	1	Total 1	Mg 1	0	0
57	BG	3	Total 3	Mg 3	0	0
57	BY	1	Total 1	Mg 1	0	0
57	DE	4	Total 4	Mg 4	0	0
57	B3	2	Total 2	Mg 2	0	0
57	CJ	1	Total 1	Mg 1	0	0
57	BR	2	Total 2	Mg 2	0	0
57	DA	677	Total 677	Mg 677	0	0
57	DP	2	Total 2	Mg 2	0	0
57	DW	4	Total 4	Mg 4	0	0
57	B7	5	Total 5	Mg 5	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	CF	1	Total 1	Mg 1	0	0
57	BV	5	Total 5	Mg 5	0	0
57	DO	1	Total 1	Mg 1	0	0
57	BO	2	Total 2	Mg 2	0	0
57	DX	1	Total 1	Mg 1	0	0
57	BZ	1	Total 1	Mg 1	0	0
57	DY	1	Total 1	Mg 1	0	0
57	CW	1	Total 1	Mg 1	0	0
57	CD	1	Total 1	Mg 1	0	0
57	BD	9	Total 9	Mg 9	0	0
57	B0	3	Total 3	Mg 3	0	0
57	CE	1	Total 1	Mg 1	0	0
57	BW	4	Total 4	Mg 4	0	0
57	AY	3	Total 3	Mg 3	0	0
57	DD	9	Total 9	Mg 9	0	0
57	CK	1	Total 1	Mg 1	0	0
57	AF	1	Total 1	Mg 1	0	0
57	DB	13	Total 13	Mg 13	0	0

- Molecule 58 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
58	AD	1	Total	Fe	S	0	0
			8	4	4		
58	CD	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	B5	1	Total	Zn	0	0
			1	1		
59	B4	1	Total	Zn	0	0
			1	1		
59	CN	1	Total	Zn	0	0
			1	1		
59	BY	1	Total	Zn	0	0
			1	1		
59	B9	1	Total	Zn	0	0
			1	1		
59	DY	1	Total	Zn	0	0
			1	1		
59	D5	1	Total	Zn	0	0
			1	1		
59	D4	1	Total	Zn	0	0
			1	1		
59	AN	1	Total	Zn	0	0
			1	1		
59	D6	1	Total	Zn	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	D9	1	Total 1	Zn 1	0	0
59	B6	1	Total 1	Zn 1	0	0

- Molecule 60 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	AX	1	Total 1	K 1	0	0
60	CX	1	Total 1	K 1	0	0

- Molecule 61 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	AA	227	Total 227	O 227	0	0
61	AE	2	Total 2	O 2	0	0
61	AJ	1	Total 1	O 1	0	0
61	AL	1	Total 1	O 1	0	0
61	AM	1	Total 1	O 1	0	0
61	AU	1	Total 1	O 1	0	0
61	AV	3	Total 3	O 3	0	0
61	AW	3	Total 3	O 3	0	0
61	AX	6	Total 6	O 6	0	0
61	AY	1	Total 1	O 1	0	0
61	BA	1383	Total 1383	O 1383	0	0
61	BB	36	Total 36	O 36	0	0
61	BD	12	Total 12	O 12	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	BE	14	Total 14	O 14	0	0
61	BF	8	Total 8	O 8	0	0
61	BG	3	Total 3	O 3	0	0
61	BI	1	Total 1	O 1	0	0
61	BO	4	Total 4	O 4	0	0
61	BP	16	Total 16	O 16	0	0
61	BQ	4	Total 4	O 4	0	0
61	BR	2	Total 2	O 2	0	0
61	BT	2	Total 2	O 2	0	0
61	BU	3	Total 3	O 3	0	0
61	BV	2	Total 2	O 2	0	0
61	BW	1	Total 1	O 1	0	0
61	BX	4	Total 4	O 4	0	0
61	BZ	1	Total 1	O 1	0	0
61	B0	3	Total 3	O 3	0	0
61	B1	1	Total 1	O 1	0	0
61	B3	2	Total 2	O 2	0	0
61	B5	2	Total 2	O 2	0	0
61	B6	1	Total 1	O 1	0	0
61	B7	2	Total 2	O 2	0	0
61	B8	8	Total 8	O 8	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	CA	185	Total 185	O 185	0	0
61	CJ	2	Total 2	O 2	0	0
61	CL	1	Total 1	O 1	0	0
61	CT	1	Total 1	O 1	0	0
61	CV	1	Total 1	O 1	0	0
61	CW	2	Total 2	O 2	0	0
61	DA	1025	Total 1025	O 1025	0	0
61	DB	9	Total 9	O 9	0	0
61	DD	19	Total 19	O 19	0	0
61	DE	11	Total 11	O 11	0	0
61	DF	3	Total 3	O 3	0	0
61	DN	2	Total 2	O 2	0	0
61	DO	1	Total 1	O 1	0	0
61	DP	16	Total 16	O 16	0	0
61	DR	1	Total 1	O 1	0	0
61	DT	3	Total 3	O 3	0	0
61	DU	2	Total 2	O 2	0	0
61	DX	3	Total 3	O 3	0	0
61	DY	2	Total 2	O 2	0	0
61	D0	3	Total 3	O 3	0	0
61	D1	1	Total 1	O 1	0	0

Continued on next page...

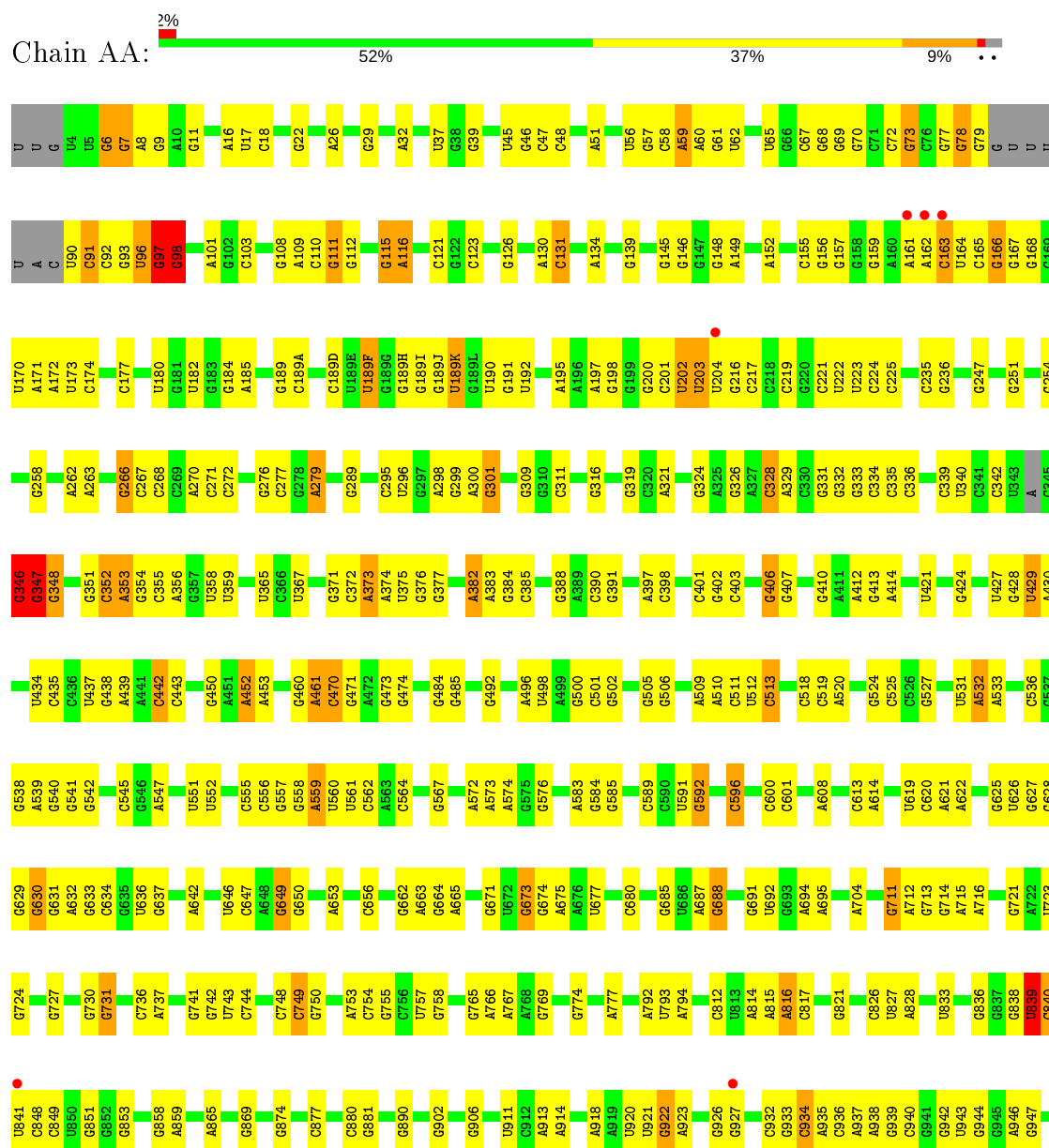
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	D3	1	Total	O	0	0
			1	1		
61	D7	3	Total	O	0	0
			3	3		
61	D8	4	Total	O	0	0
			4	4		

3 Residue-property plots

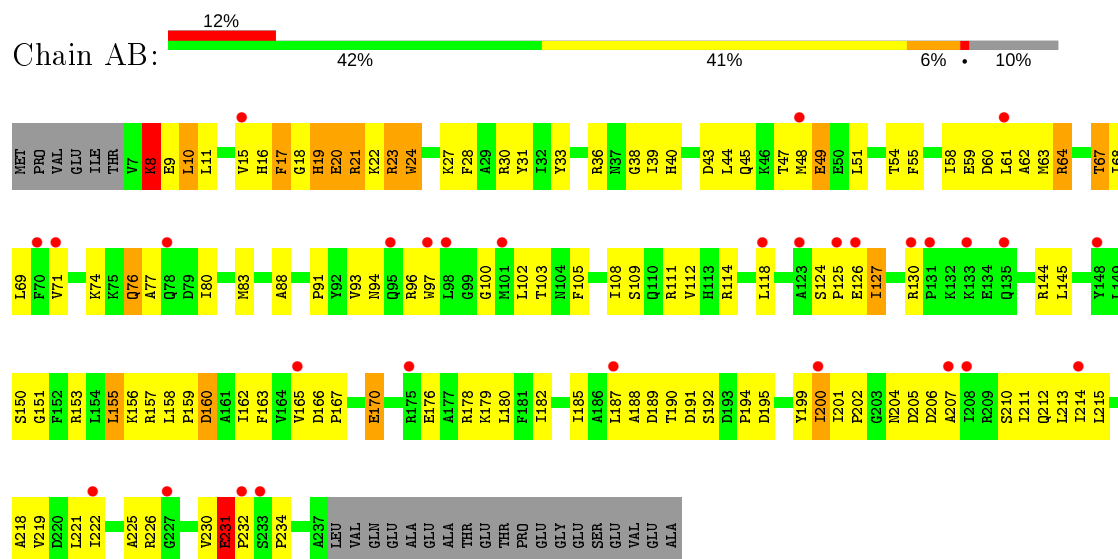
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

• Molecule 1: 16S Ribosomal RNA

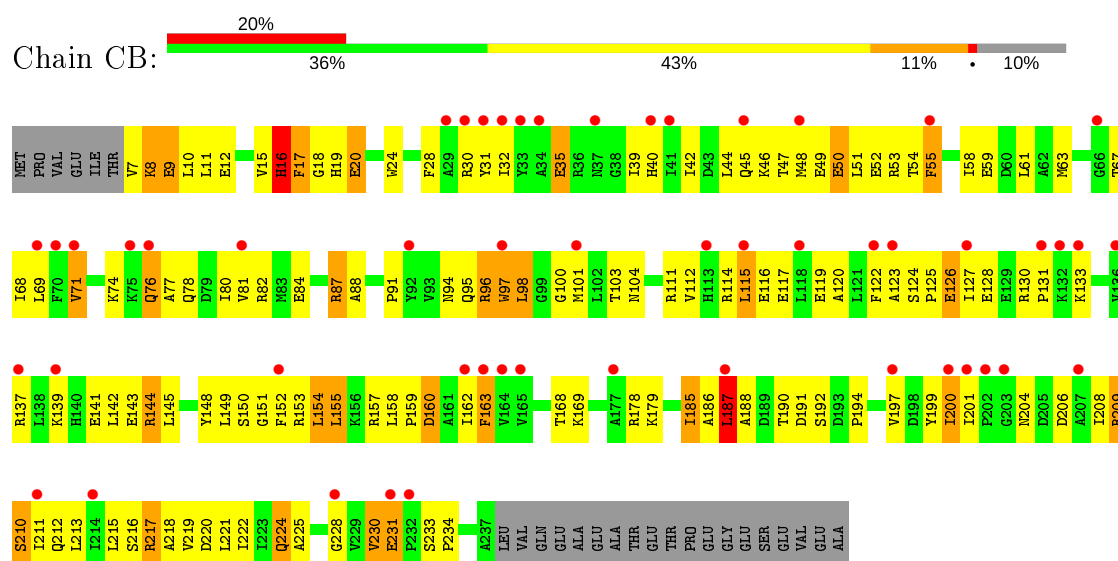


C1514	G1410	G1384	C1262	U1186	G1128	U1062	A1005	A946	U841	A737	C543	A448
G1515	C1411	G1338	C1263	G1197	C1129	C1063	C1006	G947	C848	G741	G544	C449
G1516	C1412	A1339	A1269	G1198	A1130	G1064	C1008	G948	G851	G742	G545	G450
G1517	C1413	A1340	C1270	G1199	G1131	U1065	G1007	A949	G852	G743	G546	A451
A1518	U1414	U1341	G1271	C1200	G1132	C1066	G1010	G950	G853	G744	A547	A452
A1519	G1419	C1342	G1272	A1201	G1134	A1067	G1011	G951	G854	G745	U551	G460
G1520	G1422	G1343	G1273	G1202	U1135	G1068	U1012	G952	C857	G746	U552	A461
G1529	C1423	C1344	C1203	A1204	U1136	U1070	G1013	G953	G858	G747	G556	C470
G1530	C1424	U1345	U1205	G1206	C1137	G1071	A1014	G954	A859	G748	C556	G471
A1531	U1532	U1346	C1277	U1206	G1138	G1072	G1015	G955	A860	G749	U551	G460
U1532	C1347	U1347	U1278	G1206	G1139	U1073	A1016	G956	G861	G750	U552	G461
C	U1348	A1279	U1279	U1211	C1140	G1074	G1017	G957	G862	G751	U553	G472
A	A1349	A1280	A1279	U1212	C1141	C1075	C1018	A958	C866	G752	U554	G473
C	U1350	U1281	U1280	A1213	G1142	G1076	U1019	A959	C867	G753	U555	G474
C	G1435	C1282	G1283	A1214	G1143	U1020	C1021	U960	C868	G754	U556	G475
U	U1436	C1352	G1284	G1215	C1144	G1079	G1022	U961	G869	G755	U557	G476
C	G1353	G1353	C1284	G1216	G1145	A1080	G1023	G962	A766	G756	U558	G477
C	C1354	A1285	A1285	G1217	A1146	G1081	G1024	G963	A767	G757	A572	C488
U	G1355	A1286	A1286	C1218	C1147	G1082	U1025	A964	A768	G758	A573	G492
U	G1356	A1287	A1287	C1219	U1148	U1083	G1026	A965	G769	G759	G576	G492
U	A1442A	U1288	U1288	U1219	C1149	G1084	C1027	A966	G770	G760	U580	A496
U	A1442B	A1289	A1289	U1220	U1150	U1085	G1028	A967	G771	G761	U581	U498
U	U1446	G1290	G1290	G1221	A1151	U1086	C1029	G970	G772	G762	U582	U499
U	A1447	U1291	U1291	G1222	A1152	G1087	G1030	G971	G773	G763	U583	G500
C	C1452	U1292	U1292	C1223	C1153	G1088	G1031	G972	G774	G764	U584	G501
U	G1456	G1293	G1293	G1224	G1154	A1092	G1032	G973	G775	G765	G587	G502
U	G1457	G1294	A1225	A1225	G1155	C1030A	G1033	A974	G776	G766	G588	C503
U	G1469	C1297	A1226	A1226	G1156	A1093	A1030C	A975	G777	G767	G589	C504
U	G1479	C1298	A1227	C1228	A1157	G1094	G1031	A976	G778	G768	G592	G505
G1480	A1363A	C1298	C1228	C1228	G1158	U1095	G1032	A977	G779	G769	C596	A509
G1486	U1364	A1366	A1366	G1231	U1159	C1096	G1033	A978	G780	G770	A607	A510
G1487	G1365	C1367	C1367	U1232	C1162	C1097	G1034	C979	G781	G771	A608	C511
G1490	G1370	C1367	C1367	G1233	G1163	U1098	G1035	C980	G782	G772	A609	U512
G1491	U1371	U1301	U1301	C1234	G1164	G1100	G1036	C981	G783	G773	G610	C513
A1493	U1372	G1303	G1303	U1235	C1165	A1101	G1037	U982	G784	G774	G620	C514
U1494	G1373	G1304	G1304	A1236	G1166	A1102	C1038	U983	G785	G775	G621	C518
U1495	U1374	G1305	G1305	C1237	A1169	C1103	C1039	C984	G786	G776	G622	G521
U1496	A1374	G1312	G1312	A1238	A1170	G1104	U1040	C985	G787	G777	G623	C522
G1497	U1375	U1313	U1313	U1239	G1171	C1108	A1041	A986	G788	G778	G624	A523
U1498	U1376	C1239	C1239	U1240	G1172	C1109	G1042	C988	G789	G779	G625	C528
U1499	C1378	U1315	U1315	A1243	G1173	C1110	G1043	C989	G790	G780	G626	G529
U1502	G1379	G1316	G1316	C1244	G1174	A1110	A1044	C990	G791	G781	G627	G530
A1503	C1383	C1317	C1317	A1245	G1175	C1113	G1047	U991	G792	G782	G628	U531
G1504	G1386	A1318	A1318	A1246	G1176	C1114	U1047	U992	G793	G783	G629	A532
G1505	G1387	A1319	A1319	C1246	G1177	C1115	G1048	C993	G794	G784	G630	A533
U1506	C1388	C1320	C1320	C1247	G1178	C1116	U1049	C994	G795	G785	G631	U534
A1507	U1391	C1321	C1321	A1249	A1179	C1117	G1050	A995	G796	G786	G632	C536
G1508	G1392	G1322	G1322	A1250	A1180	G1118	C1051	C996	G797	G787	G633	G537
G1509	C1393	G1323	G1323	A1251	G1181	C1119	U1052	A997	G798	G788	G634	U538
U1510	U1394	A1324	A1324	A1252	A1182	C1120	G1053	U997	G799	G789	G635	G539
U1511	G1395	C1325	C1325	G1255	A1183	G1121	A1054	C998	G800	G790	G636	G540
U1512	C1396	C1326	C1326	U1256	G1184	U1121	G1055	C999	G801	G791	G637	G541
U1513	G1397	C1327	C1327	A1257	G1185	U1122	U1056	U1000	G802	G792	G638	G542
	C1398	C1328	C1328	G1258	G1186	A1123	G1057	A1001	G803	G793	G639	G543
	C1402	G1331	G1331	G1259	G1187	G1124	G1058	G1002	G804	G794	G640	G544
		A1332	A1332	C1260	G1190	U1125	C1059	G1003	G805	G795	G641	G545
		A1333	A1333	A1261	A1191	U1126	G1060	G1004	G806	G796	G642	G546
					C1192	G1127	G1061		G807	G797	G643	G547
									G808	G798	G644	G548
									G809	G799	G645	G549
									G810	G800	G646	G550
									G811	G801	G647	G551
									G812	G802	G648	G552
									G813	G803	G649	G553
									G814	G804	G650	G554
									G815	G805	G651	G555
									G816	G806	G652	G556
									G817	G807	G653	G557
									G818	G808	G654	G558
									G819	G809	G655	G559
									G820	G810	G656	G560
									G821	G811	G657	G561
									G822	G812	G658	G562
									G823	G813	G659	G563
									G824	G814	G660	G564
									G825	G815	G661	G565
									G826	G816	G662	G566
									G827	G817	G663	G567
									G828	G818	G664	G568
									G829	G819	G665	G569
									G830	G820	G666	G570
									G831	G821	G667	G571
									G832	G822	G668	G572
									G833	G823	G669	G573
									G834	G824	G670	G574
									G835	G825	G671	G575
									G836	G826	G672	G576
									G837	G827	G673	G577
									G838	G828	G674	G578
									G839	G829	G675	G579
									G840	G830	G676	G580
									G841	G831	G677	G581
									G842	G832	G678	G582
									G843	G833	G679	G583
									G844	G834	G680	G584
									G845	G835	G681	G585
									G846	G836	G682	G586
									G847	G837	G683	G587
									G848	G838	G684	G588
									G849	G839	G685	G589
									G850	G840	G686	G590
									G851	G841	G687	G591
									G852	G842	G688	G592
									G853	G843	G689	G593
									G854	G844	G690	G594
									G855	G845	G691	G595
									G856	G846	G692	G596
									G857	G847	G693	G597
									G858	G848	G694	G598
									G859	G849	G695	G599
									G860	G850	G696	G600
									G861	G851	G697	G601
									G862	G852	G698	G602
									G863	G853	G699	G603
									G864	G854	G700	G604
									G865	G855	G701	G605
									G866	G856	G702	G606
									G867	G857	G703	G607
									G868	G858	G704	G608
									G869	G859	G705	G609
									G870	G860	G706	G610
									G871	G861	G707	G611
									G872	G862	G708	G612
									G873	G863	G709	G613
									G874	G864	G710	G614
									G875	G865	G711	G615
									G876	G866	G712	G616
									G877	G867	G713	G617
									G878	G868	G714	G618
									G879	G869	G715	G619
									G880	G870	G716	G620

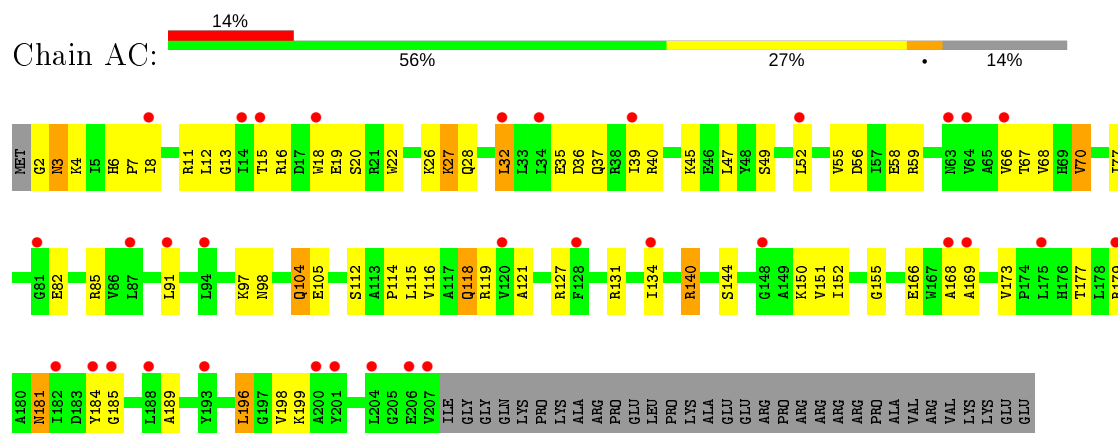
- Molecule 2: 30S ribosomal protein S2



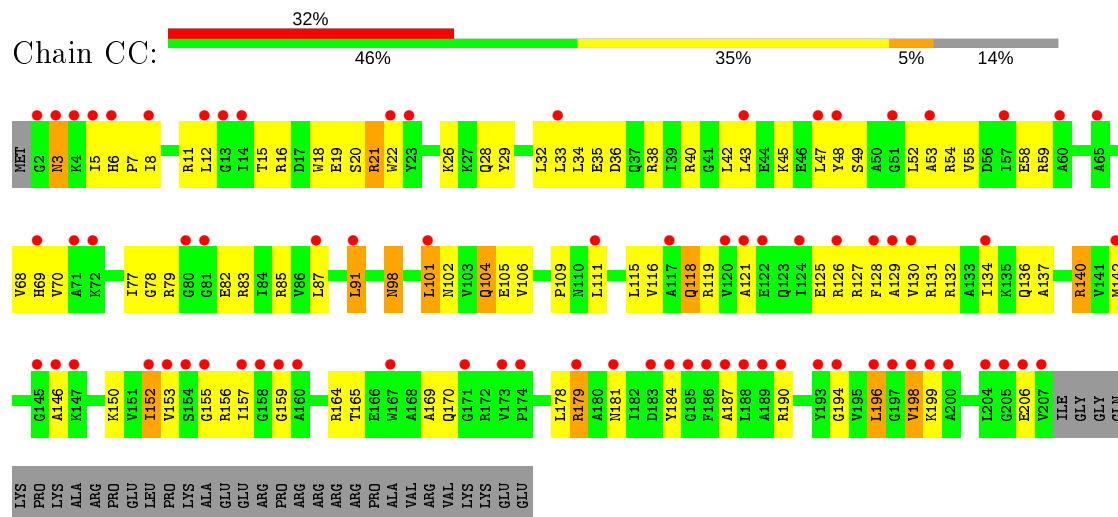
- Molecule 2: 30S ribosomal protein S2



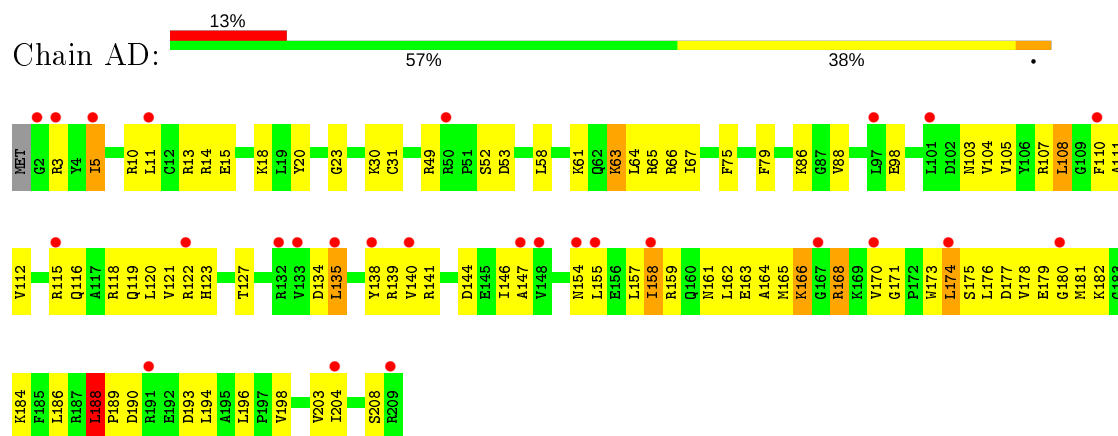
- Molecule 3: 30S ribosomal protein S3



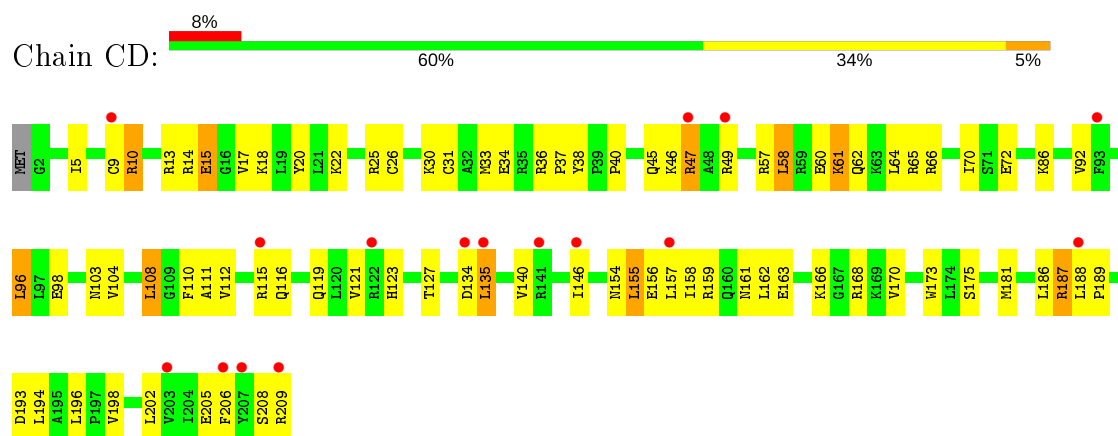
• Molecule 3: 30S ribosomal protein S3



• Molecule 4: 30S ribosomal protein S4

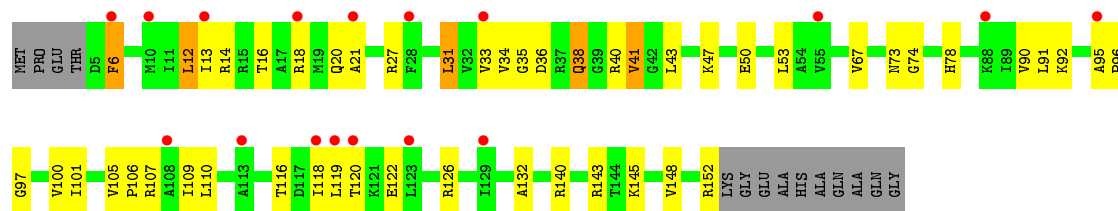


• Molecule 4: 30S ribosomal protein S4

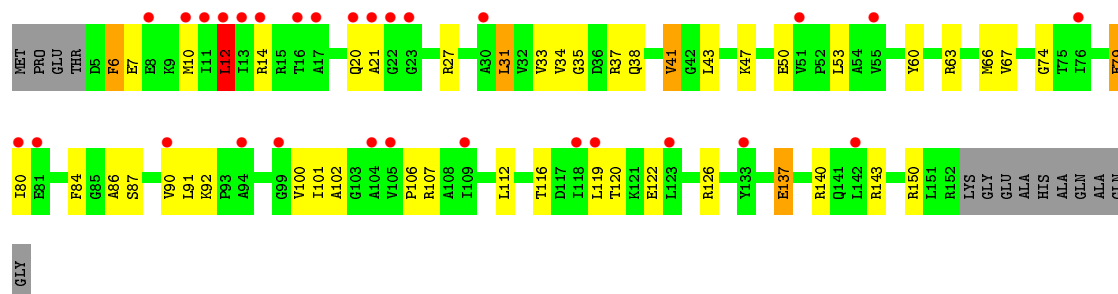


• Molecule 5: 30S ribosomal protein S5

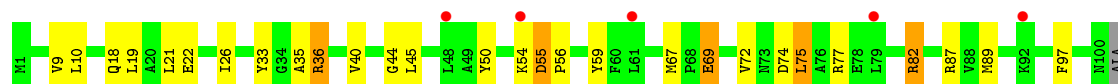
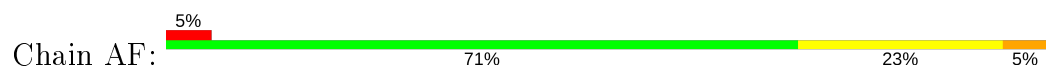




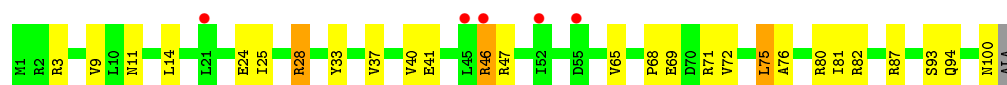
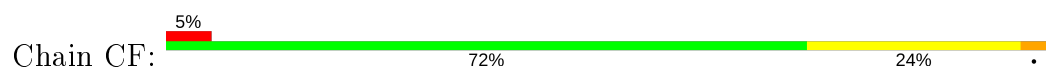
• Molecule 5: 30S ribosomal protein S5



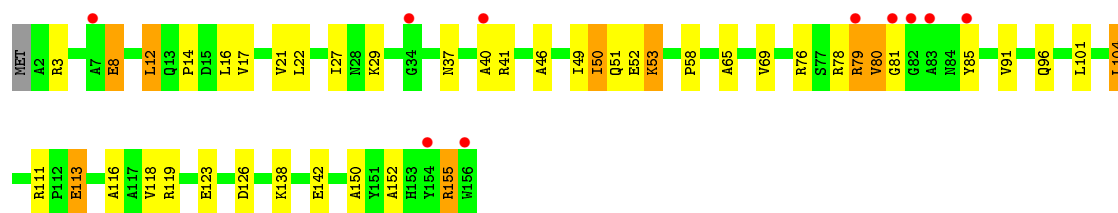
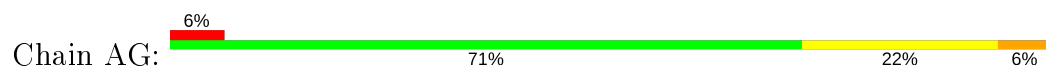
• Molecule 6: 30S ribosomal protein S6



• Molecule 6: 30S ribosomal protein S6

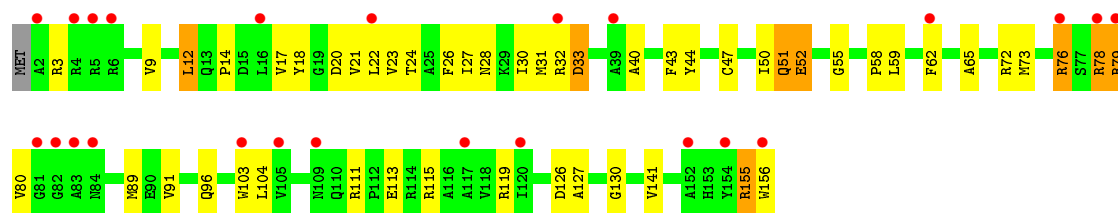


• Molecule 7: 30S ribosomal protein S7

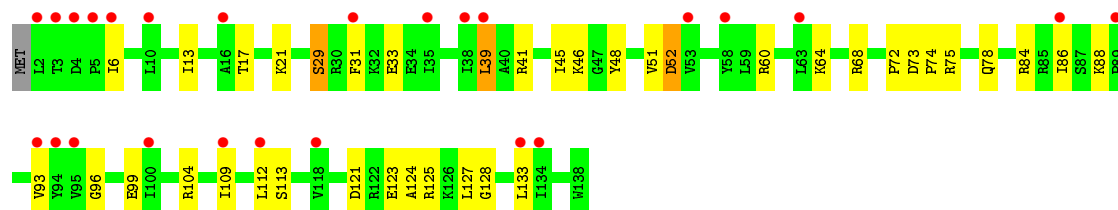
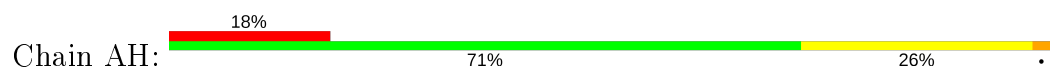


• Molecule 7: 30S ribosomal protein S7

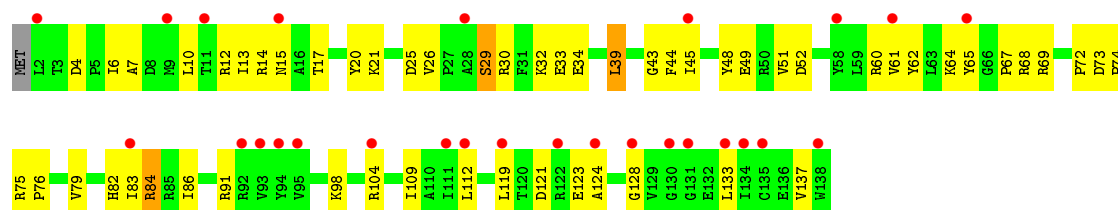




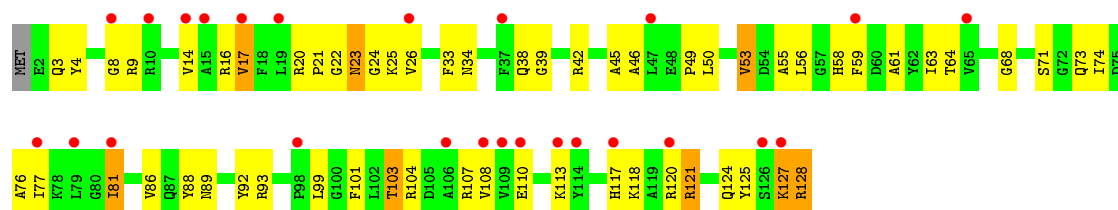
• Molecule 8: 30S ribosomal protein S8



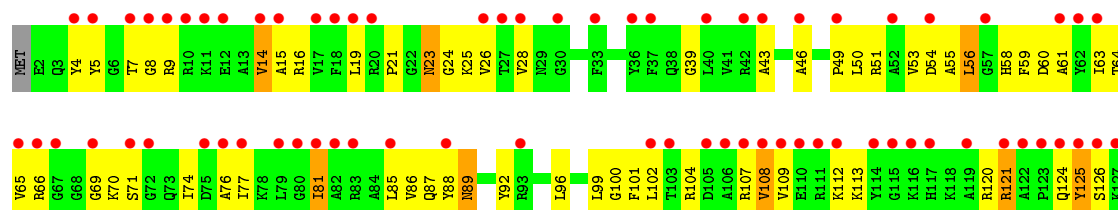
• Molecule 8: 30S ribosomal protein S8



• Molecule 9: 30S ribosomal protein S9

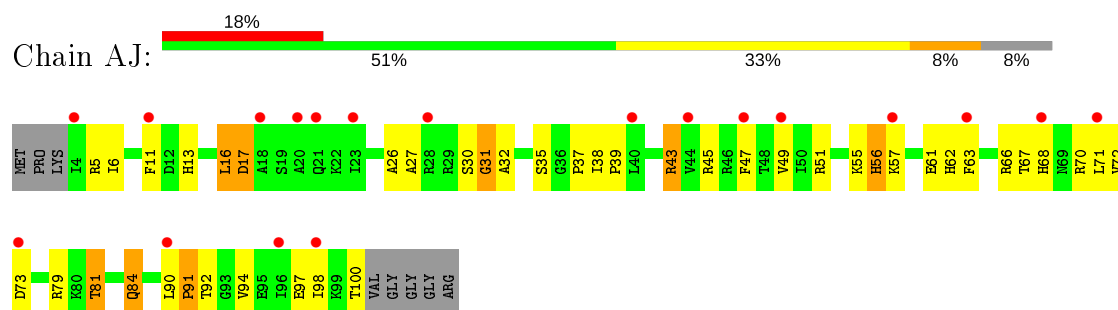


• Molecule 9: 30S ribosomal protein S9

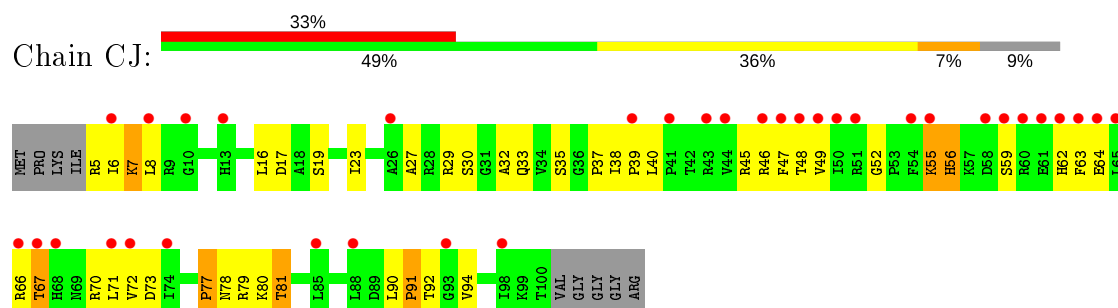




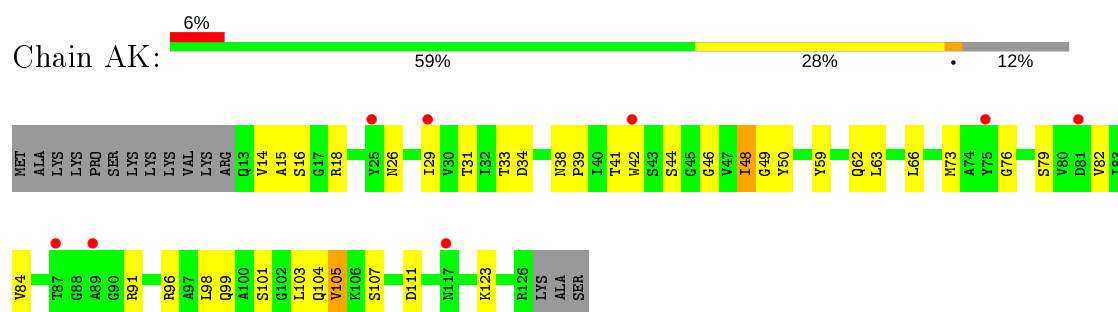
- Molecule 10: 30S ribosomal protein S10



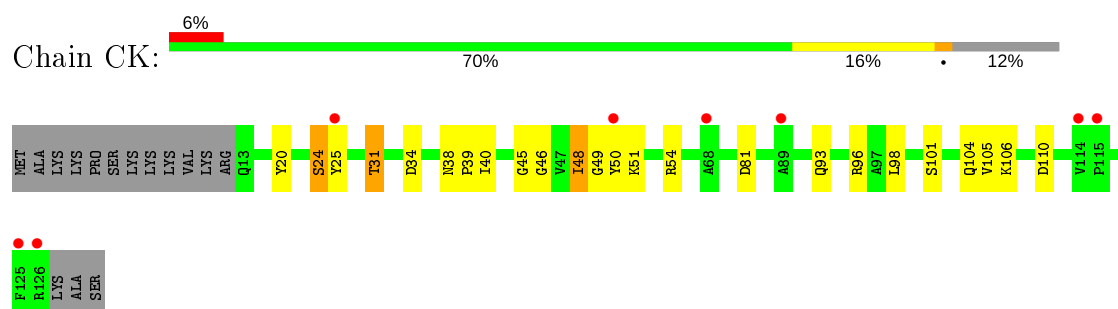
- Molecule 10: 30S ribosomal protein S10



- Molecule 11: 30S ribosomal protein S11

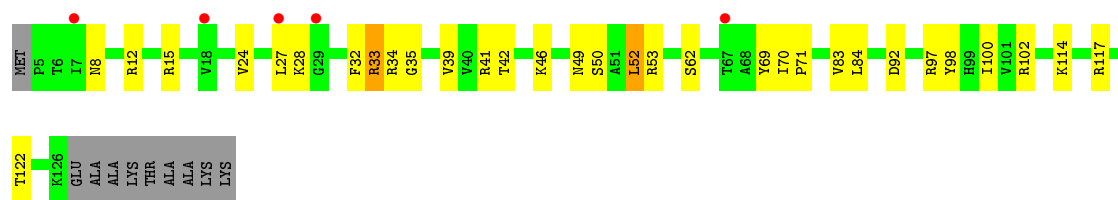


- Molecule 11: 30S ribosomal protein S11

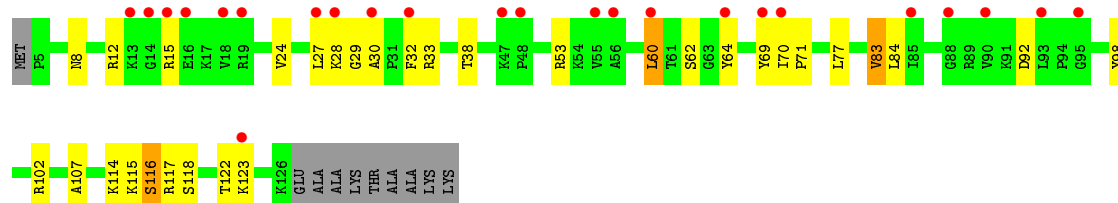


- Molecule 12: 30S ribosomal protein S12

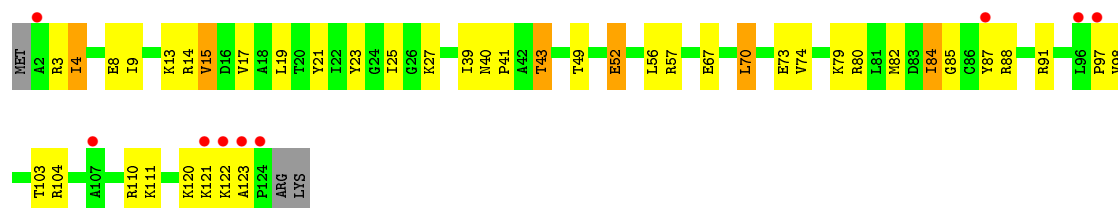




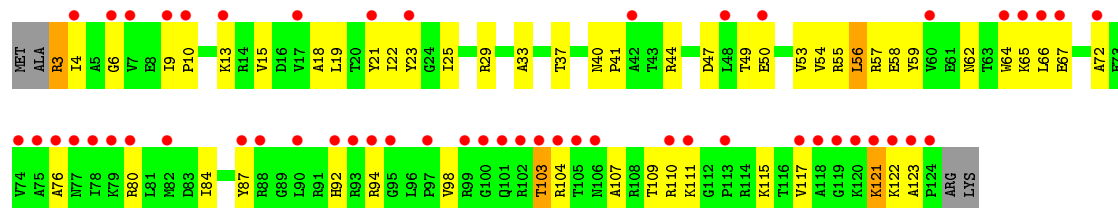
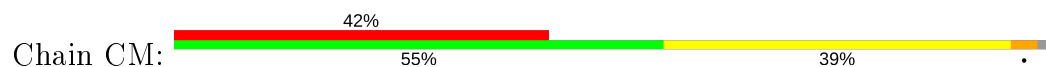
- Molecule 12: 30S ribosomal protein S12



- Molecule 13: 30S ribosomal protein S13



- Molecule 13: 30S ribosomal protein S13

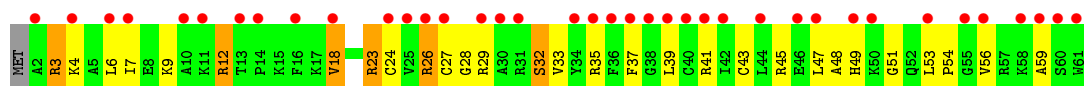


- Molecule 14: 30S ribosomal protein S14 type Z

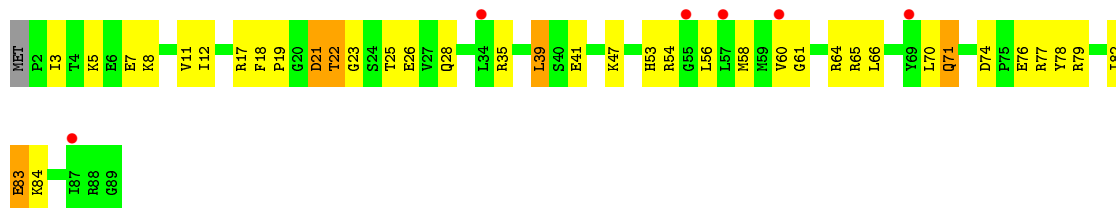


- Molecule 14: 30S ribosomal protein S14 type Z

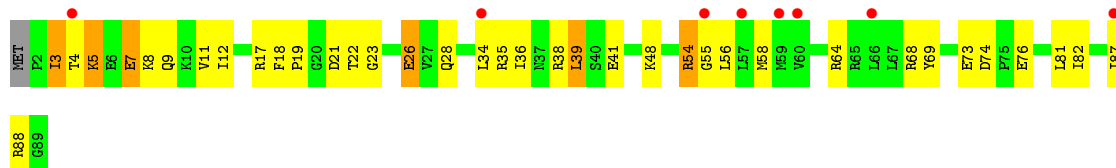




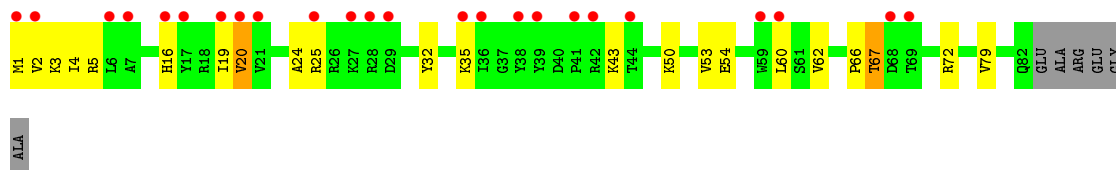
- Molecule 15: 30S ribosomal protein S15



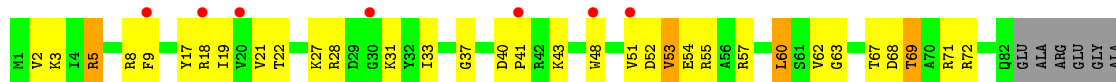
- Molecule 15: 30S ribosomal protein S15



- Molecule 16: 30S ribosomal protein S16

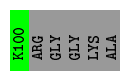


- Molecule 16: 30S ribosomal protein S16

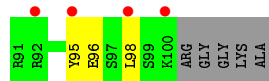
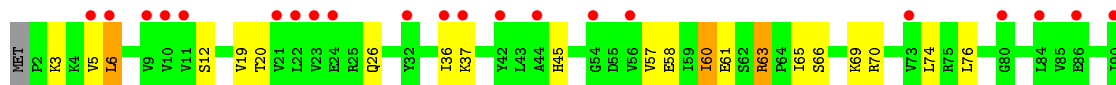
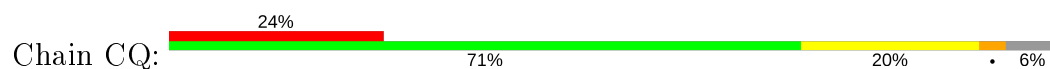


- Molecule 17: 30S ribosomal protein S17

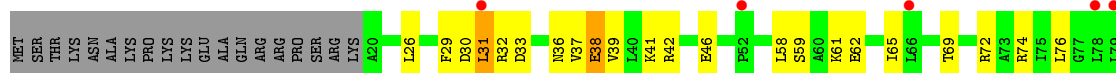




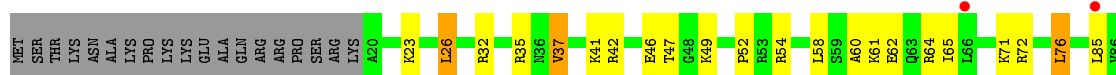
- Molecule 17: 30S ribosomal protein S17



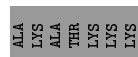
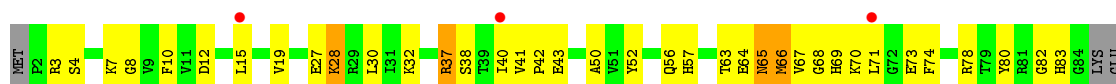
- Molecule 18: 30S ribosomal protein S18



- Molecule 18: 30S ribosomal protein S18

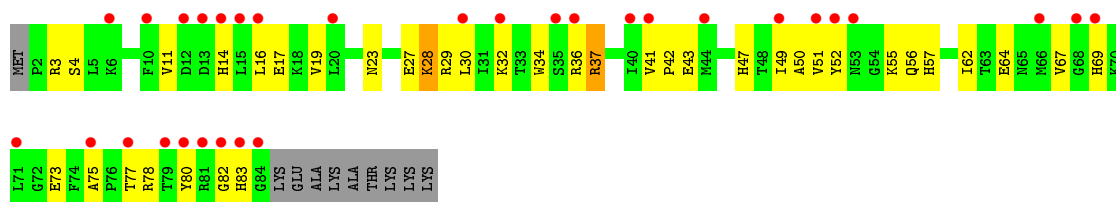


- Molecule 19: 30S ribosomal protein S19

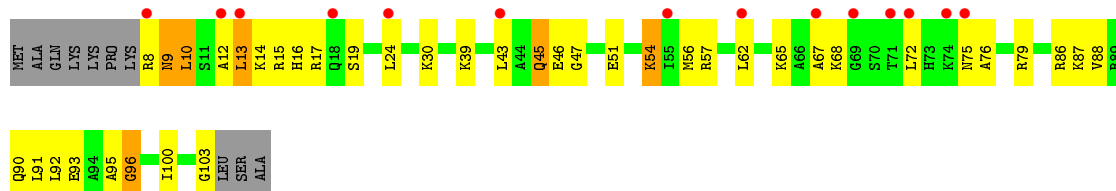


- Molecule 19: 30S ribosomal protein S19

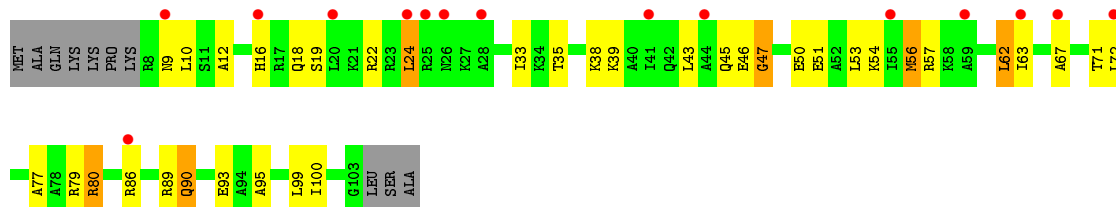




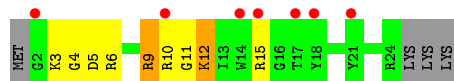
- Molecule 20: 30S ribosomal protein S20



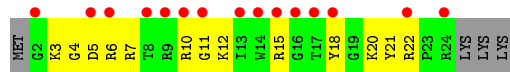
- Molecule 20: 30S ribosomal protein S20



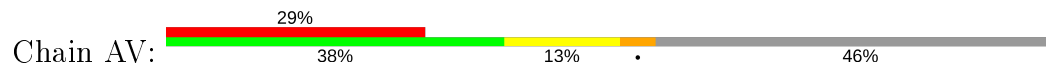
- Molecule 21: 30S ribosomal protein Thx



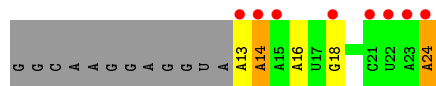
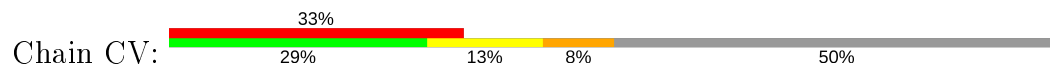
- Molecule 21: 30S ribosomal protein Thx



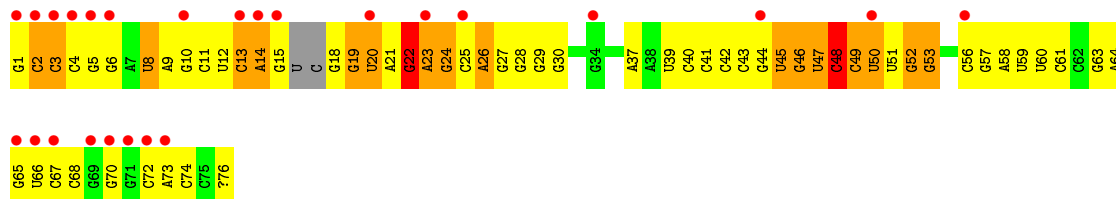
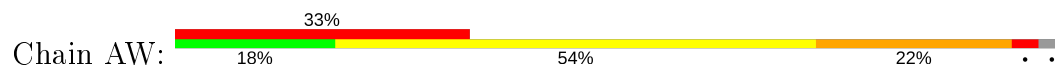
- Molecule 22: mRNA



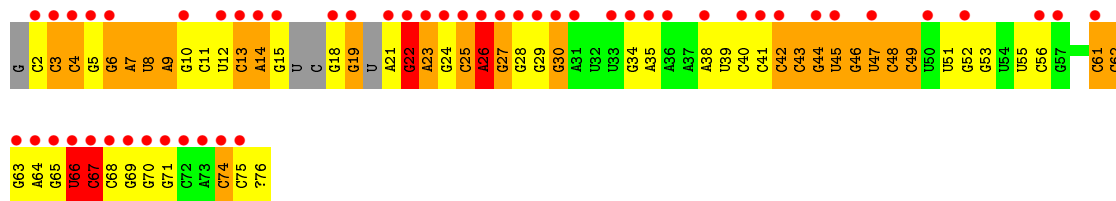
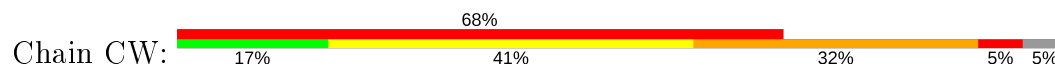
- Molecule 22: mRNA



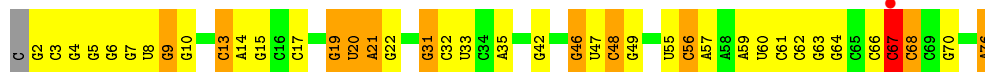
- Molecule 23: A-site tRNA



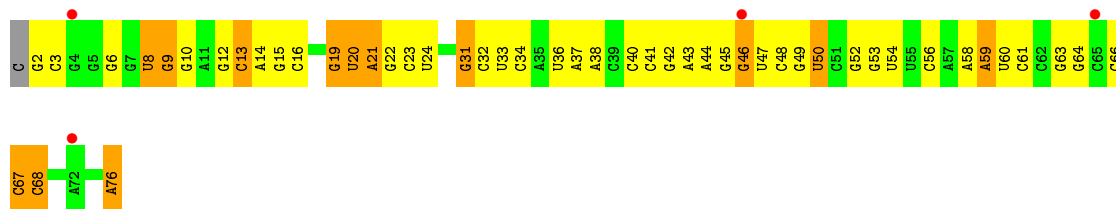
- Molecule 23: A-site tRNA



- Molecule 24: P-site tRNA

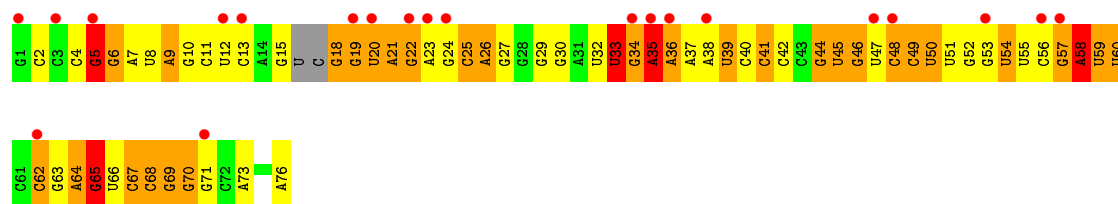


- Molecule 24: P-site tRNA

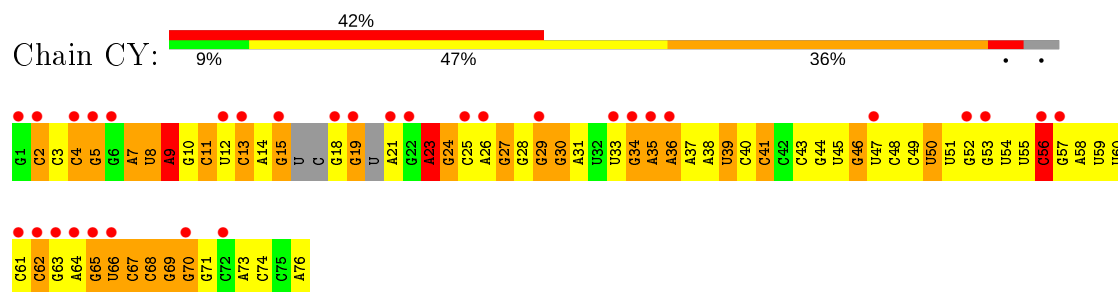


- Molecule 25: E-site tRNA

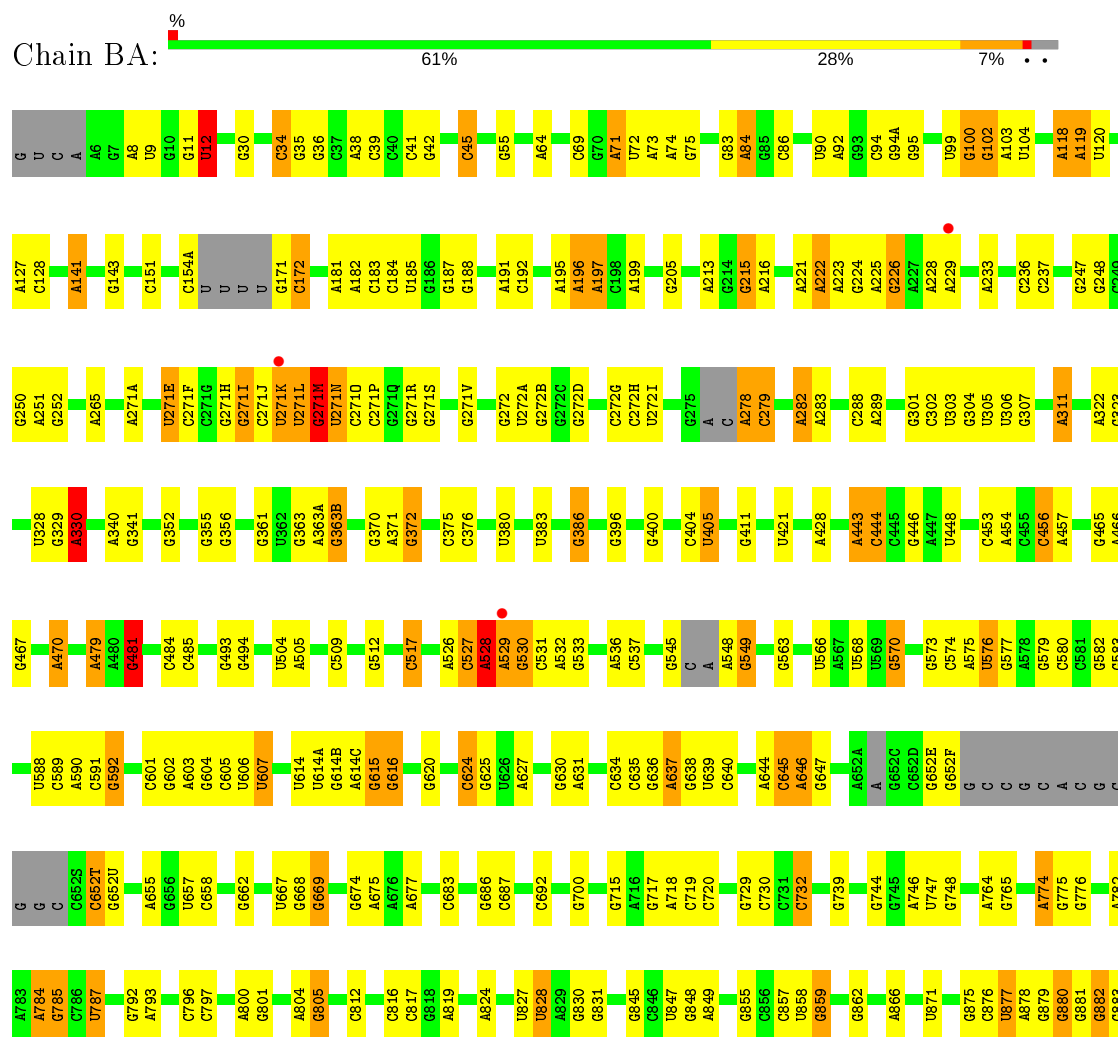




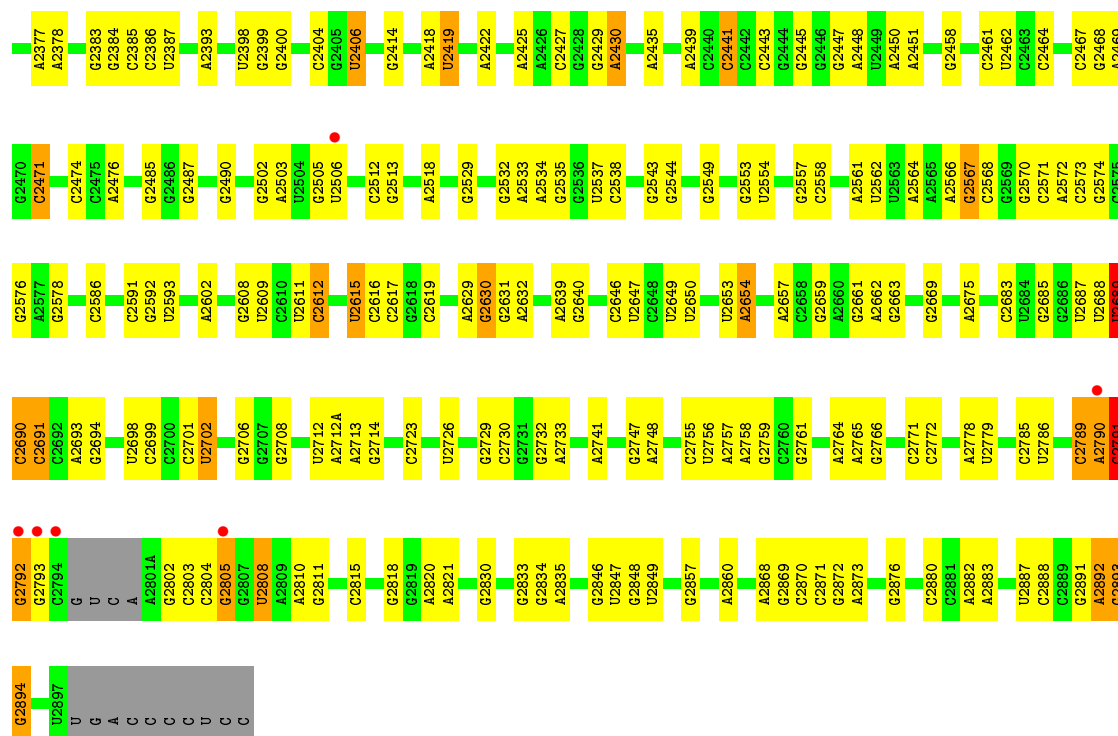
• Molecule 25: E-site tRNA



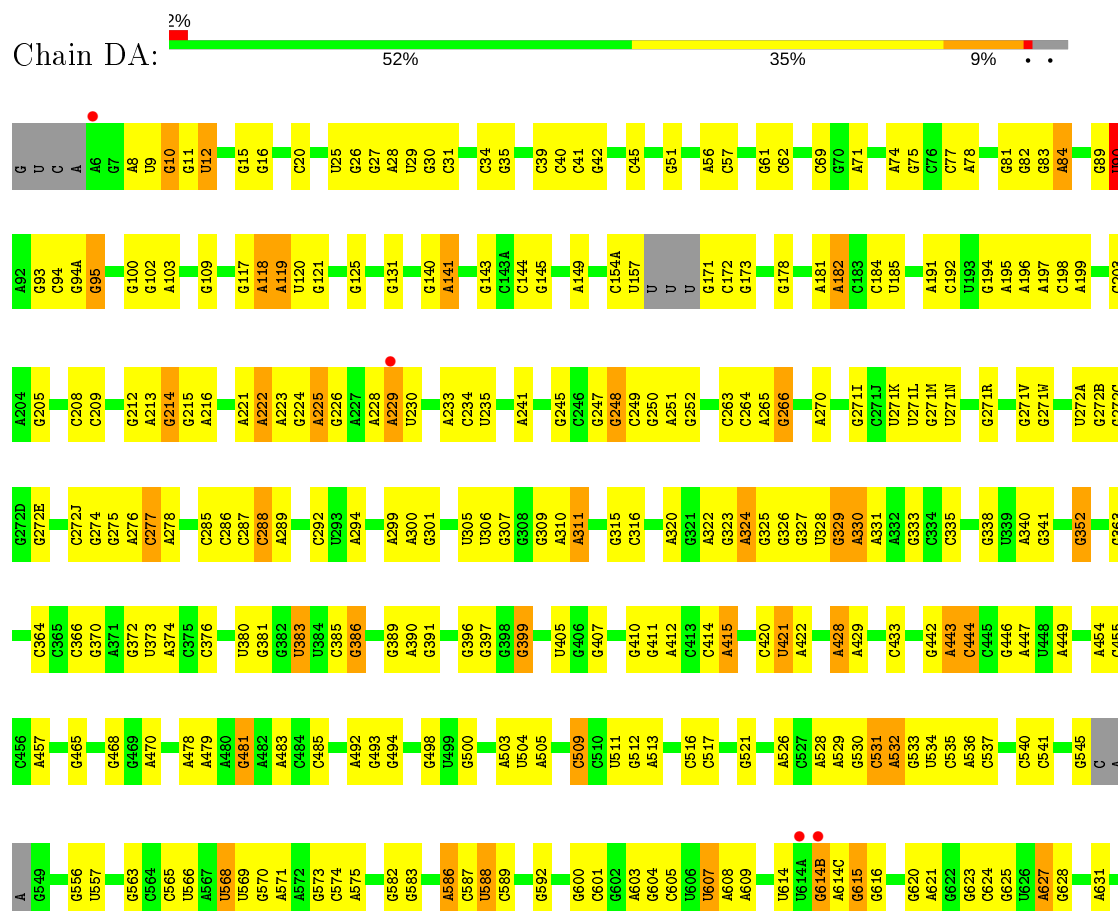
• Molecule 26: 23S Ribosomal RNA



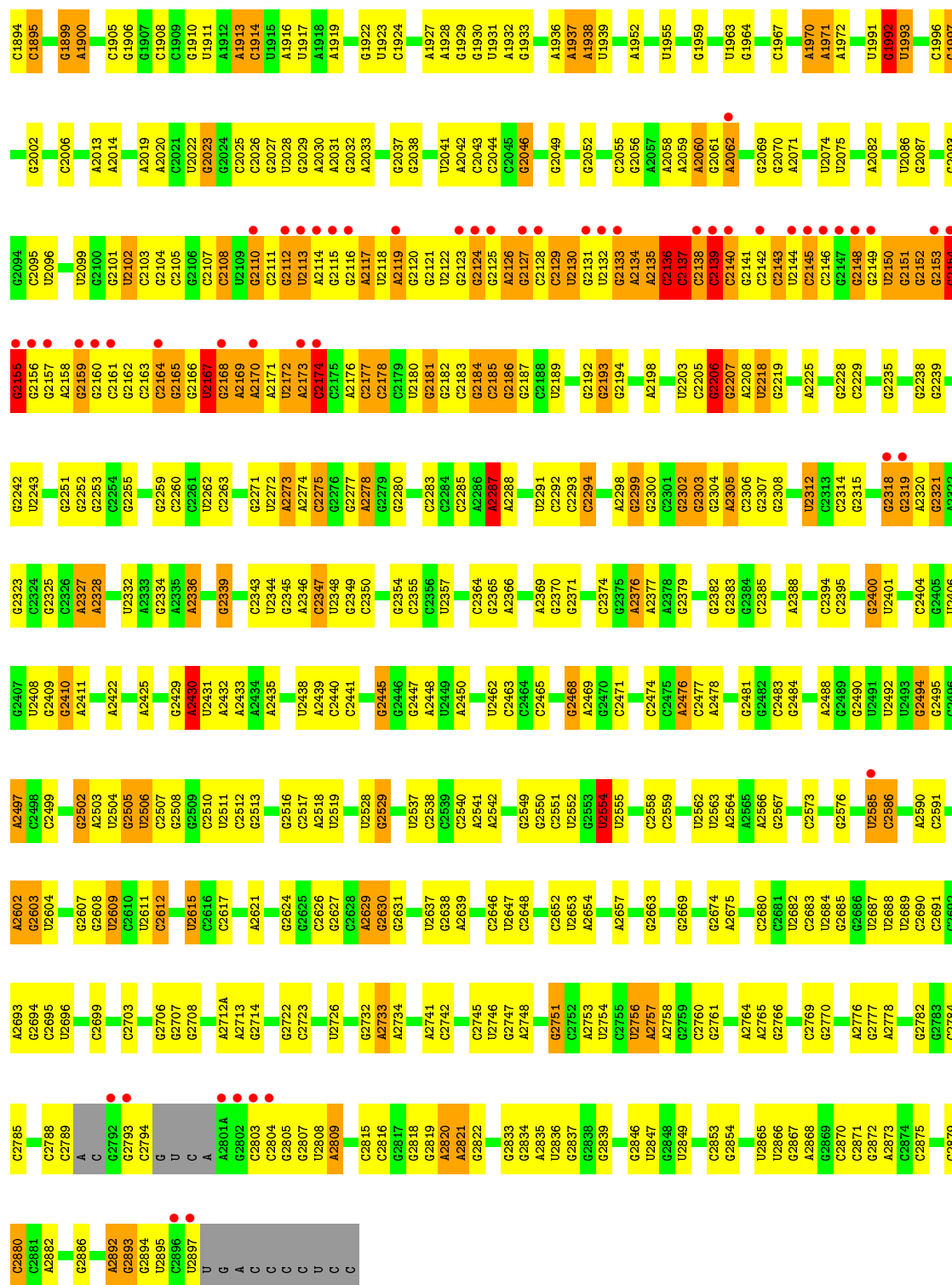
A2269	A2158	C1843	C1743	A1608	G1492	A1373	C1251	A1424	C884
A2274	G2159	A1847	C1745A	A1609	G1493	A1378	G1252	A1143	C885
C2275	C2160	A1848	G1746	A1610	A1494	A1379	A1253	G993	C886
G2276	G2161	A1849	G1747	A1611	A1495	G1380	G1256	C994	A887
G2277	C1996	U1851	G1748	A1612	A1496	A1381	G1257	C995	C888
A2278	G1997	G1858	A1749	G1630	C1506	A1384	C1258	A996	C889
G2282	A2001	A1859	G1750	G1631	A1507	G1385	G1259	C997	A890
C2283	G2010	G1860	G1751	A1631A	A1508	U1396	U1266	C998	C892
G2284	U2011	G1861	U1752	A1632	C1509	A1403	G1267	A1001	C893
C2285	G2012	G1862	A1753	G1633	A1509A	U1405	A1268	A1002	C894
A2170	A2013	A1876	A1754	A1634	U1512	U1406	C1269	A1009	A896
A2171	A2014	A1877	A1755	G1635	C1513	U1407	U1270	U1012	C897
A2172	A2015	A1878	A1756	A1636	C1514	C1408	U1271	U1013	C898
A2173	A2016	A1879	A1757	G1637	G1520	A1416	A1272	A1014	A899
A2174	A2017	A1880	A1758	A1638	G1521	C1417	A1273	C1013	A900
A2175	A2018	A1881	A1759	A1639	C1522	G1418	A1274	U1019	A901
A2176	A2019	A1882	A1760	A1640	C1523	C1419	U1275	A1020	U907
A2177	A2020	A1883	A1761	A1641	C1524	U1420	G1276	A1021	A910
A2178	A2021	A1884	A1762	A1642	C1525	U1421	C1277	A1022	A911
A2179	A2022	A1885	A1763	A1643	C1526	G1422	U1278	G1025	G916
A2180	A2023	A1886	A1764	A1644	C1527	G1423	U1279	U1026	C923
A2181	A2024	A1887	A1765	A1645	C1528	C1424	U1280	A1027	C924
A2182	A2025	A1888	A1766	A1646	C1529	U1425	A1278	A1028	G927
A2183	A2026	A1889	A1767	A1647	C1530	C1426	U1281	A1029	G928
A2184	A2027	A1890	A1768	A1648	C1531	U1427	U1282	A1030	U1033
A2185	A2028	A1891	A1769	A1649	C1532	U1428	U1283	A1031	C932
A2186	A2029	A1892	A1770	A1650	C1533	C1429	U1284	A1032	A933
A2187	A2030	A1893	A1771	A1651	C1534	U1430	U1285	A1033	A941
A2188	A2031	A1894	A1772	A1652	C1535	U1431	U1286	U1034	G944
A2189	A2032	A1895	A1773	A1653	C1536	U1432	U1287	A1035	A945
A2190	A2033	A1896	A1774	A1654	C1537	U1433	U1288	A1036	G946
A2191	A2034	A1897	A1775	A1655	C1538	U1434	U1289	A1037	G947
A2192	A2035	A1898	A1776	A1656	C1539	U1435	U1290	A1038	G948
A2193	A2036	A1899	A1777	A1657	C1540	U1436	U1291	A1039	G952
A2194	A2037	A1900	A1778	A1658	C1541	U1437	U1292	A1040	A953
A2195	A2038	A1901	A1779	A1659	C1542	U1438	U1293	A1041	G954
A2196	A2039	A1902	A1780	A1660	C1543	U1439	U1294	A1042	C955
A2197	A2040	A1903	A1781	A1661	C1544	U1440	U1295	A1043	G956
A2198	A2041	A1904	A1782	A1662	C1545	U1441	U1296	A1044	U958
A2199	A2042	A1905	A1783	A1663	C1546	U1442	U1297	A1045	A959
A2200	A2043	A1906	A1784	A1664	C1547	U1443	U1298	A1046	A960
A2201	A2044	A1907	A1785	A1665	C1548	U1444	U1299	A1047	C961
A2202	A2045	A1908	A1786	A1666	C1549	U1445	U1300	A1048	C970
A2203	A2046	A1909	A1787	A1667	C1550	U1446	U1301	A1049	C971
A2204	A2047	A1910	A1788	A1668	C1551	U1447	U1302	A1050	G972
A2205	A2048	A1911	A1789	A1669	C1552	U1448	U1303	A1051	A973
A2206	A2049	A1912	A1790	A1670	C1553	U1449	U1304	A1052	G974
A2207	A2050	A1913	A1791	A1671	C1554	U1450	U1305	A1053	C975
A2208	A2051	A1914	A1792	A1672	C1555	U1451	U1306	A1054	G
A2209	A2052	A1915	A1793	A1673	C1556	U1452	U1307	A1055	G
A2210	A2053	A1916	A1794	A1674	C1557	U1453	U1308	A1056	G
A2211	A2054	A1917	A1795	A1675	C1558	U1454	U1309	A1057	G
A2212	A2055	A1918	A1796	A1676	C1559	U1455	U1310	A1058	G
A2213	A2056	A1919	A1797	A1677	C1560	U1456	U1311	A1059	G
A2214	A2057	A1920	A1798	A1678	C1561	U1457	U1312	A1060	G
A2215	A2058	A1921	A1799	A1679	C1562	U1458	U1313	A1061	G
A2216	A2059	A1922	A1800	A1680	C1563	U1459	U1314	A1062	G
A2217	A2060	A1923	A1801	A1681	C1564	U1460	U1315	A1063	G
A2218	A2061	A1924	A1802	A1682	C1565	U1461	U1316	A1064	G
A2219	A2062	A1925	A1803	A1683	C1566	U1462	U1317	A1065	G
A2220	A2063	A1926	A1804	A1684	C1567	U1463	U1318	A1066	G
A2221	A2064	A1927	A1805	A1685	C1568	U1464	U1319	A1067	G
A2222	A2065	A1928	A1806	A1686	C1569	U1465	U1320	A1068	G
A2223	A2066	A1929	A1807	A1687	C1570	U1466	U1321	A1069	G
A2224	A2067	A1930	A1808	A1688	C1571	U1467	U1322	A1070	G
A2225	A2068	A1931	A1809	A1689	C1572	U1468	U1323	A1071	G
A2226	A2069	A1932	A1810	A1690	C1573	U1469	U1324	A1072	G
A2227	A2070	A1933	A1811	A1691	C1574	U1470	U1325	A1073	G
A2228	A2071	A1934	A1812	A1692	C1575	U1471	U1326	A1074	G
A2229	A2072	A1935	A1813	A1693	C1576	U1472	U1327	A1075	G
A2230	A2073	A1936	A1814	A1694	C1577	U1473	U1328	A1076	G
A2231	A2074	A1937	A1815	A1695	C1578	U1474	U1329	A1077	G
A2232	A2075	A1938	A1816	A1696	C1579	U1475	U1330	A1078	G
A2233	A2076	A1939	A1817	A1697	C1580	U1476	U1331	A1079	G
A2234	A2077	A1940	A1818	A1698	C1581	U1477	U1332	A1080	G
A2235	A2078	A1941	A1819	A1699	C1582	U1478	U1333	A1081	G
A2236	A2079	A1942	A1820	A1700	C1583	U1479	U1334	A1082	G
A2237	A2080	A1943	A1821	A1701	C1584	U1480	U1335	A1083	G
A2238	A2081	A1944	A1822	A1702	C1585	U1481	U1336	A1084	G
A2239	A2082	A1945	A1823	A1703	C1586	U1482	U1337	A1085	G
A2240	A2083	A1946	A1824	A1704	C1587	U1483	U1338	A1086	G
A2241	A2084	A1947	A1825	A1705	C1588	U1484	U1339	A1087	G
A2242	A2085	A1948	A1826	A1706	C1589	U1485	U1340	A1088	G
A2243	A2086	A1949	A1827	A1707	C1590	U1486	U1341	A1089	G
A2244	A2087	A1950	A1828	A1708	C1591	U1487	U1342	A1090	G
A2245	A2088	A1951	A1829	A1709	C1592	U1488	U1343	A1091	G
A2246	A2089	A1952	A1830	A1710	C1593	U1489	U1344	A1092	G
A2247	A2090	A1953	A1831	A1711	C1594	U1490	U1345	A1093	G
A2248	A2091	A1954	A1832	A1712	C1595	U1491	U1346	A1094	G
A2249	A2092	A1955	A1833	A1713	C1596	U1492	U1347	A1095	G
A2250	A2093	A1956	A1834	A1714	C1597	U1493	U1348	A1096	G
A2251	A2094	A1957	A1835	A1715	C1598	U1494	U1349	A1097	G
A2252	A2095	A1958	A1836	A1716	C1599	U1495	U1350	A1098	G
A2253	A2096	A1959	A1837	A1717	C1600	U1496	U1351	A1099	G
A2254	A2097	A1960	A1838	A1718	C1601	U1497	U1352	A1100	G
A2255	A2098	A1961	A1839	A1719	C1602	U1498	U1353	A1101	G
A2256	A2099	A1962	A1840	A1720	C1603	U1499	U1354	A1102	G
A2257	A2100	A1963	A1841	A1721	C1604	U1500	U1355	A1103	G
A2258	A2101	A1964	A1842	A1722	C1605	U1501	U1356	A1104	G
A2259	A2102	A1965	A1843	A1723	C1606	U1502	U1357	A1105	G
A2260	A2103	A1966	A1844	A1724	C1607	U1503	U1358	A1106	G
A2261	A2104	A1967	A1845	A1725	C1608	U1504	U1359	A1107	G
A2262	A2105	A1968	A1846	A1726	C1609	U1505	U1360	A1108	G
A2263	A2106	A1969	A1847	A1727	C1610	U1506	U1361	A1109	G
A2264	A2107	A1970	A1848	A1728	C1611	U1507	U1362	A1110	G
A2265	A2108	A1971	A1849	A1729	C1612	U1508	U1363	A1111	G
A2266	A2109	A1972	A1850	A1730	C1613	U1509	U1364	A1112	G
A2267	A2110	A1973	A1851	A1731	C1614	U1510	U1365	A1113	G
A2268	A2111	A1974	A1852	A1732	C1615	U1511	U1366	A1114	G
A2269	A2112	A1975	A1853	A1733	C1616	U1512	U1367	A1115	G
A2270	A2113	A1976	A1854	A1734	C1617	U1513	U1368	A1116	G
A2271	A2114	A1977	A1855	A1735	C1618	U1514	U1369	A1117	G
A2272	A2115	A1978	A1856	A1736	C1619	U1515	U1370	A1118	G
A2273	A2116	A1979	A1857	A1737	C1620	U1516	U1371	A1119	G
A2274	A2117	A1980	A1858	A1738	C1621	U1517	U1372	A1120	G
A2275	A2118	A1981	A1859	A1739	C1622	U1518	U1373	A1121	G
A2276	A2119	A1982	A1860	A1740	C1623	U1519	U1374	A1122	G
A2277	A2120	A1983	A1861	A1741	C1624	U1520	U1375	A1123	G
A2278	A2121	A1984	A1862	A1742	C1625	U1521	U1376	A1124	G
A2279	A2122	A1985	A1863	A1743	C1626	U1522	U1377	A1125	G
A2280	A2123	A1986	A1864	A1744	C1627	U1523	U1378	A1126	G
A2281	A2124	A1987	A1865	A1745	C1628	U1524	U1379	A1127	G
A2282	A2125	A1988	A1866	A1746	C1629	U1525	U1380	A1128	G
A2283	A2126	A1989	A1867	A1747	C1630	U1526	U1381	A1129	G
A2284	A2127	A1990	A1868	A1748	C1631	U1527	U1382	A1130	G
A2285	A2128	A1991	A1869	A1749	C1632	U1528	U1383	A1131	G
A2286	A2129	A1992	A1870	A1750	C1633	U1529	U1384	A1132	G
A2287	A2130	A1993	A1871	A1751	C1634	U1530	U1385	A1133	G
A2288	A2131	A1994	A1872	A1752	C1635	U1531	U1386	A1134	G
A2289	A2132	A1995	A1873	A1753	C1636	U1532	U1387	A1135	G
A2290	A2133	A1996	A1874	A1754	C1637	U1533	U1388	A1136	G
A2291	A2134	A1997	A1875	A1755	C1638	U1534	U1389	A1137</	



• Molecule 26: 23S Ribosomal RNA

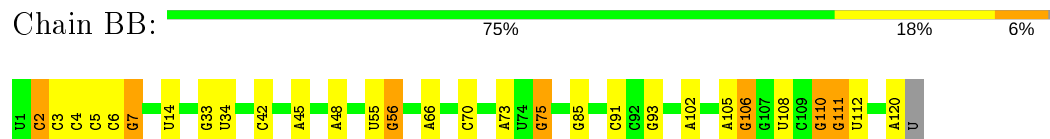


U1794	C1653	C1543	A1471	C1370	U1283	G1179	C	G1042	G966	A887	G809	C721	A837
C1795	A1654	A1544	A1472	G1371	G1284	G1180	A	C1043	C967	C888	G809	C721	G638
U1796	A1655	A1545	G1473	U1372	A1285	G1181	C	G	C971	A890	U810	U724	U639
C1797	C1656	C1546	G1473	G1372	G1286	G1183	U	A	C971	A891	U811	U725	C640
U1798	C1657	C1547	A1477	A1378	U1287	G1184	G	G	G974	C883	U813	G726	G641
G1799	A1658	A1554	G1478	A1379	C1288	C1185	U	A	C975	C894	C816	A643	G642
C1800	A1659	A1555	G1482	G1380	A1278	G1196	C	C	A983	U895	C817	A644	C645
A1801	A1660	A1556	G1484	A1381	A1279	G1197	A	C	A984	A896	C818	A645	C646
A1802	C1670	A1557	G1485	G1382	G1270	U1188	C	C	A985	C897	C819	A646	C647
A1803	A1671	A1558	A1486	A1383	U1271	A1189	U	A	G987	A898	A820	A734	G647
C1804	C1672	A1559	G1487	U1394	U1272	G1196	C	C	A988	A899	A821	G648	G649
U1805	G1673	A1560	G1488	A1395	A1278	G1197	A	C	G989	A900	A821	G649	G649
A1809	G1674	A1561	U1489	A1396	A1279	U1198	C	C	A990	A901	U740	A652B	A652B
A1812	U1688	C1575	A1490	C1399	G1283	U1199	G	G	C991	C902	U827	G652C	G652C
A1815	A1689	U1576	G1491	A1405	A1284	U1200	A	A	C992	C903	U828	C652D	C652D
C1817	C1693	C1493	C1493	U1406	G1285	G1201	G	G	C993	C904	G744	G745	G652E
G1816	U1696	A1494	A1494	A1406	A1286	G1202	G	G	C994	A910	G830	G746	G
G1817	G1697	A1495	U1497	G1410	U1287	A1203	U	U	C995	A911	G831	G747	G
C1835	A1698	A1580	C1498	C1411	U1288	U1205	G	G	A996	C912	G832	G748	C
C1836	G1699	A1581	U1499	A1412	U1289	G1209	C	C	C998	U839	G833	G749	C
C1837	A1700	A1582	U1503	U1415	U1290	A1210	U	U	C999	C914	U839	A752	C
C1838	G1703	A1583	C1504	G1416	U1291	U1211	U	U	A1000	A917	C840	C754	A
G1839	U1720	A1584	A1507	C1417	U1300	U1212	A	A	G1002	A918	G848	C755	C
C1842	C1721	G1593	A1508	G1418	A1301	G1219	G	G	C1005	G921	U851	G760	C
A1722	A1722	C1594	A1509	U1419	A1302	A1220	A	A	C1006	G922	G852	A761	G
U1739	U1596	G1595	A1509A	G1421	C1304	C1221	G	G	C1007	C923	G853	U762	G
A1847	A1597	A1597	U1512	G1422	G1305	G1222	C	C	C1008	G927	G854	G763	C
A1848	C1598	C1598	C1513	G1423	G1306	G1223	A	A	G1011	G928	C855	A764	C
U1851	C1604	C1604	U1514	A1427	G1310	U1224	G	G	C1012	G929	C856	G765	C652T
A1853	A1608	A1608	U1515	G1428	U1313	G1225	C	C	C1013	G932	C857	G770	G652U
A1854	A1609	A1609	G1519	G1429	C1314	U1226	A	A	U1014	G933	U858	A774	A655
G1857	C1611	C1611	U1520	G1430	C1315	G1229	U	U	G1015	A934	U860	A775	G656
C1858	C1612	C1612	G1523	U1431	G1316	C1230	C	C	G1016	G937	A861	G776	U657
U1865	G1626	G1626	G1524	A1434	G1317	G1231	U	U	C1017	U937	G862	G777	C658
C1866	G1627	G1627	G1525	C1437	C1327	G1232	U	U	C1018	G938	A863	G778	G659
A1876	G1630	G1630	G1526	A1445	A1336	G1235	A	A	A1020	A941	G864	A782	G662
A1877	C1631	C1631	A1528A	C1446	G1337	G1236	U	U	A1021	G942	C865	A783	G668
G1878	G1635	G1635	C1531	G1447	U1352	U1240	G	G	U1022	U943	A866	A784	G669
U1779	C1636	C1636	A1449	A1448	U1353	A1241	A	A	G1023	G944	U868	G785	G668
A1780	A1637	A1637	G1450	G1450	A1354	A1242	U	U	G1024	G945	G869	G786	G669
C1781	U	U	G1459	U1359	A1354	A1243	C	C	U1025	G946	A870	A788	G674
C1782	A	A	G1459	A1360	A1354	A1244	G	G	U1026	G950	G874	C791	G686
A1884	C1536	C1536	C1463	A1360	A1354	A1245	C	C	A1027	C951	G875	G792	C692
C1886	G1537	G1537	C1464	A1360	A1354	A1246	G	G	A1032	G952	A878	G793	C698
A1887	G1538	G1538	C1465	A1360	A1354	A1247	U	U	U1033	G953	G879	G794	G699
A1887	G1539	G1539	G1466	A1360	A1354	A1248	A	A	G1034	G954	G880	C795	A699
G1888	U1540	U1540	C1467	A1360	A1354	A1249	U	U	U1035	A957	G881	C797	G700
A1889	C1648	C1648	C1467	A1360	A1354	A1250	A	A	G1036	U958	G882	G798	U709
A1890	A1791	A1791	C1467	A1360	A1354	A1251	C	C	G1037	A959	G883	U803	U710
									G1038	C961	C884	A804	G715
									G1039		C886	G805	

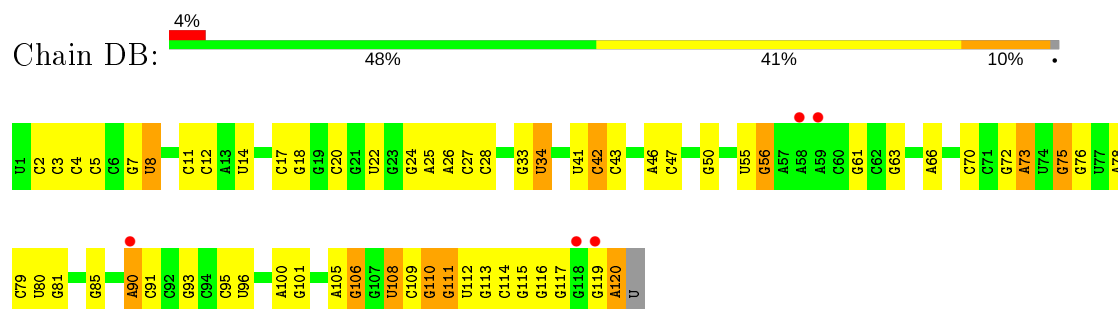


- Molecule 27: 5S Ribosomal RNA

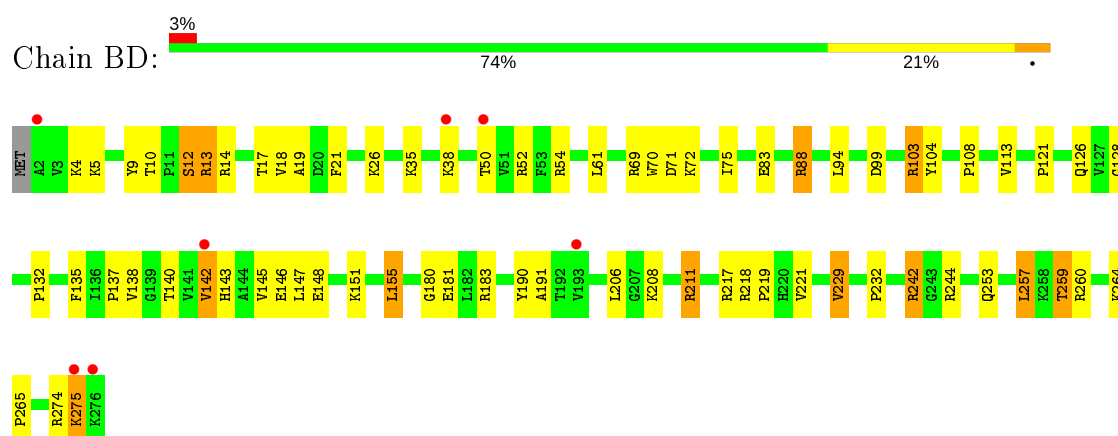
Chain BB:



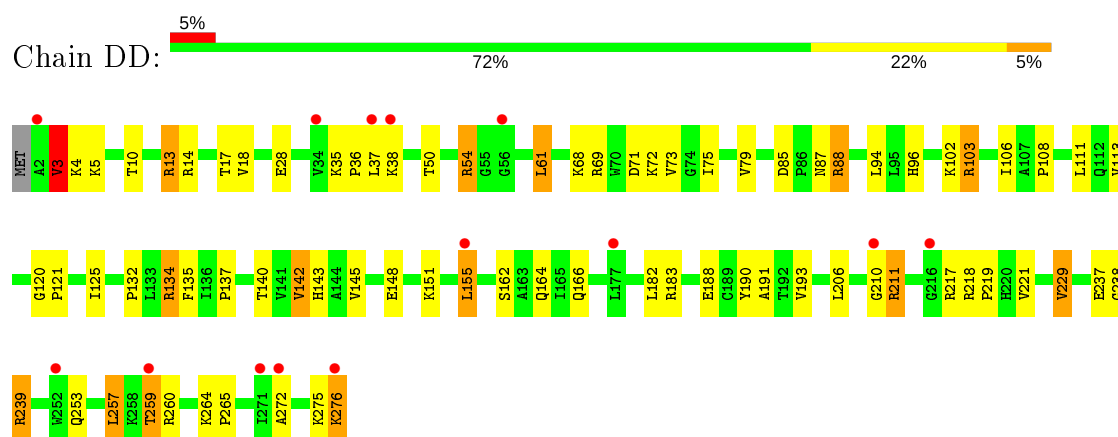
- Molecule 27: 5S Ribosomal RNA



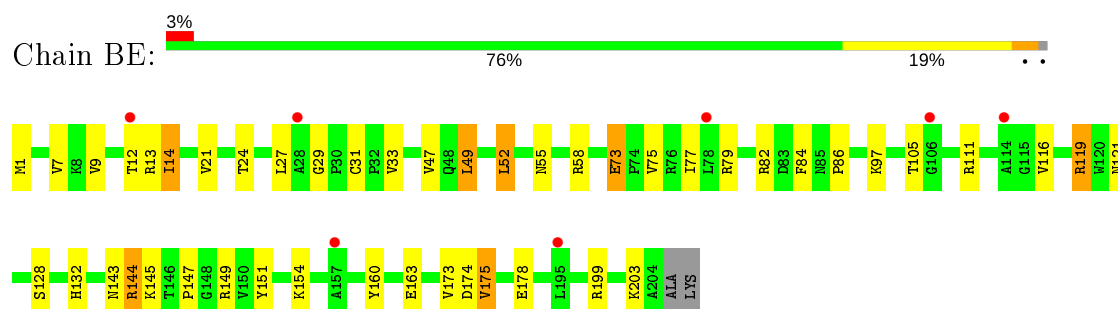
- Molecule 28: 50S ribosomal protein L2



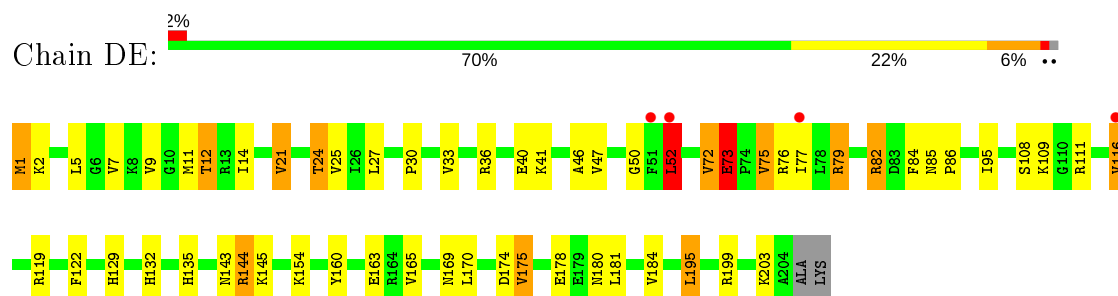
- Molecule 28: 50S ribosomal protein L2



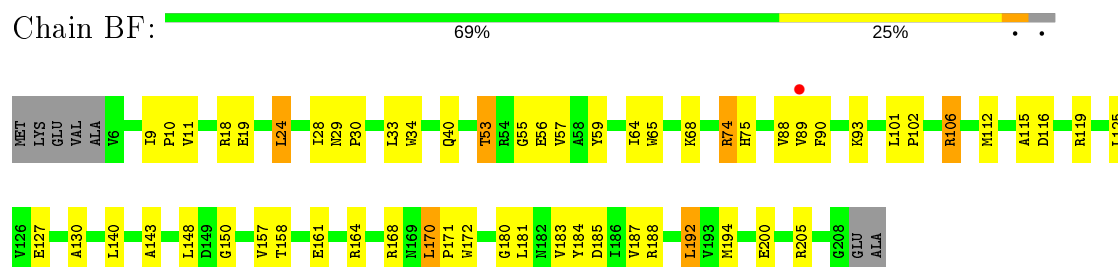
- Molecule 29: 50S ribosomal protein L3



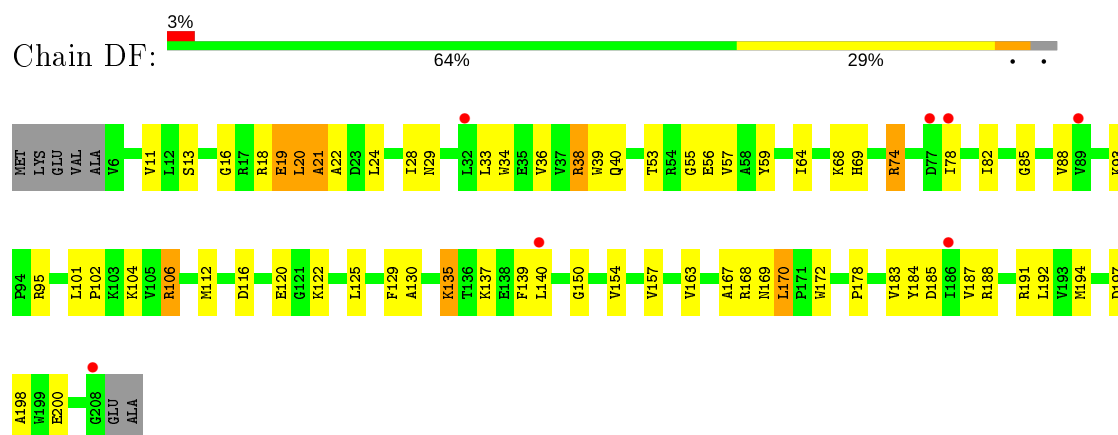
- Molecule 29: 50S ribosomal protein L3



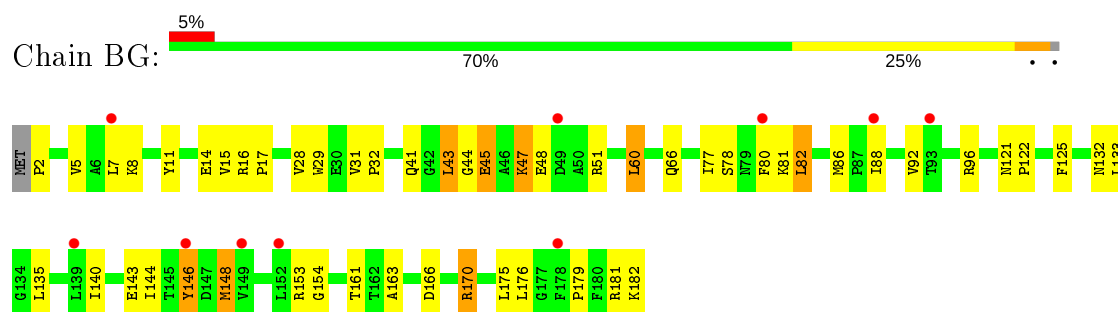
- Molecule 30: 50S ribosomal protein L4



- Molecule 30: 50S ribosomal protein L4

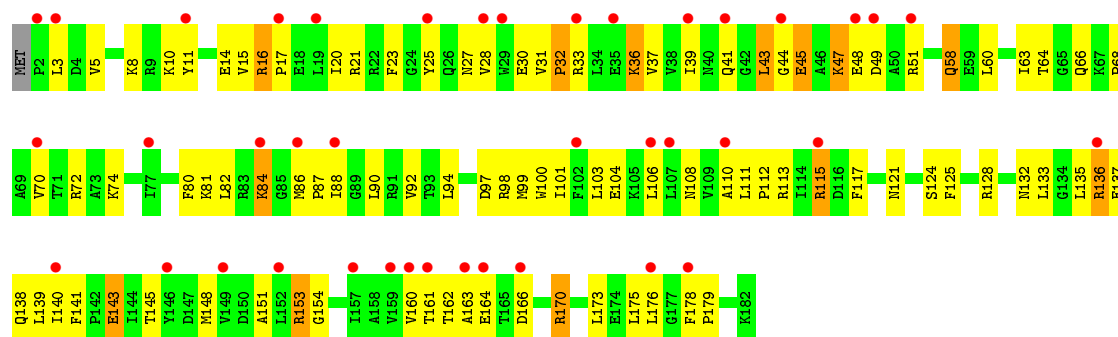


- Molecule 31: 50S ribosomal protein L5

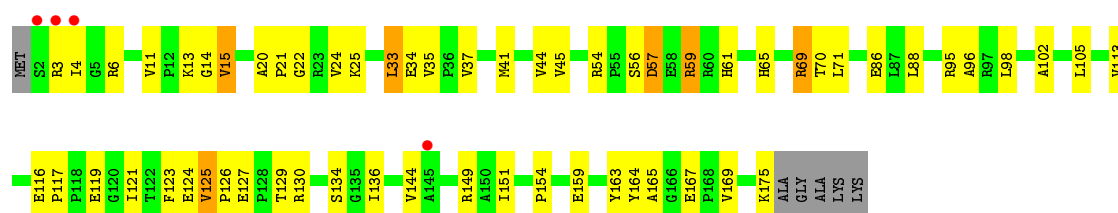


- Molecule 31: 50S ribosomal protein L5

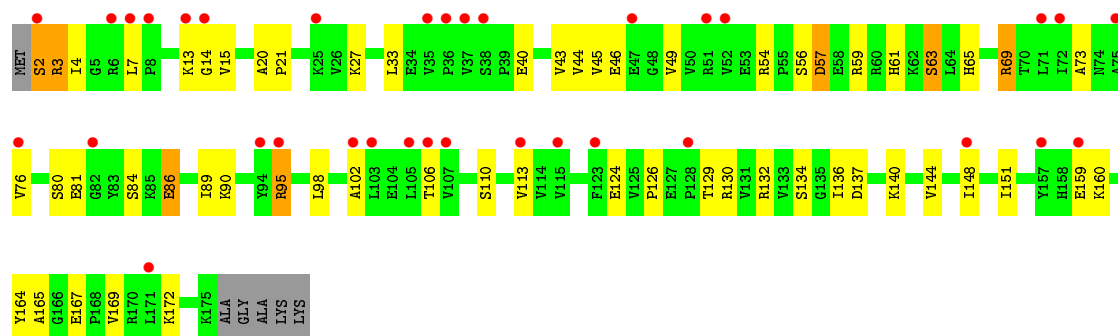




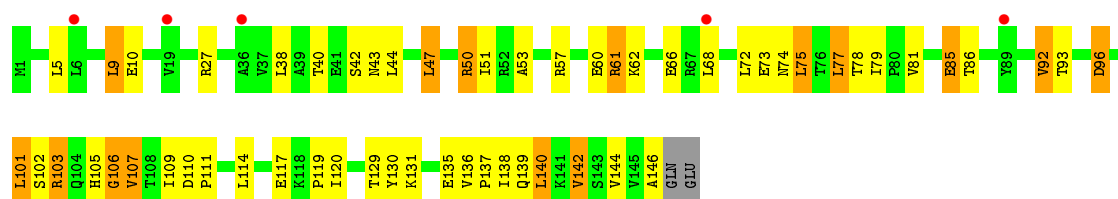
- Molecule 32: 50S ribosomal protein L6



- Molecule 32: 50S ribosomal protein L6

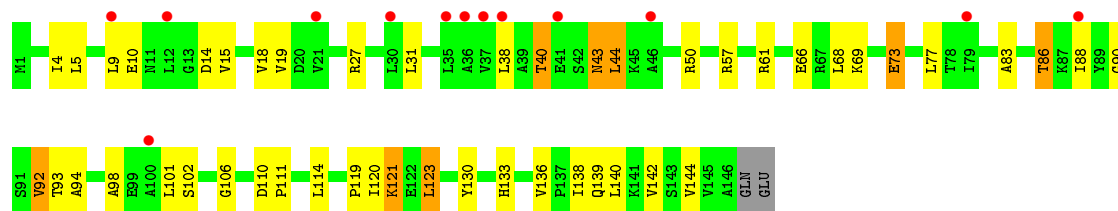


- Molecule 33: 50S ribosomal protein L9

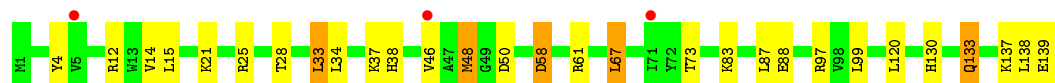
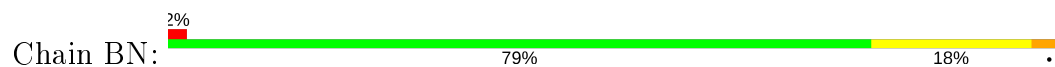


- Molecule 33: 50S ribosomal protein L9

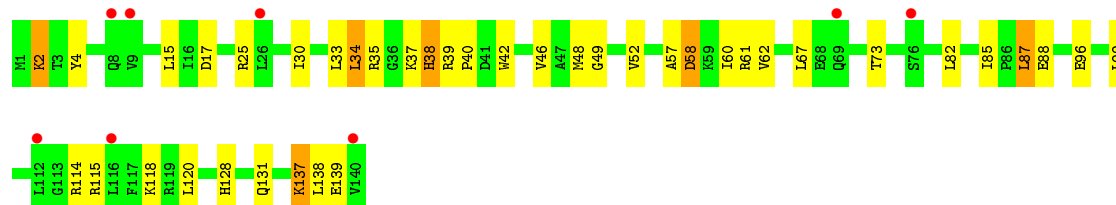
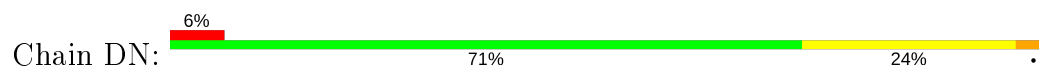




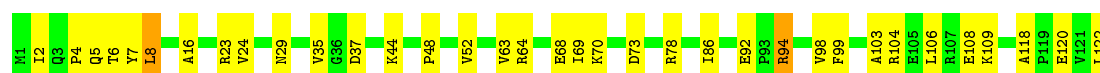
- Molecule 34: 50S ribosomal protein L13



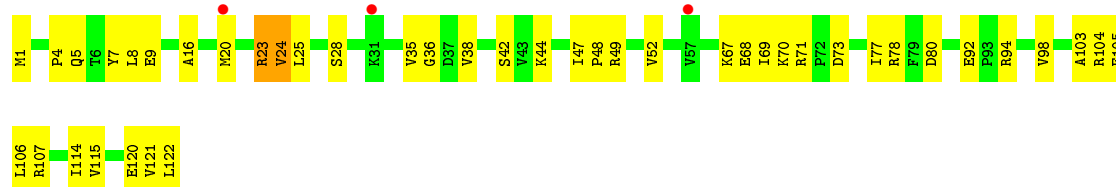
- Molecule 34: 50S ribosomal protein L13



- Molecule 35: 50S ribosomal protein L14



- Molecule 35: 50S ribosomal protein L14

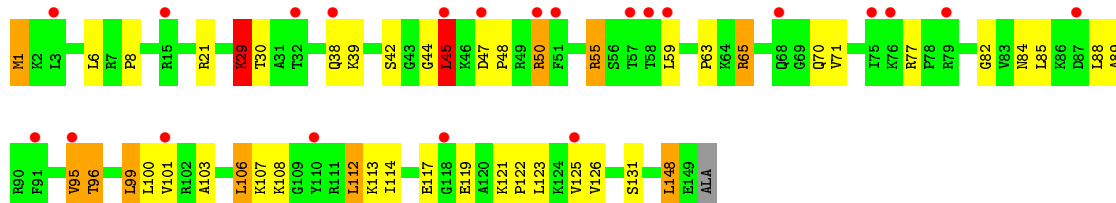


- Molecule 36: 50S ribosomal protein L15

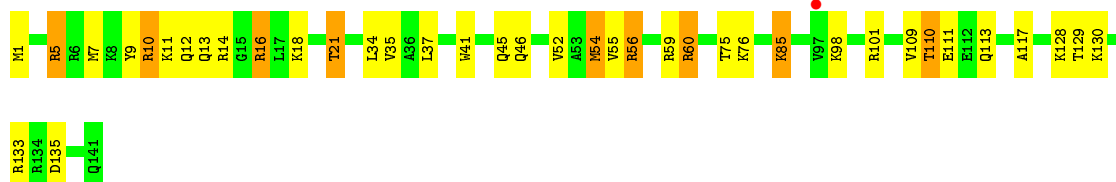
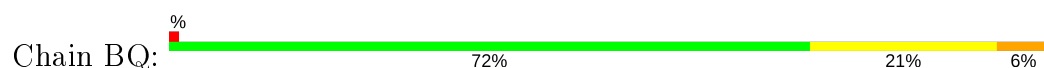




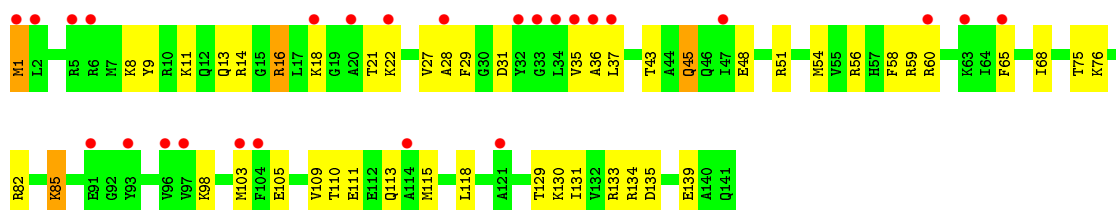
- Molecule 36: 50S ribosomal protein L15



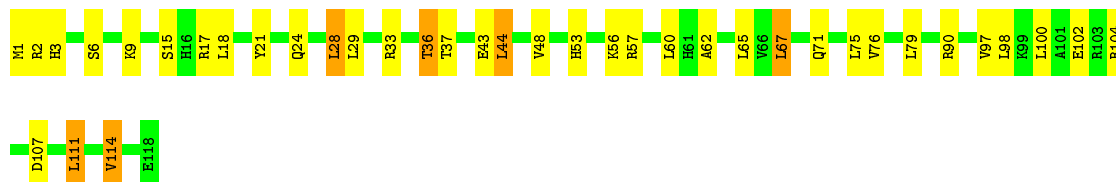
- Molecule 37: 50S ribosomal protein L16



- Molecule 37: 50S ribosomal protein L16

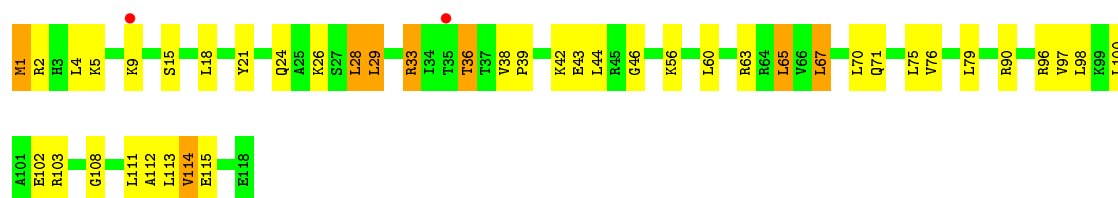


- Molecule 38: 50S ribosomal protein L17



- Molecule 38: 50S ribosomal protein L17

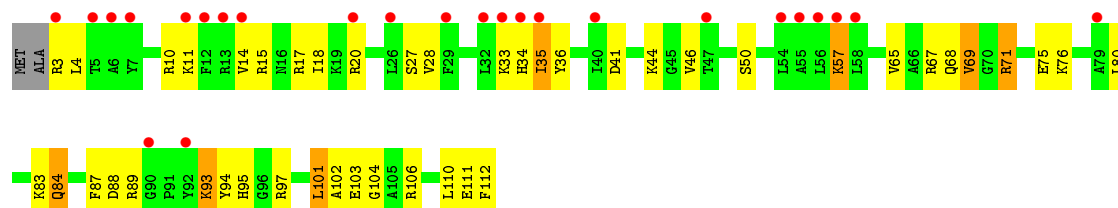




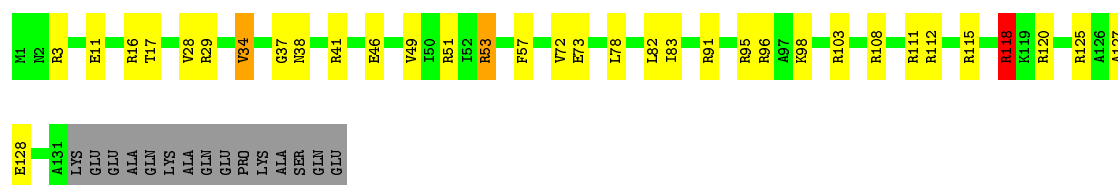
- Molecule 39: 50S ribosomal protein L18



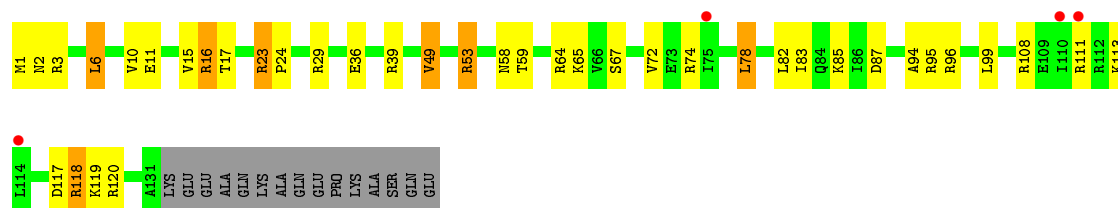
- Molecule 39: 50S ribosomal protein L18



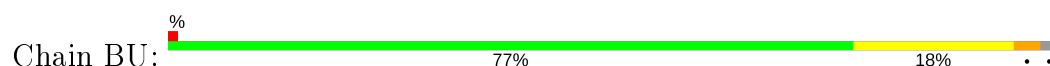
- Molecule 40: 50S ribosomal protein L19



- Molecule 40: 50S ribosomal protein L19

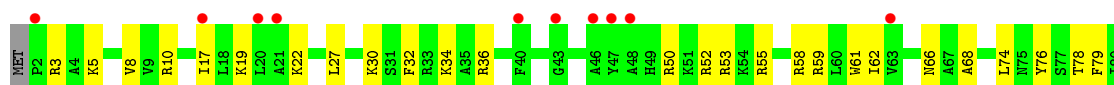


- Molecule 41: 50S ribosomal protein L20

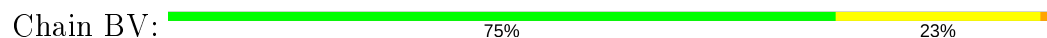




- Molecule 41: 50S ribosomal protein L20



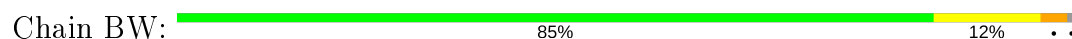
- Molecule 42: 50S ribosomal protein L21



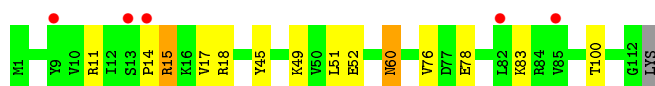
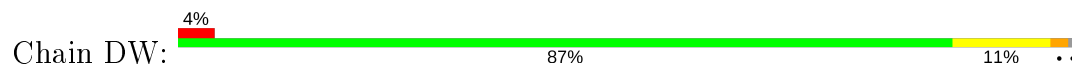
- Molecule 42: 50S ribosomal protein L21



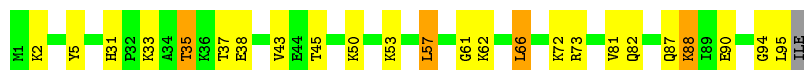
- Molecule 43: 50S ribosomal protein L22



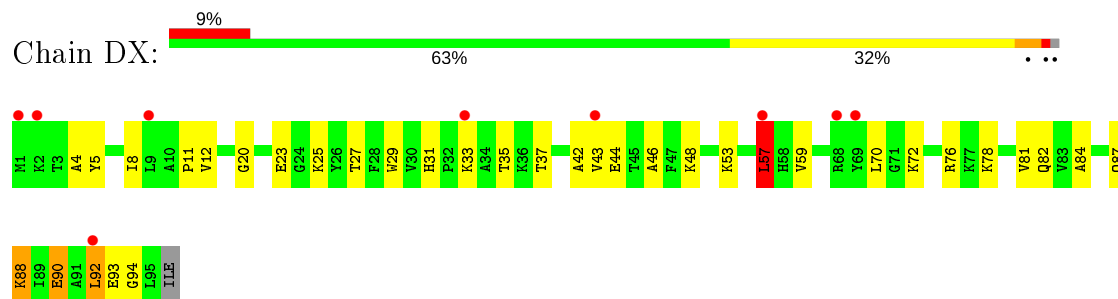
- Molecule 43: 50S ribosomal protein L22



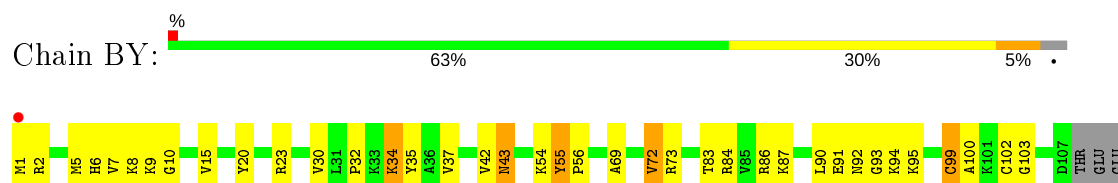
- Molecule 44: 50S ribosomal protein L23



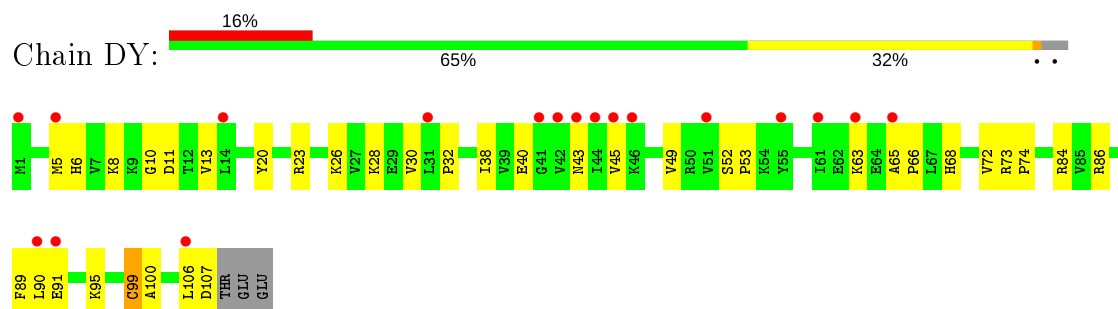
- Molecule 44: 50S ribosomal protein L23



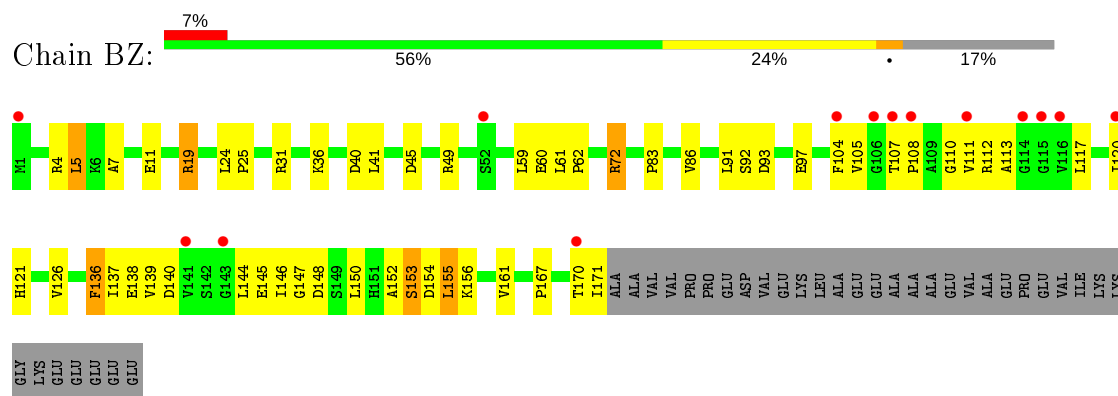
- Molecule 45: 50S ribosomal protein L24



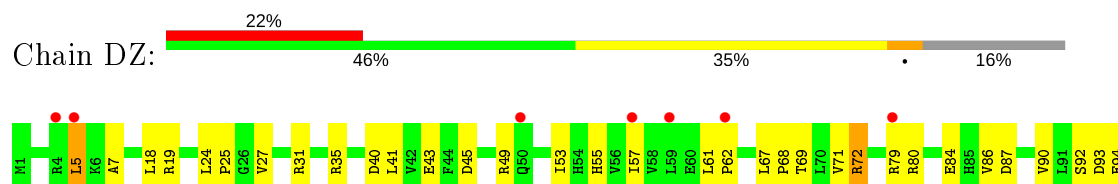
- Molecule 45: 50S ribosomal protein L24

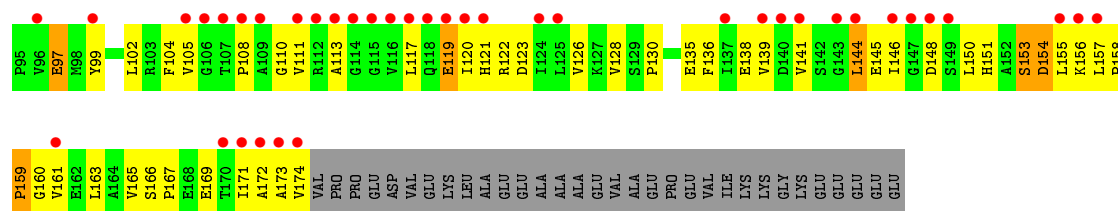


- Molecule 46: 50S ribosomal protein L25

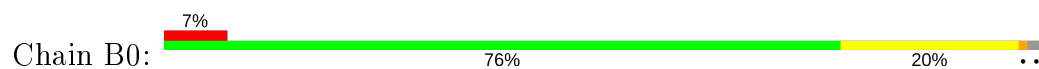


- Molecule 46: 50S ribosomal protein L25

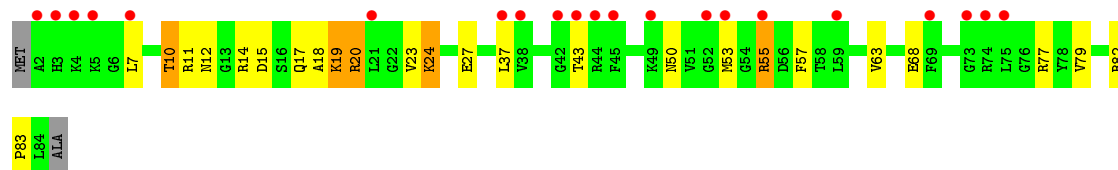




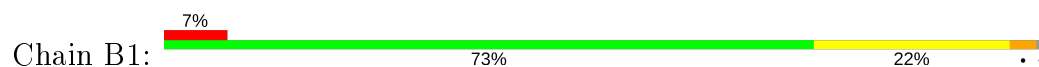
- Molecule 47: 50S ribosomal protein L27



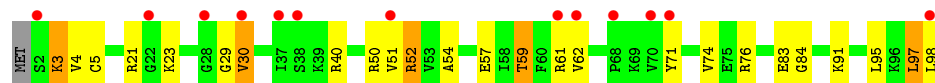
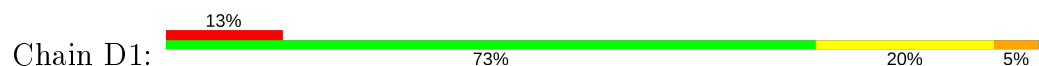
- Molecule 47: 50S ribosomal protein L27



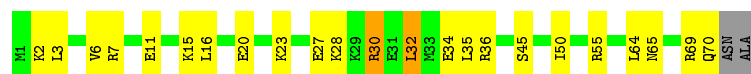
- Molecule 48: 50S ribosomal protein L28



- Molecule 48: 50S ribosomal protein L28

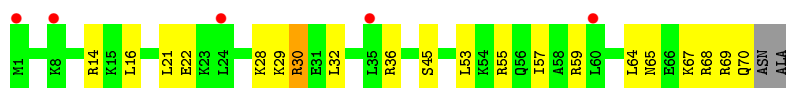


- Molecule 49: 50S ribosomal protein L29



- Molecule 49: 50S ribosomal protein L29





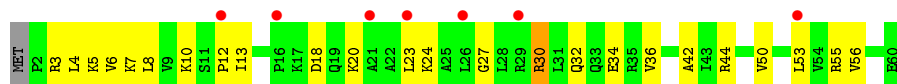
- Molecule 50: 50S ribosomal protein L30

Chain B3: 73% 20% 5% .



- Molecule 50: 50S ribosomal protein L30

Chain D3: 12% 58% 38% . .



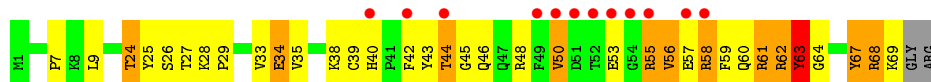
- Molecule 51: 50S ribosomal protein L31

Chain B4: 7% 56% 25% 13% . .



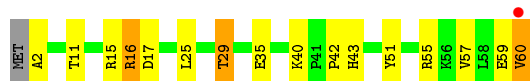
- Molecule 51: 50S ribosomal protein L31

Chain D4: 17% 48% 32% 15% . .



- Molecule 52: 50S ribosomal protein L32

Chain B5: 2% 72% 22% 5% .

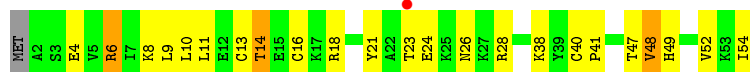


- Molecule 52: 50S ribosomal protein L32

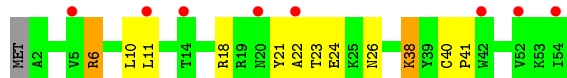
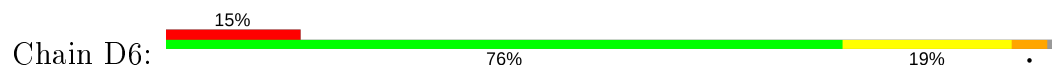
Chain D5: 3% 72% 23% . .



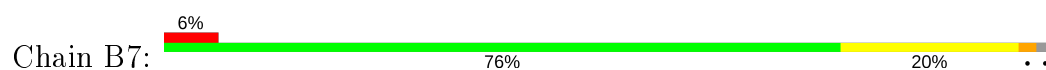
- Molecule 53: 50S ribosomal protein L33



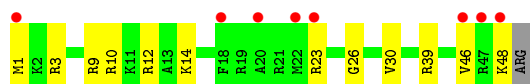
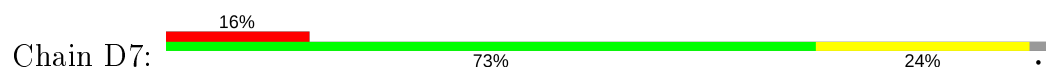
- Molecule 53: 50S ribosomal protein L33



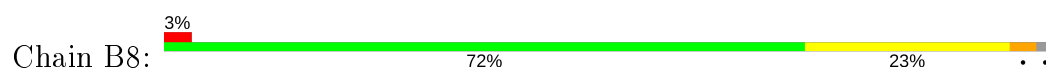
- Molecule 54: 50S ribosomal protein L34



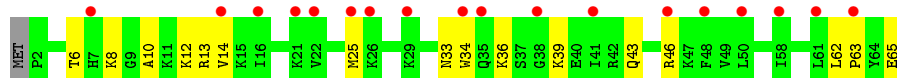
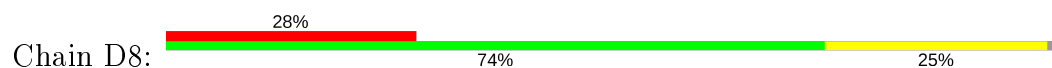
- Molecule 54: 50S ribosomal protein L34



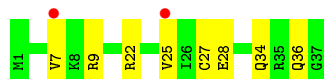
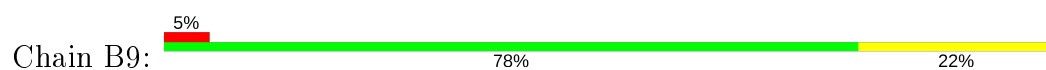
- Molecule 55: 50S ribosomal protein L35



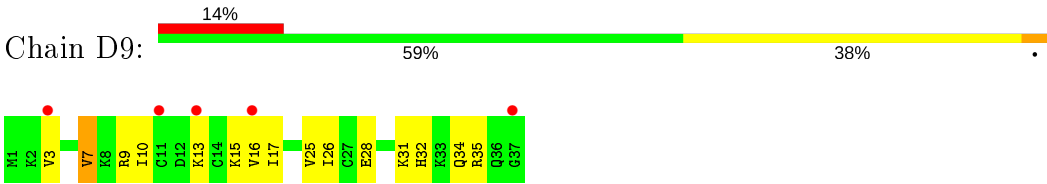
- Molecule 55: 50S ribosomal protein L35



- Molecule 56: 50S ribosomal protein L36



● Molecule 56: 50S ribosomal protein L36



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.32Å 450.06Å 622.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	152.51 – 2.55 255.92 – 2.55	Depositor EDS
% Data completeness (in resolution range)	95.8 (152.51-2.55) 95.8 (255.92-2.55)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 2.55Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.233 , 0.280 0.233 , 0.280	Depositor DCC
R_{free} test set	90444 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	50.6	Xtriage
Anisotropy	0.115	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 58.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	297141	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.64% 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: 5MU, ZN, 31M, MIA, SF4, MG, 5MC, 4SU, 7MG, K, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	AA	0.37	0/36049	0.91	42/56261 (0.1%)
1	CA	0.40	6/36170 (0.0%)	1.00	88/56452 (0.2%)
2	AB	0.31	0/1881	0.60	0/2542
2	CB	0.33	0/1860	0.65	1/2518 (0.0%)
3	AC	0.28	0/1576	0.52	0/2130
3	CC	0.32	0/1566	0.61	0/2119
4	AD	0.29	0/1689	0.58	2/2267 (0.1%)
4	CD	0.30	0/1704	0.54	0/2284
5	AE	0.30	0/1145	0.55	0/1543
5	CE	0.31	0/1149	0.62	1/1548 (0.1%)
6	AF	0.28	0/819	0.49	0/1111
6	CF	0.31	0/829	0.52	0/1123
7	AG	0.27	0/1250	0.51	0/1679
7	CG	0.28	0/1254	0.53	0/1683
8	AH	0.27	0/1108	0.50	0/1494
8	CH	0.27	0/1108	0.52	0/1494
9	AI	0.30	0/1002	0.59	0/1346
9	CI	0.30	0/997	0.57	0/1343
10	AJ	0.28	0/722	0.59	0/982
10	CJ	0.31	0/727	0.59	0/988
11	AK	0.28	0/844	0.60	1/1145 (0.1%)
11	CK	0.28	0/848	0.53	0/1149
12	AL	0.30	0/946	0.52	0/1274
12	CL	0.30	0/946	0.55	0/1274
13	AM	0.28	0/969	0.61	0/1302
13	CM	0.29	0/961	0.57	0/1291
14	AN	0.30	0/501	0.50	0/664
14	CN	0.33	0/501	0.57	0/664
15	AO	0.28	0/739	0.55	0/985
15	CO	0.30	0/739	0.54	0/985
16	AP	0.28	0/697	0.52	0/939
16	CP	0.31	0/693	0.51	0/935

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.28	0/836	0.53	0/1117
17	CQ	0.29	0/836	0.50	0/1117
18	AR	0.27	0/560	0.56	0/746
18	CR	0.28	0/560	0.56	0/746
19	AS	0.29	0/667	0.58	0/900
19	CS	0.32	0/661	0.67	0/893
20	AT	0.28	0/730	0.58	0/965
20	CT	0.28	0/729	0.52	0/965
21	AU	0.26	0/203	0.52	0/266
21	CU	0.35	0/203	0.52	0/266
22	AV	0.41	0/310	0.94	0/480
22	CV	0.45	0/282	1.06	1/437 (0.2%)
23	AW	0.47	0/1577	1.18	6/2454 (0.2%)
23	CW	0.59	0/1531	1.46	25/2379 (1.1%)
24	AX	0.51	0/1725	1.17	14/2689 (0.5%)
24	CX	0.44	0/1725	1.12	10/2689 (0.4%)
25	AY	0.62	0/1602	1.43	22/2493 (0.9%)
25	CY	0.64	0/1579	1.46	32/2455 (1.3%)
26	BA	0.48	2/68013 (0.0%)	0.95	84/106165 (0.1%)
26	DA	0.42	1/67542 (0.0%)	0.94	72/105428 (0.1%)
27	BB	0.41	0/2878	0.88	0/4490
27	DB	0.44	0/2878	0.94	0/4490
28	BD	0.37	0/2186	0.59	0/2944
28	DD	0.33	0/2186	0.55	0/2944
29	BE	0.36	0/1592	0.57	0/2149
29	DE	0.34	0/1592	0.60	1/2149 (0.0%)
30	BF	0.35	0/1619	0.55	0/2193
30	DF	0.32	0/1615	0.58	0/2188
31	BG	0.31	0/1450	0.54	0/1959
31	DG	0.33	0/1449	0.57	0/1958
32	BH	0.33	0/1356	0.54	0/1834
32	DH	0.30	0/1356	0.52	0/1834
33	BI	0.29	0/1100	0.60	0/1501
33	DI	0.28	0/1076	0.57	0/1471
34	BN	0.32	0/1144	0.53	0/1543
34	DN	0.31	0/1144	0.54	0/1543
35	BO	0.34	0/943	0.58	1/1269 (0.1%)
35	DO	0.31	0/943	0.51	0/1269
36	BP	0.34	0/1152	0.58	0/1533
36	DP	0.31	0/1152	0.59	0/1533
37	BQ	0.34	0/1143	0.53	0/1527
37	DQ	0.31	0/1143	0.52	0/1527
38	BR	0.35	0/982	0.58	0/1312

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DR	0.29	0/982	0.52	0/1312
39	BS	0.31	0/887	0.63	2/1180 (0.2%)
39	DS	0.29	0/880	0.61	0/1172
40	BT	0.33	0/1105	0.59	1/1477 (0.1%)
40	DT	0.29	0/1097	0.56	0/1468
41	BU	0.37	0/977	0.56	0/1301
41	DU	0.31	0/977	0.50	0/1301
42	BV	0.39	0/782	0.58	0/1049
42	DV	0.32	0/782	0.64	2/1049 (0.2%)
43	BW	0.38	0/897	0.57	0/1205
43	DW	0.31	0/897	0.52	0/1205
44	BX	0.39	0/764	0.59	1/1025 (0.1%)
44	DX	0.32	0/764	0.56	1/1025 (0.1%)
45	BY	0.34	0/819	0.57	0/1095
45	DY	0.31	0/819	0.55	0/1095
46	BZ	0.31	0/1379	0.61	0/1873
46	DZ	0.29	0/1390	0.57	0/1890
47	B0	0.35	0/662	0.57	0/881
47	D0	0.29	0/662	0.49	0/881
48	B1	0.34	0/762	0.56	0/1014
48	D1	0.32	0/762	0.54	0/1014
49	B2	0.32	0/590	0.56	0/781
49	D2	0.27	0/590	0.46	0/781
50	B3	0.36	0/474	0.58	0/635
50	D3	0.27	0/469	0.50	0/630
51	B4	0.35	0/571	0.71	0/768
51	D4	0.34	0/545	0.70	0/737
52	B5	0.38	0/469	0.60	0/635
52	D5	0.33	0/469	0.52	0/635
53	B6	0.36	0/460	0.51	0/613
53	D6	0.30	0/456	0.48	0/608
54	B7	0.39	0/426	0.55	0/561
54	D7	0.33	0/426	0.59	0/561
55	B8	0.36	0/519	0.58	0/684
55	D8	0.32	0/525	0.52	0/691
56	B9	0.35	0/310	0.51	0/407
56	D9	0.31	0/310	0.56	0/407
All	All	0.40	9/316594 (0.0%)	0.88	410/473970 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	AB	0	4
7	AG	0	2
7	CG	0	1
20	CT	0	1
28	BD	0	1
39	BS	0	1
51	B4	0	2
51	D4	0	1
All	All	0	13

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	CA	1154	G	N1-C2	-11.01	1.28	1.37
1	CA	1154	G	C6-N1	-10.68	1.32	1.39
1	CA	1119	C	N3-C4	-9.86	1.27	1.33
1	CA	1154	G	N7-C5	-7.17	1.34	1.39
26	BA	330	A	N9-C4	-6.79	1.33	1.37
26	BA	1021	A	N9-C4	-5.85	1.34	1.37
26	DA	2287	A	N9-C4	-5.40	1.34	1.37
1	CA	1154	G	C5-C4	5.28	1.42	1.38
1	CA	1119	C	C2-N3	-5.06	1.31	1.35

All (410) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CA	1119	C	N1-C2-O2	32.18	138.21	118.90
1	CA	1154	G	N3-C2-N2	24.48	137.03	119.90
1	CA	1154	G	C5-C6-O6	24.01	143.00	128.60
1	CA	1154	G	N1-C2-N2	-21.95	96.45	116.20
1	CA	1119	C	N3-C2-O2	-20.26	107.72	121.90
1	CA	1119	C	C2-N3-C4	18.04	128.92	119.90
1	CA	1119	C	C2-N1-C1'	16.83	137.32	118.80
1	CA	1154	G	C5-C6-N1	-16.70	103.15	111.50
1	CA	1154	G	C6-N1-C2	15.37	134.32	125.10
1	CA	1119	C	C5-C4-N4	13.49	129.64	120.20
1	CA	1119	C	C6-N1-C1'	-13.30	104.84	120.80
26	DA	2139	C	N1-C2-O2	11.63	125.88	118.90
1	CA	1119	C	N3-C4-N4	-11.16	110.19	118.00
1	CA	1001(A)	G	N3-C4-N9	10.62	132.37	126.00
23	CW	67	C	C5-C6-N1	10.56	126.28	121.00
1	CA	1154	G	C4-N9-C1'	10.47	140.11	126.50
25	AY	64	A	N1-C6-N6	-10.40	112.36	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	CY	23	A	N1-C6-N6	10.31	124.79	118.60
1	CA	1154	G	N1-C6-O6	-10.16	113.81	119.90
25	CY	66	U	C5-C4-O4	-10.02	119.89	125.90
25	AY	64	A	C5-C6-N6	9.87	131.59	123.70
26	BA	330	A	C2-N3-C4	-9.84	105.68	110.60
1	CA	1154	G	C2-N3-C4	-9.82	106.99	111.90
26	DA	2585	U	C5-C4-O4	-9.67	120.10	125.90
26	BA	2140	C	N1-C2-O2	9.55	124.63	118.90
1	CA	1119	C	C6-N1-C2	-9.51	116.49	120.30
26	DA	2174	C	C2-N1-C1'	9.37	129.11	118.80
1	CA	1119	C	C5-C6-N1	9.24	125.62	121.00
26	DA	2139	C	C2-N1-C1'	9.23	128.95	118.80
26	BA	1639	U	O5'-P-OP2	-9.22	97.40	105.70
1	CA	1054	C	P-O3'-C3'	9.21	130.75	119.70
26	DA	2152	G	C5-C6-O6	-9.21	123.08	128.60
1	CA	79	G	C5-C6-O6	9.02	134.01	128.60
24	AX	14	A	C4-C5-C6	8.97	121.48	117.00
1	CA	1154	G	C8-N9-C1'	-8.97	115.34	127.00
25	CY	4	C	N1-C2-O2	8.94	124.27	118.90
24	AX	46	G	C6-N1-C2	-8.94	119.74	125.10
24	CX	46	G	C6-N1-C2	-8.92	119.75	125.10
26	DA	2152	G	N1-C6-O6	8.87	125.22	119.90
26	BA	2140	C	N3-C2-O2	-8.83	115.72	121.90
1	CA	1004	A	O4'-C1'-N9	8.50	115.00	108.20
1	CA	1119	C	N1-C2-N3	-8.44	113.29	119.20
23	CW	7	A	N1-C6-N6	8.42	123.65	118.60
24	AX	14	A	C5-N7-C8	8.39	108.10	103.90
26	BA	1021	A	C2-N3-C4	-8.31	106.45	110.60
1	AA	1030(B)	C	C2-N1-C1'	8.24	127.86	118.80
26	DA	2136	C	N1-C2-O2	8.23	123.84	118.90
1	CA	1001(A)	G	N3-C4-C5	-8.21	124.49	128.60
23	CW	67	C	C2-N3-C4	8.09	123.95	119.90
1	AA	1137	C	C6-N1-C2	-8.06	117.07	120.30
26	BA	2140	C	C2-N1-C1'	8.06	127.67	118.80
25	CY	68	C	C2-N1-C1'	7.99	127.59	118.80
26	DA	2152	G	N9-C4-C5	-7.99	102.20	105.40
26	DA	2152	G	N3-C4-N9	7.99	130.79	126.00
24	CX	14	A	C4-C5-C6	7.97	120.98	117.00
39	BS	67	ARG	NE-CZ-NH1	-7.95	116.32	120.30
1	AA	1036	G	C4-N9-C1'	7.92	136.79	126.50
11	AK	18	ARG	NE-CZ-NH1	-7.89	116.36	120.30
1	CA	1001(A)	G	C4-N9-C1'	7.85	136.70	126.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CA	1154	G	C4-C5-C6	7.84	123.51	118.80
26	BA	2140	C	C6-N1-C2	-7.82	117.17	120.30
23	CW	22	G	N3-C2-N2	-7.75	114.47	119.90
1	AA	1030(B)	C	N1-C2-O2	7.75	123.55	118.90
26	DA	2139	C	N3-C2-O2	-7.71	116.50	121.90
26	DA	2152	G	C6-C5-N7	-7.69	125.79	130.40
1	CA	1126	U	C2-N1-C1'	7.68	126.92	117.70
26	BA	226	G	O4'-C1'-N9	7.68	114.34	108.20
26	DA	2167	U	N1-C2-O2	7.67	128.17	122.80
25	CY	66	U	N3-C4-O4	7.66	124.76	119.40
1	AA	1054	C	P-O3'-C3'	7.60	128.81	119.70
1	AA	346	G	C4-N9-C1'	7.56	136.32	126.50
25	CY	68	C	N3-C2-O2	-7.46	116.67	121.90
25	CY	56	C	C2-N1-C1'	7.45	126.99	118.80
1	CA	1001(A)	G	C8-N9-C1'	-7.43	117.34	127.00
25	CY	7	A	C6-N1-C2	-7.43	114.14	118.60
25	CY	68	C	N1-C2-O2	7.39	123.34	118.90
1	CA	1054	C	O4'-C1'-N1	7.39	114.11	108.20
26	BA	887	A	O4'-C1'-N9	7.35	114.08	108.20
26	BA	12	U	C2-N1-C1'	7.29	126.45	117.70
26	BA	1022	G	N3-C2-N2	-7.29	114.80	119.90
26	BA	1963	U	C2-N1-C1'	7.25	126.40	117.70
26	DA	2167	U	C2-N1-C1'	7.25	126.40	117.70
26	DA	2139	C	C6-N1-C1'	-7.22	112.13	120.80
26	DA	2152	G	C4-C5-N7	7.19	113.68	110.80
35	BO	8	LEU	CA-CB-CG	7.19	131.83	115.30
23	CW	45	U	C2-N1-C1'	7.17	126.31	117.70
26	DA	2174	C	C6-N1-C1'	-7.16	112.20	120.80
26	DA	2206	G	C4-N9-C1'	-7.14	117.22	126.50
24	AX	14	A	C5-C6-N1	-7.14	114.13	117.70
23	CW	44	G	C5-C6-O6	-7.13	124.32	128.60
1	AA	254	G	O5'-P-OP1	-7.09	99.32	105.70
1	AA	1036	G	C8-N9-C1'	-7.08	117.79	127.00
26	DA	2155	G	N3-C2-N2	7.07	124.85	119.90
26	BA	512	G	O4'-C1'-N9	7.04	113.83	108.20
26	DA	2167	U	N3-C2-O2	-7.03	117.28	122.20
24	AX	22	G	C5-N7-C8	-7.00	100.80	104.30
26	DA	2152	G	C8-N9-C1'	-6.95	117.96	127.00
26	DA	1372	U	C5-C4-O4	-6.92	121.75	125.90
26	DA	2137	C	C6-N1-C2	-6.90	117.54	120.30
1	AA	1137	C	C5-C6-N1	6.88	124.44	121.00
25	CY	23	A	C6-C5-N7	-6.85	127.51	132.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	CW	67	C	C2-N1-C1'	6.84	126.32	118.80
26	DA	2155	G	C6-N1-C2	6.83	129.20	125.10
23	CW	22	G	N3-C4-N9	-6.82	121.91	126.00
26	DA	893	C	C2-N1-C1'	6.82	126.30	118.80
26	DA	2585	U	C6-N1-C1'	-6.80	111.67	121.20
25	AY	5	G	N3-C4-N9	6.80	130.08	126.00
44	DX	57	LEU	CA-CB-CG	6.80	130.94	115.30
26	DA	2585	U	C2-N1-C1'	6.79	125.85	117.70
1	AA	346	G	O4'-C1'-N9	6.76	113.61	108.20
26	BA	271(M)	G	OP1-P-O3'	6.75	120.05	105.20
44	BX	57	LEU	CA-CB-CG	6.75	130.82	115.30
26	BA	624	C	O5'-P-OP1	-6.73	99.64	105.70
1	CA	1003	G	C4-N9-C1'	6.73	135.25	126.50
24	AX	22	G	C4-C5-C6	-6.69	114.79	118.80
23	CW	45	U	N1-C2-O2	6.69	127.48	122.80
1	CA	1154	G	N3-C4-N9	6.66	130.00	126.00
25	AY	4	C	N3-C2-O2	-6.61	117.27	121.90
26	BA	748	G	O4'-C1'-N9	6.61	113.49	108.20
1	CA	754	C	C2-N1-C1'	6.59	126.05	118.80
23	CW	7	A	C5-C6-N6	-6.57	118.45	123.70
26	DA	2152	G	C4-N9-C1'	6.55	135.02	126.50
25	CY	7	A	C5-C6-N1	6.53	120.96	117.70
1	CA	1001(A)	G	C6-C5-N7	-6.51	126.49	130.40
26	BA	2061	G	O5'-P-OP2	-6.50	99.84	105.70
23	CW	67	C	N1-C2-O2	6.49	122.79	118.90
25	AY	4	C	N1-C2-O2	6.48	122.79	118.90
26	BA	1142(A)	A	C2-N3-C4	-6.48	107.36	110.60
25	CY	56	C	C6-N1-C1'	-6.48	113.03	120.80
24	CX	22	G	N1-C6-O6	-6.45	116.03	119.90
25	CY	7	A	N3-C4-N9	6.45	132.56	127.40
23	CW	67	C	C6-N1-C2	-6.44	117.72	120.30
25	AY	33	U	N3-C2-O2	-6.42	117.71	122.20
26	DA	1372	U	N3-C4-O4	6.41	123.89	119.40
26	BA	330	A	N1-C2-N3	6.39	132.50	129.30
1	CA	998	G	N3-C4-N9	-6.39	122.17	126.00
26	BA	141	A	N7-C8-N9	6.38	116.99	113.80
25	AY	58	A	C4-N9-C1'	6.37	137.76	126.30
23	CW	66	U	C2-N1-C1'	6.36	125.33	117.70
26	BA	1992	G	P-O3'-C3'	6.36	127.33	119.70
24	AX	22	G	N3-C4-N9	-6.32	122.21	126.00
26	DA	2206	G	C8-N9-C1'	6.31	135.21	127.00
1	AA	1054	C	N3-C2-O2	-6.31	117.48	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BA	372	G	O4'-C1'-N9	6.30	113.24	108.20
23	CW	3	C	N1-C2-O2	6.29	122.67	118.90
26	BA	1256	G	N9-C4-C5	-6.28	102.89	105.40
1	AA	1397	C	C2-N1-C1'	6.28	125.70	118.80
1	AA	346	G	C8-N9-C4	-6.27	103.89	106.40
26	BA	330	A	N3-C4-C5	6.27	131.19	126.80
26	DA	1531	C	C2-N1-C1'	6.25	125.68	118.80
26	BA	1300	U	P-O3'-C3'	6.25	127.19	119.70
24	CX	46	G	C5-C6-N1	6.24	114.62	111.50
23	AW	15	G	N3-C2-N2	6.24	124.27	119.90
25	AY	69	G	N3-C4-N9	6.24	129.74	126.00
1	CA	1003	G	N7-C8-N9	6.20	116.20	113.10
23	AW	48	C	N1-C2-O2	-6.20	115.18	118.90
1	CA	1154	G	N3-C4-C5	-6.19	125.50	128.60
1	CA	96	U	O4'-C1'-N1	6.19	113.15	108.20
25	CY	23	A	C4-C5-C6	6.18	120.09	117.00
25	CY	23	A	C5-C6-N6	-6.17	118.77	123.70
25	AY	33	U	C2-N1-C1'	6.16	125.09	117.70
1	CA	1030(B)	C	C5-C6-N1	6.15	124.08	121.00
25	AY	68	C	N1-C2-O2	6.13	122.58	118.90
24	AX	14	A	C8-N9-C1'	-6.13	116.67	127.70
26	BA	1176	G	OP1-P-O3'	6.13	118.69	105.20
25	CY	4	C	N3-C2-O2	-6.13	117.61	121.90
1	AA	1054	C	C6-N1-C2	-6.12	117.85	120.30
1	CA	1052	U	N1-C2-O2	6.11	127.08	122.80
1	AA	1030(B)	C	N3-C2-O2	-6.11	117.62	121.90
1	CA	1256	A	O4'-C1'-N9	-6.11	103.31	108.20
1	CA	1119	C	C4-C5-C6	-6.11	114.35	117.40
26	BA	528	A	C2-N3-C4	-6.10	107.55	110.60
24	CX	46	G	N3-C2-N2	-6.07	115.65	119.90
1	CA	1064	G	P-O3'-C3'	6.07	126.98	119.70
25	AY	50	U	C2-N3-C4	6.05	130.63	127.00
26	BA	2036	C	O5'-P-OP1	-6.04	100.26	105.70
26	BA	330	A	N3-C4-N9	-6.04	122.57	127.40
1	CA	754	C	N1-C2-O2	6.00	122.50	118.90
26	BA	141	A	C5-N7-C8	-6.00	100.90	103.90
26	BA	787	U	O5'-P-OP1	-5.99	100.31	105.70
26	BA	271(M)	G	P-O3'-C3'	5.99	126.89	119.70
26	DA	1531	C	N1-C2-O2	5.98	122.49	118.90
26	DA	2140	C	C2-N1-C1'	5.98	125.38	118.80
25	AY	33	U	N1-C2-O2	5.97	126.98	122.80
1	CA	1030	C	C2-N1-C1'	5.96	125.36	118.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BA	2248	C	O5'-P-OP2	-5.95	100.34	105.70
1	CA	65	U	P-O3'-C3'	5.95	126.84	119.70
1	AA	1030(B)	C	C6-N1-C1'	-5.94	113.67	120.80
26	BA	1992	G	C8-N9-C4	-5.94	104.02	106.40
26	BA	1776	G	O5'-P-OP2	-5.94	100.35	105.70
23	CW	22	G	N9-C4-C5	5.94	107.78	105.40
26	BA	2615	U	O5'-P-OP1	-5.92	100.37	105.70
39	BS	67	ARG	NE-CZ-NH2	5.92	123.26	120.30
1	CA	1030(B)	C	C6-N1-C2	-5.92	117.93	120.30
26	BA	933	A	O4'-C1'-N9	5.92	112.93	108.20
25	AY	69	G	N3-C4-C5	-5.91	125.64	128.60
1	AA	347	G	P-O3'-C3'	5.91	126.79	119.70
23	AW	3	C	C2-N1-C1'	5.91	125.30	118.80
26	BA	1021	A	N1-C2-N3	5.91	132.25	129.30
25	CY	56	C	N1-C2-O2	5.89	122.43	118.90
24	AX	46	G	C5-C6-N1	5.88	114.44	111.50
26	DA	614	U	N3-C2-O2	-5.88	118.08	122.20
24	AX	22	G	C8-N9-C1'	5.86	134.62	127.00
24	AX	14	A	C4-N9-C1'	5.86	136.84	126.30
1	CA	687	A	P-O3'-C3'	5.85	126.72	119.70
23	CW	3	C	C2-N3-C4	5.84	122.82	119.90
1	CA	1023	G	N3-C4-N9	5.83	129.50	126.00
24	CX	14	A	C5-N7-C8	5.82	106.81	103.90
1	CA	1067	A	P-O3'-C3'	5.81	126.67	119.70
26	DA	2139	C	C5-C6-N1	5.81	123.91	121.00
1	CA	997	U	C5-C4-O4	5.79	129.38	125.90
26	BA	1022	G	N3-C4-N9	-5.76	122.54	126.00
1	AA	839	U	P-O3'-C3'	5.75	126.60	119.70
23	CW	66	U	P-O3'-C3'	5.74	126.59	119.70
26	BA	1828	G	C5-C6-O6	-5.73	125.16	128.60
26	BA	528	A	C5-N7-C8	-5.73	101.04	103.90
25	AY	35	A	O5'-P-OP2	-5.72	100.55	105.70
26	BA	845	G	O4'-C1'-N9	5.71	112.77	108.20
26	DA	1204	A	O4'-C1'-N9	5.70	112.76	108.20
1	CA	1039	C	N1-C2-O2	5.69	122.32	118.90
26	BA	1493	C	N1-C2-O2	5.69	122.31	118.90
1	CA	1125	U	O3'-P-O5'	5.69	114.81	104.00
26	BA	1963	U	N1-C2-O2	5.68	126.78	122.80
23	CW	45	U	C6-N1-C1'	-5.68	113.25	121.20
1	AA	1067	A	P-O3'-C3'	5.68	126.51	119.70
1	CA	1039	C	C5-C4-N4	-5.68	116.23	120.20
1	CA	1001(A)	G	N9-C4-C5	-5.67	103.13	105.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	DE	72	VAL	C-N-CA	5.66	135.86	121.70
1	CA	79	G	N1-C6-O6	-5.66	116.50	119.90
1	AA	1054	C	C2-N1-C1'	5.66	125.02	118.80
25	CY	5	G	N3-C4-C5	-5.64	125.78	128.60
1	AA	1125	U	P-O3'-C3'	5.64	126.47	119.70
25	CY	50	U	C5-C4-O4	5.64	129.28	125.90
1	AA	346	G	N3-C4-C5	-5.63	125.79	128.60
42	DV	100	ARG	NE-CZ-NH1	5.63	123.11	120.30
26	DA	214	G	O4'-C1'-N9	5.62	112.70	108.20
26	DA	2137	C	O4'-C1'-N1	5.61	112.69	108.20
26	DA	893	C	N1-C2-O2	5.60	122.26	118.90
23	AW	22	G	N1-C6-O6	5.60	123.26	119.90
26	BA	1372	U	N3-C4-O4	5.59	123.32	119.40
1	CA	1154	G	C5-N7-C8	5.59	107.09	104.30
26	DA	748	G	C4-N9-C1'	-5.59	119.24	126.50
1	CA	1021	G	O4'-C1'-N9	5.58	112.66	108.20
1	AA	346	G	C8-N9-C1'	-5.57	119.76	127.00
26	BA	1176	G	P-O3'-C3'	5.57	126.38	119.70
26	DA	1937	A	O4'-C1'-N9	5.56	112.65	108.20
42	DV	38	LEU	CA-CB-CG	5.56	128.09	115.30
25	AY	58	A	C8-N9-C1'	-5.56	117.69	127.70
1	AA	1022	G	N3-C2-N2	5.55	123.78	119.90
1	CA	1126	U	N1-C2-O2	5.55	126.68	122.80
1	CA	1493	A	P-O3'-C3'	5.55	126.36	119.70
26	DA	2174	C	C5-C6-N1	5.54	123.77	121.00
1	CA	1225	A	C5-C6-N6	5.53	128.13	123.70
23	CW	6	G	C4-C5-N7	5.53	113.01	110.80
23	CW	6	G	N9-C4-C5	-5.53	103.19	105.40
24	AX	22	G	N3-C4-C5	5.53	131.36	128.60
1	AA	991	U	P-O3'-C3'	5.52	126.33	119.70
25	AY	58	A	P-O3'-C3'	5.52	126.33	119.70
25	CY	69	G	N3-C4-N9	5.52	129.31	126.00
26	DA	2140	C	N1-C2-O2	5.52	122.21	118.90
26	BA	570	G	C5-C6-O6	-5.52	125.29	128.60
26	BA	1256	G	C4-C5-N7	5.52	113.01	110.80
24	CX	34	C	C2-N1-C1'	5.52	124.87	118.80
25	CY	68	C	C6-N1-C1'	-5.51	114.19	120.80
24	AX	67	C	N1-C2-O2	5.50	122.20	118.90
26	DA	2139	C	N3-C4-C5	5.49	124.10	121.90
1	AA	1028	C	O4'-C1'-N1	5.48	112.59	108.20
1	CA	1154	G	C6-C5-N7	-5.48	127.11	130.40
26	DA	383	U	O4'-C1'-N1	5.48	112.58	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BA	1936	A	O4'-C1'-N9	5.46	112.57	108.20
1	CA	90	U	N1-C2-N3	5.46	118.18	114.90
26	BA	1187	G	N1-C6-O6	-5.46	116.62	119.90
26	BA	383	U	C2-N1-C1'	-5.46	111.15	117.70
26	BA	2789	C	N1-C2-O2	-5.46	115.62	118.90
1	AA	1054	C	N1-C2-O2	5.46	122.17	118.90
1	CA	1286	A	C8-N9-C4	-5.45	103.62	105.80
26	BA	2689	U	N3-C2-O2	-5.45	118.39	122.20
1	AA	1285	A	P-O3'-C3'	5.44	126.23	119.70
26	BA	847	U	C2-N1-C1'	-5.44	111.17	117.70
26	BA	12	U	N1-C2-O2	5.43	126.60	122.80
26	DA	1300	U	P-O3'-C3'	5.43	126.22	119.70
24	CX	22	G	C5-N7-C8	-5.43	101.59	104.30
26	DA	2685	G	N1-C6-O6	-5.42	116.65	119.90
1	AA	347	G	OP1-P-O3'	5.41	117.09	105.20
26	DA	2585	U	O4'-C1'-N1	-5.40	103.88	108.20
26	DA	2321	G	C4-N9-C1'	5.40	133.52	126.50
1	AA	1502	A	N1-C2-N3	5.39	132.00	129.30
1	AA	97	G	N3-C4-N9	5.39	129.24	126.00
26	BA	1530	C	P-O3'-C3'	5.38	126.16	119.70
23	CW	26	A	C5-C6-N6	-5.38	119.39	123.70
26	DA	1313	U	C2-N1-C1'	5.38	124.16	117.70
23	AW	50	U	C5-C4-O4	-5.38	122.67	125.90
26	BA	1204	A	O4'-C1'-N9	5.38	112.50	108.20
25	CY	7	A	C6-C5-N7	-5.38	128.54	132.30
26	BA	945	A	C2-N3-C4	-5.38	107.91	110.60
26	BA	576	U	O5'-P-OP1	-5.37	100.86	105.70
26	BA	1698	A	O4'-C1'-N9	5.37	112.50	108.20
1	CA	1286	A	N7-C8-N9	5.37	116.48	113.80
26	BA	944	G	C4-N9-C1'	5.36	133.47	126.50
25	CY	5	G	O4'-C1'-N9	5.36	112.49	108.20
1	CA	1529	G	C4-N9-C1'	5.36	133.47	126.50
1	AA	1278	U	C5-C6-N1	5.36	125.38	122.70
26	DA	1530	C	P-O3'-C3'	5.36	126.13	119.70
25	CY	68	C	C6-N1-C2	-5.35	118.16	120.30
25	CY	5	G	C2-N3-C4	5.35	114.58	111.90
24	CX	46	G	C5-C6-O6	-5.35	125.39	128.60
26	DA	1698	A	O4'-C1'-N9	5.35	112.48	108.20
23	CW	67	C	C4-C5-C6	-5.34	114.73	117.40
1	AA	1042	G	O4'-C1'-N9	5.34	112.47	108.20
2	CB	187	LEU	CA-CB-CG	5.34	127.58	115.30
26	BA	12	U	N3-C2-O2	-5.33	118.47	122.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BA	2593	U	N3-C4-O4	-5.33	115.67	119.40
1	AA	1030(B)	C	C6-N1-C2	-5.32	118.17	120.30
25	CY	5	G	N3-C4-N9	5.32	129.19	126.00
1	CA	1126	U	C6-N1-C1'	-5.31	113.76	121.20
25	CY	24	G	N3-C4-N9	5.31	129.19	126.00
25	AY	50	U	N3-C4-C5	-5.31	111.42	114.60
1	CA	992	U	P-O3'-C3'	5.30	126.06	119.70
1	CA	1206	G	C5-C6-O6	-5.30	125.42	128.60
26	BA	1614	A	O5'-P-OP1	-5.30	100.93	105.70
26	BA	1045	A	O5'-P-OP1	5.29	117.04	110.70
1	CA	1502	A	N1-C2-N3	5.29	131.94	129.30
26	BA	1175	U	P-O3'-C3'	5.28	126.04	119.70
23	CW	66	U	C5-C6-N1	5.28	125.34	122.70
4	AD	174	LEU	CA-CB-CG	5.26	127.41	115.30
23	AW	3	C	N1-C2-O2	5.26	122.06	118.90
1	CA	79	G	C6-N1-C2	5.26	128.25	125.10
26	DA	2629	A	O4'-C1'-N9	5.25	112.40	108.20
4	AD	188	LEU	CA-CB-CG	5.24	127.36	115.30
1	CA	1323	G	N3-C4-N9	5.24	129.15	126.00
5	CE	12	LEU	CA-CB-CG	5.24	127.35	115.30
25	CY	60	U	N3-C2-O2	-5.24	118.53	122.20
24	AX	22	G	C4-N9-C1'	-5.24	119.69	126.50
26	BA	1315	C	O5'-P-OP2	-5.24	100.99	105.70
1	CA	1126	U	P-O5'-C5'	5.23	129.27	120.90
1	CA	1126	U	C5-C6-N1	5.22	125.31	122.70
1	CA	1158	C	C2-N1-C1'	5.22	124.55	118.80
25	CY	7	A	N9-C4-C5	-5.22	103.71	105.80
26	BA	2789	C	C2-N1-C1'	-5.21	113.07	118.80
26	BA	1963	U	C6-N1-C1'	-5.21	113.91	121.20
1	CA	1003	G	C8-N9-C4	-5.21	104.32	106.40
1	CA	1183	A	P-O3'-C3'	5.21	125.95	119.70
1	CA	1158	C	N1-C2-O2	5.20	122.02	118.90
26	DA	2554	U	O5'-P-OP2	-5.20	101.02	105.70
26	DA	2154	G	N9-C1'-C2'	-5.20	106.28	112.00
1	CA	1220	G	N3-C4-N9	-5.20	122.88	126.00
1	CA	998	G	N9-C4-C5	5.19	107.48	105.40
26	BA	481	G	O4'-C1'-N9	5.19	112.35	108.20
26	BA	195	A	P-O3'-C3'	5.19	125.92	119.70
26	BA	141	A	O4'-C1'-N9	5.18	112.35	108.20
26	BA	527	C	N3-C2-O2	-5.18	118.27	121.90
26	DA	945	A	O4'-C1'-N9	5.18	112.35	108.20
25	CY	7	A	C5-C6-N6	-5.18	119.56	123.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1150	U	C2-N3-C4	5.17	130.10	127.00
1	AA	1502	A	N7-C8-N9	5.17	116.39	113.80
1	CA	1030	C	C6-N1-C1'	-5.17	114.59	120.80
1	AA	754	C	C2-N1-C1'	5.17	124.49	118.80
26	BA	2791	C	C6-N1-C2	-5.17	118.23	120.30
25	AY	5	G	N3-C4-C5	-5.17	126.02	128.60
1	AA	97	G	N3-C4-C5	-5.16	126.02	128.60
1	CA	848	C	C5-C6-N1	5.16	123.58	121.00
26	DA	2137	C	C6-N1-C1'	5.16	126.99	120.80
26	DA	914	C	N1-C2-O2	5.15	121.99	118.90
26	DA	748	G	C8-N9-C1'	5.15	133.69	127.00
1	CA	266	G	C4-N9-C1'	5.14	133.19	126.50
26	BA	265	A	O4'-C1'-N9	5.14	112.31	108.20
26	BA	1021	A	C5-N7-C8	-5.13	101.33	103.90
26	BA	2471	C	N1-C2-O2	5.13	121.98	118.90
25	AY	6	G	N9-C4-C5	-5.12	103.35	105.40
25	AY	18	G	C4-N9-C1'	-5.12	119.84	126.50
25	AY	45	U	C5-C6-N1	5.12	125.26	122.70
1	CA	60	A	P-O3'-C3'	5.12	125.84	119.70
1	CA	1158	C	C6-N1-C2	-5.11	118.26	120.30
25	CY	69	G	N3-C4-C5	-5.11	126.05	128.60
24	CX	22	G	C4-C5-C6	-5.10	115.74	118.80
26	BA	517	C	C6-N1-C2	-5.10	118.26	120.30
26	BA	2187	G	C5-C6-O6	5.10	131.66	128.60
23	CW	66	U	C5-C4-O4	-5.10	122.84	125.90
22	CV	24	A	O4'-C1'-N9	5.09	112.28	108.20
25	CY	9	A	C4-C5-C6	-5.09	114.45	117.00
1	AA	1397	C	O4'-C1'-N1	5.09	112.27	108.20
26	DA	893	C	C6-N1-C2	-5.08	118.27	120.30
26	DA	2430	A	O4'-C1'-N9	5.08	112.26	108.20
26	DA	893	C	C5-C6-N1	5.08	123.54	121.00
26	DA	2621	A	C8-N9-C4	5.07	107.83	105.80
26	DA	214	G	C4-N9-C1'	-5.07	119.91	126.50
26	DA	1992	G	P-O3'-C3'	5.06	125.78	119.70
1	CA	1003	G	C8-N9-C1'	-5.06	120.42	127.00
1	CA	955	U	C2-N3-C4	5.06	130.04	127.00
1	AA	346	G	N7-C8-N9	5.06	115.63	113.10
1	CA	79	G	N3-C4-N9	-5.06	122.97	126.00
1	CA	90	U	O4'-C1'-N1	5.06	112.25	108.20
26	BA	2848	G	O4'-C1'-N9	5.05	112.24	108.20
26	DA	1558	A	P-O3'-C3'	5.05	125.77	119.70
23	CW	22	G	N1-C2-N2	5.05	120.75	116.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	DA	1791	A	O5'-P-OP1	-5.05	101.16	105.70
26	DA	2136	C	N3-C2-O2	-5.04	118.37	121.90
26	BA	2553	G	N3-C4-C5	-5.04	126.08	128.60
25	AY	65	G	N9-C4-C5	5.04	107.42	105.40
1	AA	98	G	N3-C4-N9	5.04	129.02	126.00
26	BA	383	U	O4'-C1'-N1	5.04	112.23	108.20
1	AA	1035	A	N1-C2-N3	5.03	131.82	129.30
40	BT	118	ARG	NE-CZ-NH1	5.02	122.81	120.30
26	DA	512	G	O4'-C1'-N9	5.02	112.22	108.20
26	DA	1131	G	O4'-C1'-N9	5.01	112.21	108.20
26	DA	1899	G	N3-C4-N9	5.01	129.01	126.00
26	BA	774	A	C8-N9-C4	-5.01	103.80	105.80
26	BA	933	A	N7-C8-N9	5.01	116.30	113.80
26	DA	90	U	C2-N1-C1'	5.00	123.70	117.70
26	DA	2140	C	C6-N1-C2	-5.00	118.30	120.30

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	AB	18	GLY	Peptide
2	AB	231	GLU	Peptide
2	AB	8	LYS	Peptide
2	AB	9	GLU	Peptide
7	AG	78	ARG	Peptide
7	AG	79	ARG	Peptide
51	B4	52	THR	Peptide
51	B4	59	PHE	Peptide
28	BD	274	ARG	Peptide
39	BS	58	LEU	Peptide
7	CG	78	ARG	Peptide
20	CT	9	ASN	Peptide
51	D4	67	TYR	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32205	0	16254	495	0
1	CA	32312	0	16307	663	0
2	AB	1846	0	1867	92	0
2	CB	1825	0	1828	102	0
3	AC	1552	0	1546	53	0
3	CC	1542	0	1517	81	0
4	AD	1659	0	1676	73	0
4	CD	1674	0	1714	61	0
5	AE	1129	0	1185	34	0
5	CE	1133	0	1191	33	0
6	AF	806	0	793	24	0
6	CF	816	0	808	18	0
7	AG	1231	0	1238	28	0
7	CG	1235	0	1249	37	0
8	AH	1088	0	1126	26	0
8	CH	1088	0	1126	42	0
9	AI	983	0	986	47	0
9	CI	978	0	966	47	0
10	AJ	709	0	650	35	0
10	CJ	714	0	672	36	0
11	AK	829	0	825	20	0
11	CK	833	0	836	14	0
12	AL	930	0	980	24	0
12	CL	930	0	980	27	0
13	AM	958	0	1002	31	0
13	CM	950	0	988	39	0
14	AN	492	0	529	16	0
14	CN	492	0	529	33	0
15	AO	728	0	760	20	0
15	CO	728	0	760	31	0
16	AP	681	0	697	12	0
16	CP	677	0	686	23	0
17	AQ	823	0	891	22	0
17	CQ	823	0	891	15	0
18	AR	555	0	618	17	0
18	CR	555	0	618	16	0
19	AS	652	0	662	31	0
19	CS	646	0	644	42	0
20	AT	728	0	798	32	0
20	CT	727	0	796	25	0
21	AU	199	0	208	8	0
21	CU	199	0	208	10	0
22	AV	277	0	140	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	CV	252	0	130	7	0
23	AW	1607	0	839	55	0
23	CW	1560	0	803	55	0
24	AX	1625	0	828	34	0
24	CX	1625	0	828	33	0
25	AY	1581	0	805	96	0
25	CY	1561	0	796	79	0
26	BA	60729	0	30621	669	0
26	DA	60311	0	30409	876	0
27	BB	2573	0	1306	19	0
27	DB	2573	0	1306	50	0
28	BD	2136	0	2218	51	0
28	DD	2136	0	2218	61	0
29	BE	1559	0	1618	30	0
29	DE	1559	0	1618	45	0
30	BF	1584	0	1625	47	0
30	DF	1580	0	1619	50	0
31	BG	1425	0	1443	38	0
31	DG	1424	0	1434	66	0
32	BH	1330	0	1407	28	0
32	DH	1330	0	1407	30	0
33	BI	1085	0	1114	41	0
33	DI	1061	0	1080	25	0
34	BN	1117	0	1183	17	0
34	DN	1117	0	1184	27	0
35	BO	933	0	996	20	0
35	DO	933	0	996	29	0
36	BP	1135	0	1212	38	0
36	DP	1135	0	1212	43	0
37	BQ	1122	0	1179	31	0
37	DQ	1122	0	1179	35	0
38	BR	968	0	1033	18	0
38	DR	968	0	1033	28	0
39	BS	877	0	938	23	0
39	DS	870	0	923	34	0
40	BT	1091	0	1151	27	0
40	DT	1083	0	1136	31	0
41	BU	959	0	1019	17	0
41	DU	959	0	1019	38	0
42	BV	771	0	830	13	0
42	DV	771	0	830	25	0
43	BW	886	0	939	12	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	DW	886	0	940	9	0
44	BX	750	0	814	16	0
44	DX	750	0	814	23	0
45	BY	806	0	881	23	0
45	DY	806	0	881	26	0
46	BZ	1349	0	1355	44	0
46	DZ	1360	0	1363	61	0
47	B0	653	0	674	14	0
47	D0	653	0	674	20	0
48	B1	755	0	826	18	0
48	D1	755	0	826	18	0
49	B2	588	0	643	11	0
49	D2	588	0	643	12	0
50	B3	469	0	518	9	0
50	D3	464	0	514	12	0
51	B4	558	0	544	22	0
51	D4	532	0	503	31	0
52	B5	455	0	465	11	0
52	D5	455	0	465	12	0
53	B6	453	0	473	13	0
53	D6	449	0	469	9	0
54	B7	418	0	467	9	0
54	D7	418	0	467	10	0
55	B8	511	0	571	21	0
55	D8	517	0	582	10	0
56	B9	307	0	335	7	0
56	D9	307	0	335	13	0
57	AA	214	0	0	0	0
57	AE	3	0	0	0	0
57	AF	1	0	0	0	0
57	AK	1	0	0	0	0
57	AM	1	0	0	0	0
57	AN	2	0	0	0	0
57	AW	4	0	0	0	0
57	AX	15	0	0	0	0
57	AY	3	0	0	0	0
57	B0	3	0	0	0	0
57	B1	1	0	0	0	0
57	B2	1	0	0	0	0
57	B3	2	0	0	0	0
57	B4	1	0	0	0	0
57	B5	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	B6	2	0	0	0	0
57	B7	5	0	0	0	0
57	B8	1	0	0	0	0
57	B9	1	0	0	0	0
57	BA	812	0	0	0	0
57	BB	20	0	0	0	0
57	BD	9	0	0	0	0
57	BE	8	0	0	0	0
57	BF	9	0	0	0	0
57	BG	3	0	0	0	0
57	BN	6	0	0	0	0
57	BO	2	0	0	0	0
57	BP	5	0	0	0	0
57	BQ	5	0	0	0	0
57	BR	2	0	0	0	0
57	BU	8	0	0	0	0
57	BV	5	0	0	0	0
57	BW	4	0	0	0	0
57	BX	3	0	0	0	0
57	BY	1	0	0	0	0
57	BZ	1	0	0	0	0
57	CA	170	0	0	0	0
57	CD	1	0	0	0	0
57	CE	1	0	0	0	0
57	CF	1	0	0	0	0
57	CJ	1	0	0	0	0
57	CK	1	0	0	0	0
57	CT	1	0	0	0	0
57	CV	1	0	0	0	0
57	CW	1	0	0	0	0
57	CX	3	0	0	1	0
57	D0	1	0	0	0	0
57	D3	1	0	0	0	0
57	D8	1	0	0	0	0
57	DA	677	0	0	0	0
57	DB	13	0	0	0	0
57	DD	9	0	0	0	0
57	DE	4	0	0	0	0
57	DF	4	0	0	0	0
57	DG	1	0	0	0	0
57	DN	1	0	0	0	0
57	DO	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	DP	2	0	0	0	0
57	DQ	4	0	0	0	0
57	DR	1	0	0	0	0
57	DU	2	0	0	0	0
57	DV	3	0	0	0	0
57	DW	4	0	0	0	0
57	DX	1	0	0	0	0
57	DY	1	0	0	0	0
58	AD	8	0	0	0	0
58	CD	8	0	0	0	0
59	AN	1	0	0	0	0
59	B4	1	0	0	0	0
59	B5	1	0	0	0	0
59	B6	1	0	0	0	0
59	B9	1	0	0	0	0
59	BY	1	0	0	0	0
59	CN	1	0	0	0	0
59	D4	1	0	0	0	0
59	D5	1	0	0	0	0
59	D6	1	0	0	0	0
59	D9	1	0	0	0	0
59	DY	1	0	0	0	0
60	AX	1	0	0	0	0
60	CX	1	0	0	0	0
61	AA	227	0	0	17	0
61	AE	2	0	0	0	0
61	AJ	1	0	0	0	0
61	AL	1	0	0	1	0
61	AM	1	0	0	0	0
61	AU	1	0	0	1	0
61	AV	3	0	0	0	0
61	AW	3	0	0	0	0
61	AX	6	0	0	2	0
61	AY	1	0	0	0	0
61	B0	3	0	0	0	0
61	B1	1	0	0	0	0
61	B3	2	0	0	0	0
61	B5	2	0	0	0	0
61	B6	1	0	0	0	0
61	B7	2	0	0	0	0
61	B8	8	0	0	1	0
61	BA	1383	0	0	61	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	BB	36	0	0	1	0
61	BD	12	0	0	1	0
61	BE	14	0	0	4	0
61	BF	8	0	0	0	0
61	BG	3	0	0	0	0
61	BI	1	0	0	0	0
61	BO	4	0	0	0	0
61	BP	16	0	0	3	0
61	BQ	4	0	0	0	0
61	BR	2	0	0	0	0
61	BT	2	0	0	0	0
61	BU	3	0	0	0	0
61	BV	2	0	0	0	0
61	BW	1	0	0	0	0
61	BX	4	0	0	0	0
61	BZ	1	0	0	0	0
61	CA	185	0	0	17	0
61	CJ	2	0	0	1	0
61	CL	1	0	0	0	0
61	CT	1	0	0	0	0
61	CV	1	0	0	0	0
61	CW	2	0	0	0	0
61	D0	3	0	0	0	0
61	D1	1	0	0	0	0
61	D3	1	0	0	1	0
61	D7	3	0	0	0	0
61	D8	4	0	0	0	0
61	DA	1025	0	0	79	0
61	DB	9	0	0	0	0
61	DD	19	0	0	4	0
61	DE	11	0	0	0	0
61	DF	3	0	0	0	0
61	DN	2	0	0	1	0
61	DO	1	0	0	0	0
61	DP	16	0	0	2	0
61	DR	1	0	0	0	0
61	DT	3	0	0	0	0
61	DU	2	0	0	0	0
61	DX	3	0	0	0	0
61	DY	2	0	0	0	0
All	All	297141	0	196251	5228	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 11.

All (5228) 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)
25:CY:7:A:N6	25:CY:66:U:H3	1.37	1.21
25:AY:49:C:N4	25:AY:65:G:H1	1.44	1.16
26:DA:2139:C:N4	26:DA:2152:G:H1	1.42	1.16
1:CA:1000:U:H3	1:CA:1041:A:N6	1.44	1.15
1:CA:1002:G:H1	1:CA:1038:C:N4	1.48	1.12
26:BA:2136:C:N4	26:BA:2155:G:H1	1.51	1.08
26:DA:2138:C:N4	26:DA:2153:G:H1	1.54	1.03
26:DA:2121:G:H1	26:DA:2177:C:N4	1.54	1.02
23:AW:26:A:H61	23:AW:44:G:H1	1.04	1.02
2:CB:16:HIS:HB2	2:CB:204:ASN:HB3	1.36	1.01
25:CY:19:G:N2	25:CY:56:C:N3	2.08	1.01
25:CY:19:G:H1	25:CY:56:C:N4	1.58	1.01
1:CA:999:C:H42	1:CA:1042:G:H1	1.07	1.01
25:CY:50:U:H3	25:CY:64:A:N6	1.58	1.00
26:BA:1019:U:HO2'	26:BA:1021:A:H2	1.07	1.00
2:CB:16:HIS:HB3	2:CB:210:SER:HB2	1.44	1.00
1:CA:1162:C:H42	1:CA:1174:G:H1	1.01	0.99
2:AB:16:HIS:HB2	2:AB:204:ASN:HB3	1.41	0.98
25:CY:8:4SU:HN3	25:CY:14:A:H62	1.10	0.98
26:DA:2124:G:H1	26:DA:2174:C:N4	1.62	0.97
26:BA:1798:U:H5'	28:BD:259:THR:HG22	1.47	0.97
26:BA:993:G:OP1	41:BU:50:ARG:NH2	1.98	0.97
25:AY:7:A:H61	25:AY:66:U:H3	1.11	0.97
1:CA:1162:C:N4	1:CA:1174:G:H1	1.63	0.96
1:AA:1502:A:H2	1:AA:1505:G:H1	1.10	0.96
7:AG:50:ILE:HD11	7:AG:58:PRO:HA	1.48	0.95
26:BA:2123:G:H1	26:BA:2175:C:H42	1.12	0.95
23:CW:66:U:H3'	23:CW:67:C:H5''	1.49	0.95
25:CY:51:U:H3	25:CY:63:G:H1	1.13	0.95
27:DB:22:U:H3	27:DB:61:G:H1	1.11	0.94
25:AY:49:C:N3	25:AY:65:G:N2	2.14	0.94
24:AX:5:G:H1	24:AX:68:C:N4	1.65	0.94
1:CA:76:C:N4	1:CA:93:G:H1	1.66	0.93
42:DV:100:ARG:HH11	42:DV:100:ARG:HG3	1.33	0.93
23:AW:29:G:H1	23:AW:41:C:H42	1.16	0.93
25:CY:50:U:H3	25:CY:64:A:H61	0.96	0.92
1:CA:76:C:H42	1:CA:93:G:H1	0.97	0.92
46:BZ:153:SER:HB3	46:BZ:167:PRO:HB3	1.49	0.92

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:BA:2136:C:H42	26:BA:2155:G:H1	0.96	0.92
5:CE:100:VAL:O	5:CE:107:ARG:NH2	2.02	0.92
2:CB:179:LYS:HA	8:CH:72:PRO:HG3	1.51	0.91
23:AW:50:U:H3	23:AW:64:A:H61	1.02	0.91
26:BA:517:C:OP1	52:B5:16:ARG:NH2	2.04	0.91
26:DA:2124:G:H1	26:DA:2174:C:H42	1.17	0.91
26:DA:1204:A:H2	26:DA:1241:A:H62	1.19	0.90
24:AX:5:G:H1	24:AX:68:C:H42	0.92	0.90
26:DA:2206:G:H3'	26:DA:2207:G:C8	2.07	0.89
25:CY:15:G:N1	25:CY:48:C:N3	2.19	0.89
25:AY:26:A:H61	25:AY:44:G:H1	1.14	0.88
25:CY:9:A:N6	25:CY:23:A:OP2	2.06	0.88
1:CA:922:G:H4'	5:CE:20:GLN:HA	1.56	0.88
1:CA:1000:U:H3	1:CA:1041:A:H61	0.88	0.88
1:CA:1502:A:H2	1:CA:1505:G:H1	1.22	0.87
1:AA:664:G:H22	1:AA:741:G:H1	1.19	0.87
1:CA:1002:G:N2	1:CA:1038:C:N3	2.23	0.87
47:B0:11:ARG:O	47:B0:14:ARG:NH2	2.07	0.87
23:AW:50:U:H3	23:AW:64:A:N6	1.71	0.87
26:DA:994:C:OP1	41:DU:53:ARG:NH2	2.08	0.87
23:AW:76:31M:H5'	23:AW:76:31M:H8	1.56	0.87
26:DA:1689:A:H62	26:DA:1698:A:H2	1.20	0.86
26:DA:1798:U:H5'	28:DD:259:THR:HG22	1.55	0.86
1:AA:1025:U:O2	1:AA:1036:G:O6	1.93	0.86
29:BE:47:VAL:HG21	29:BE:86:PRO:HD2	1.57	0.86
26:DA:397:G:N7	61:DA:4625:HOH:O	2.08	0.86
1:CA:664:G:H22	1:CA:741:G:H1	1.24	0.86
26:DA:827:U:OP1	61:DA:4303:HOH:O	1.91	0.85
1:CA:1360:A:OP2	14:CN:35:ARG:NH2	2.10	0.85
26:DA:1169:G:H1	26:DA:1180:C:H42	1.23	0.85
26:DA:2130:U:H4'	26:DA:2133:G:H4'	1.58	0.85
10:AJ:35:SER:HB3	10:AJ:73:ASP:HB2	1.59	0.85
30:DF:53:THR:HG22	30:DF:56:GLU:HG3	1.58	0.84
26:BA:1689:A:H62	26:BA:1698:A:H2	1.25	0.84
26:DA:2430:A:OP2	61:DA:4303:HOH:O	1.94	0.84
26:BA:631:A:OP1	36:BP:65:ARG:NH1	2.10	0.84
7:CG:79:ARG:HE	7:CG:80:VAL:HG23	1.42	0.84
26:DA:2138:C:N3	26:DA:2153:G:N2	2.24	0.84
26:BA:100:G:O2'	49:B2:7:ARG:NH2	2.10	0.84
26:BA:2287:A:H62	26:BA:2344:U:H3	1.23	0.84
9:CI:51:ARG:HG2	9:CI:56:LEU:HD21	1.60	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:36:C:OP1	12:CL:123:LYS:NZ	2.11	0.84
33:BI:92:VAL:HG13	33:BI:120:ILE:HB	1.60	0.83
1:CA:427:U:OP1	4:CD:13:ARG:NH2	2.11	0.83
23:AW:26:A:N6	23:AW:44:G:H1	1.75	0.83
30:DF:53:THR:HG23	30:DF:55:GLY:H	1.44	0.83
23:AW:6:G:H1	23:AW:67:C:N4	1.77	0.82
10:CJ:7:LYS:HG3	10:CJ:71:LEU:HD12	1.60	0.82
29:DE:11:MET:HG2	29:DE:24:THR:HB	1.61	0.82
25:AY:50:U:O4	25:AY:64:A:N1	2.13	0.82
26:BA:1176:G:H1'	26:BA:1177:A:H5'	1.59	0.82
35:DO:35:VAL:HG11	35:DO:103:ALA:HB3	1.62	0.82
3:AC:40:ARG:NH2	3:AC:55:VAL:O	2.12	0.82
3:CC:58:GLU:HB3	10:CJ:92:THR:HG21	1.59	0.82
26:BA:885:C:H3'	26:BA:886:C:H5''	1.61	0.82
25:CY:31:A:N1	25:CY:39:PSU:O2	2.13	0.82
36:DP:100:LEU:HD12	36:DP:112:LEU:HD11	1.60	0.82
26:BA:2100:G:H1	26:BA:2189:U:H3	1.27	0.82
23:CW:4:C:N4	23:CW:69:G:H1	1.77	0.82
25:CY:19:G:H1	25:CY:56:C:H42	0.85	0.82
4:AD:158:ILE:H	4:AD:158:ILE:HD13	1.45	0.81
1:CA:1029:C:N3	1:CA:1032:G:N2	2.28	0.81
19:AS:50:ALA:HB1	19:AS:57:HIS:HB3	1.62	0.81
46:BZ:117:LEU:HD11	46:BZ:144:LEU:HD22	1.61	0.81
1:CA:1029:C:N4	1:CA:1032:G:N1	2.29	0.81
26:DA:2136:C:HO2'	26:DA:2137:C:H6	1.29	0.81
26:DA:2139:C:H42	26:DA:2152:G:H1	0.83	0.81
1:CA:1153:C:H42	1:CA:1154:G:H21	1.28	0.81
26:BA:279:C:H42	26:BA:361:G:H1	1.26	0.81
26:DA:2124:G:N2	26:DA:2174:C:N3	2.28	0.81
46:DZ:126:VAL:HG11	46:DZ:161:VAL:HG23	1.61	0.81
26:BA:1530:C:O2'	26:BA:1531:C:O5'	1.99	0.81
26:DA:2114:A:N6	26:DA:2119:A:N7	2.28	0.81
26:BA:2723:C:OP1	38:BR:3:HIS:ND1	2.12	0.81
1:CA:999:C:N4	1:CA:1042:G:H1	1.77	0.81
26:DA:2121:G:N2	26:DA:2177:C:N3	2.27	0.81
1:CA:201:C:H42	1:CA:216:G:H1	1.28	0.80
32:BH:59:ARG:HB2	32:BH:59:ARG:HH11	1.43	0.80
19:CS:50:ALA:HB1	19:CS:57:HIS:HB3	1.62	0.80
26:DA:2114:A:N1	26:DA:2171:A:N6	2.29	0.80
1:AA:407:G:H5''	4:AD:115:ARG:HG2	1.62	0.80
39:BS:25:ARG:NH1	39:BS:42:ASP:OD1	2.14	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:DA:1315:C:OP2	61:DA:4172:HOH:O	1.99	0.80
26:DA:529:A:N6	26:DA:2041:U:O2	2.14	0.80
1:CA:985:C:H42	1:CA:1220:G:H1	1.24	0.80
1:AA:742:G:OP2	15:AO:35:ARG:NH2	2.12	0.80
1:CA:1317:C:N3	19:CS:37:ARG:NH2	2.30	0.80
26:DA:2819:G:N7	61:DA:4078:HOH:O	2.15	0.80
26:BA:1466:G:HO2'	26:BA:1546:C:HO2'	1.22	0.79
25:CY:53:G:O6	25:CY:61:C:N4	2.16	0.79
26:DA:2139:C:N3	26:DA:2152:G:N2	2.26	0.79
25:AY:19:G:N2	25:AY:56:C:N3	2.30	0.79
25:CY:19:G:N1	25:CY:56:C:N4	2.23	0.79
1:CA:1133:G:H1	1:CA:1141:C:H42	1.26	0.79
25:CY:8:4SU:S4	25:CY:14:A:N7	2.56	0.79
26:DA:2682:U:OP2	61:DA:3832:HOH:O	2.00	0.79
1:CA:1000:U:O2	1:CA:1041:A:N1	2.15	0.79
26:DA:1530:C:O2'	26:DA:1531:C:O5'	2.01	0.79
26:BA:1506:C:H2'	26:BA:1507:A:H8	1.47	0.79
26:BA:2683:C:O2	35:BO:70:LYS:NZ	2.15	0.79
35:BO:35:VAL:HG11	35:BO:103:ALA:HB3	1.64	0.79
1:CA:1024:G:H2'	1:CA:1025:U:H5''	1.62	0.79
26:DA:2138:C:H42	26:DA:2153:G:H1	0.80	0.79
9:CI:71:SER:HA	9:CI:74:ILE:HD12	1.65	0.78
23:CW:29:G:H1	23:CW:41:C:H42	1.29	0.78
26:BA:2808:U:O2	26:BA:2892:A:N6	2.15	0.78
1:CA:656:C:O2'	15:CO:28:GLN:NE2	2.15	0.78
26:DA:1324:G:N7	61:DA:3887:HOH:O	2.15	0.78
1:CA:582:U:OP1	15:CO:68:ARG:NH2	2.16	0.78
26:BA:2141:G:H1	26:BA:2149:G:H22	1.31	0.78
1:CA:975:A:H4'	1:CA:976:G:H5''	1.64	0.78
1:AA:1158:C:H5	1:AA:1181:G:H1	1.32	0.78
1:AA:156:G:N2	1:AA:165:C:O2	2.17	0.78
5:CE:122:GLU:O	5:CE:126:ARG:NH1	2.16	0.78
47:D0:11:ARG:O	47:D0:14:ARG:NH2	2.17	0.78
26:BA:2123:G:H1	26:BA:2175:C:N4	1.81	0.78
25:CY:15:G:N2	25:CY:48:C:H42	1.82	0.78
26:DA:2608:G:N7	61:DA:4023:HOH:O	2.17	0.78
46:DZ:19:ARG:NH1	46:DZ:84:GLU:O	2.17	0.78
26:DA:1648:C:OP1	61:DA:4215:HOH:O	2.01	0.78
9:AI:50:LEU:HD23	9:AI:81:ILE:HD11	1.67	0.77
25:CY:62:C:H2'	25:CY:63:G:H8	1.49	0.77
1:AA:559:A:OP1	5:AE:126:ARG:NH2	2.18	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:DA:2287:A:H62	26:DA:2344:U:H3	1.30	0.77
1:CA:1151:A:HO2'	1:CA:1152:A:H8	1.32	0.77
1:CA:985:C:N4	1:CA:1220:G:H1	1.81	0.77
13:AM:3:ARG:HD2	13:AM:9:ILE:HG12	1.65	0.77
26:BA:2136:C:N3	26:BA:2155:G:N2	2.27	0.77
1:CA:1255:G:OP1	10:CJ:45:ARG:NH2	2.17	0.77
26:BA:998:C:OP1	61:BA:4663:HOH:O	2.02	0.77
46:BZ:72:ARG:NH2	46:BZ:97:GLU:O	2.18	0.77
3:CC:129:ALA:HB3	3:CC:132:ARG:HB2	1.67	0.77
25:CY:25:C:H2'	25:CY:26:A:H8	1.47	0.77
1:AA:1260:C:O2	1:AA:1275:A:N6	2.17	0.77
33:BI:129:THR:HG22	33:BI:139:GLN:HE22	1.48	0.77
23:CW:19:G:H1	23:CW:56:C:H42	1.33	0.77
25:AY:7:A:N6	25:AY:66:U:H3	1.82	0.77
23:AW:53:G:OP1	37:BQ:60:ARG:NH2	2.17	0.77
1:AA:1422:G:H5''	35:BO:48:PRO:HB3	1.67	0.76
26:BA:927:G:N7	61:BA:4413:HOH:O	2.17	0.76
1:CA:1025:U:H3	1:CA:1036:G:H1	1.32	0.76
37:DQ:135:ASP:OD2	46:DZ:49:ARG:NH2	2.18	0.76
26:BA:400:G:N7	61:BA:5004:HOH:O	2.17	0.76
1:CA:838:G:H1	1:CA:848:C:N4	1.84	0.76
26:BA:1452:A:OP2	61:BA:4011:HOH:O	2.02	0.76
42:BV:40:LEU:HB2	42:BV:46:VAL:HG13	1.67	0.76
30:BF:18:ARG:NH2	30:BF:127:GLU:OE1	2.18	0.76
1:CA:1422:G:H5''	35:DO:48:PRO:HB3	1.67	0.76
23:CW:4:C:N3	23:CW:69:G:N2	2.34	0.76
26:DA:143:G:H4'	44:DX:35:THR:HG21	1.68	0.76
26:DA:2723:C:H5''	38:DR:1:MET:HE2	1.66	0.76
1:AA:975:A:H4'	1:AA:976:G:H5''	1.67	0.76
26:BA:2103:C:H42	26:BA:2186:G:H1	1.30	0.76
28:DD:238:GLY:O	61:DD:408:HOH:O	2.03	0.76
12:AL:71:PRO:O	12:AL:102:ARG:NH1	2.18	0.76
1:CA:1054:C:O2'	1:CA:1055:A:O5'	2.02	0.76
56:D9:25:VAL:HB	56:D9:34:GLN:HB2	1.66	0.76
3:CC:98:ASN:N	3:CC:98:ASN:OD1	2.19	0.76
26:BA:11:G:H2'	26:BA:12:U:H5''	1.68	0.76
26:DA:880:G:N1	26:DA:898:C:O2	2.18	0.76
51:D4:38:LYS:O	51:D4:40:HIS:N	2.17	0.76
13:CM:25:ILE:HD11	13:CM:66:LEU:HD13	1.68	0.75
36:BP:126:VAL:HG12	36:BP:148:LEU:HD22	1.66	0.75
2:CB:17:PHE:HB2	2:CB:44:LEU:HD11	1.66	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:DA:792:G:O6	61:DA:4162:HOH:O	2.03	0.75
29:DE:14:ILE:HG13	29:DE:21:VAL:HG13	1.68	0.75
36:DP:29:LYS:HG3	36:DP:30:THR:N	2.01	0.75
1:AA:532:A:H2	1:AA:1206:G:H21	1.35	0.75
24:AX:6:G:H1	24:AX:67:C:H42	1.34	0.75
26:BA:1332:G:OP1	61:BA:4653:HOH:O	2.03	0.75
42:BV:76:LYS:HB2	42:BV:81:TYR:HB3	1.68	0.75
23:CW:49:C:N4	23:CW:65:G:O6	2.20	0.75
23:CW:4:C:H42	23:CW:69:G:H1	1.33	0.75
6:CF:9:VAL:HB	6:CF:87:ARG:HB2	1.68	0.75
10:AJ:17:ASP:OD1	10:AJ:70:ARG:NH1	2.20	0.75
1:CA:1013:G:N2	1:CA:1016:A:OP2	2.19	0.75
26:DA:631:A:OP1	36:DP:65:ARG:NH1	2.20	0.75
1:CA:1456:G:O6	20:CT:54:LYS:NZ	2.16	0.75
26:DA:2638:G:OP2	29:DE:82:ARG:NH2	2.19	0.75
1:AA:1183:A:H3'	1:AA:1184:G:H5''	1.69	0.75
26:BA:271(R):G:OP1	48:B1:76:ARG:NH1	2.19	0.75
26:BA:307:G:H21	26:BA:330:A:H62	1.35	0.75
1:CA:1149:C:O2'	1:CA:1280:A:N1	2.18	0.75
1:AA:574:A:OP2	61:AA:4005:HOH:O	2.05	0.75
1:AA:78:G:N2	1:AA:91:C:N3	2.35	0.75
23:AW:29:G:H1	23:AW:41:C:N4	1.84	0.75
23:AW:6:G:N2	23:AW:67:C:N3	2.34	0.75
35:BO:64:ARG:NH2	35:BO:99:PHE:O	2.20	0.75
3:CC:179:ARG:HD2	3:CC:206:GLU:HB2	1.68	0.75
15:CO:54:ARG:NH1	15:CO:58:MET:SD	2.59	0.75
1:AA:1314:C:OP2	19:AS:4:SER:OG	2.05	0.74
1:AA:642:A:N3	8:AH:113:SER:OG	2.20	0.74
26:BA:301:G:OP2	45:BY:84:ARG:NH2	2.19	0.74
1:AA:1036:G:H21	1:AA:1037:C:H1'	1.51	0.74
26:BA:2741:A:OP1	56:B9:22:ARG:NH2	2.17	0.74
19:CS:42:PRO:HG3	51:D4:61:ARG:HG2	1.69	0.74
26:DA:1189:A:OP2	61:DA:4184:HOH:O	2.04	0.74
4:CD:104:VAL:HG11	4:CD:146:ILE:HD13	1.68	0.74
27:DB:76:G:N2	27:DB:101:G:O6	2.19	0.74
20:AT:10:LEU:HB3	20:AT:12:ALA:H	1.52	0.74
28:DD:148:GLU:HB2	28:DD:151:LYS:HD2	1.68	0.74
46:DZ:72:ARG:NH2	46:DZ:97:GLU:O	2.21	0.74
26:BA:2467:C:OP2	61:BA:5096:HOH:O	2.05	0.74
4:CD:154:ASN:HA	4:CD:159:ARG:HH21	1.53	0.74
1:CA:958:A:N6	19:CS:77:THR:O	2.20	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:DA:1815:A:OP2	28:DD:54:ARG:NH2	2.19	0.74
26:DA:449:A:OP2	61:DA:4657:HOH:O	2.05	0.74
1:CA:811:C:N4	61:CA:4023:HOH:O	2.20	0.74
25:AY:50:U:H3	25:AY:64:A:H2	1.35	0.74
23:CW:2:C:N3	23:CW:71:G:O6	2.21	0.74
23:CW:7:A:N1	23:CW:66:U:O4	2.19	0.74
26:DA:2169:A:O2'	26:DA:2170:A:O5'	2.06	0.74
27:DB:75:G:N2	46:DZ:87:ASP:OD1	2.21	0.74
26:BA:1840:G:N7	61:BA:4332:HOH:O	2.20	0.74
26:DA:2049:G:N7	61:DA:3798:HOH:O	2.19	0.74
26:DA:884:C:N4	26:DA:892:G:O6	2.20	0.74
2:AB:195:ASP:O	8:AH:68:ARG:NH2	2.21	0.74
28:BD:17:THR:O	28:BD:211:ARG:NH2	2.21	0.74
3:CC:150:LYS:HG3	3:CC:169:ALA:HB2	1.70	0.74
1:CA:1226:C:O2'	13:CM:111:LYS:NZ	2.20	0.74
26:DA:1314:C:OP1	61:DA:4172:HOH:O	2.04	0.74
4:AD:104:VAL:HG11	4:AD:146:ILE:HD13	1.69	0.74
26:BA:568:U:O4	61:BA:4141:HOH:O	2.05	0.74
36:DP:96:THR:H	36:DP:99:LEU:HD21	1.53	0.74
1:AA:911:U:OP2	12:AL:97:ARG:NH1	2.21	0.73
3:AC:15:THR:HG21	3:AC:181:ASN:HA	1.69	0.73
25:CY:62:C:H2'	25:CY:63:G:C8	2.23	0.73
49:D2:22:GLU:OE2	49:D2:68:ARG:NH2	2.21	0.73
1:AA:1505:G:O2'	22:AV:13:A:O2'	2.05	0.73
26:BA:1602:U:O4	61:BA:4228:HOH:O	2.06	0.73
26:BA:2187:G:O2'	26:BA:2188:C:OP1	2.07	0.73
1:CA:1291:G:H4'	9:CI:39:GLY:HA3	1.68	0.73
25:CY:31:A:C6	25:CY:39:PSU:O2	2.41	0.73
26:DA:2121:G:H1	26:DA:2177:C:H42	0.80	0.73
29:DE:77:ILE:HD13	29:DE:195:LEU:HD13	1.70	0.73
51:D4:40:HIS:O	51:D4:44:THR:N	2.17	0.73
51:D4:40:HIS:HB3	51:D4:43:TYR:HB2	1.71	0.73
51:B4:53:GLU:C	51:B4:55:ARG:H	1.92	0.73
5:CE:80:ILE:HG22	5:CE:91:LEU:HB2	1.71	0.73
27:DB:20:C:N4	27:DB:63:G:O6	2.19	0.73
26:DA:1959:G:N7	61:DA:4503:HOH:O	2.21	0.73
26:DA:2815:C:H5'	52:D5:29:THR:HG21	1.71	0.73
1:CA:742:G:OP2	15:CO:35:ARG:NH2	2.21	0.73
26:DA:1352:U:OP2	61:DA:3767:HOH:O	2.06	0.73
4:CD:187:ARG:NH2	4:CD:193:ASP:OD2	2.22	0.73
25:CY:18:G:N2	25:CY:55:PSU:N3	2.37	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:972:C:O2'	10:AJ:55:LYS:O	2.05	0.73
1:CA:1348:U:H4'	9:CI:120:ARG:HD2	1.71	0.73
11:CK:20:TYR:HB2	11:CK:31:THR:HG22	1.69	0.73
26:DA:11:G:N7	61:DA:4280:HOH:O	2.20	0.73
27:DB:24:G:N2	27:DB:27:C:N3	2.32	0.73
4:AD:15:GLU:HG2	4:AD:63:LYS:HB3	1.71	0.73
51:B4:59:PHE:H	51:B4:59:PHE:HD1	1.35	0.73
3:CC:43:LEU:HD21	3:CC:91:LEU:HD13	1.69	0.73
23:AW:52:G:H4'	37:BQ:56:ARG:HH22	1.54	0.72
25:AY:26:A:N6	25:AY:44:G:H1	1.85	0.72
12:CL:24:VAL:HG13	12:CL:98:TYR:HE1	1.53	0.72
1:CA:390:C:O3'	16:CP:28:ARG:NH2	2.22	0.72
25:CY:36:A:H2'	25:CY:37:MIA:O4'	1.89	0.72
31:DG:136:ARG:HD2	31:DG:137:GLU:HG3	1.70	0.72
26:DA:2562:U:H1'	35:DO:23:ARG:HH11	1.53	0.72
36:BP:94:GLU:OE2	36:BP:124:LYS:NZ	2.22	0.72
26:DA:741:G:OP2	61:DA:4224:HOH:O	2.05	0.72
1:AA:1348:U:H4'	9:AI:120:ARG:HD2	1.72	0.72
45:BY:92:ASN:HB3	45:BY:94:LYS:H	1.52	0.72
25:CY:31:A:N1	25:CY:39:PSU:C2	2.57	0.72
26:BA:1507:A:O2'	26:BA:1508:A:O4'	2.06	0.72
1:CA:976:G:H5'	1:CA:1358:U:O2'	1.89	0.72
26:DA:1449:A:O2'	26:DA:1529:G:N2	2.22	0.72
36:DP:126:VAL:HG12	36:DP:148:LEU:HD22	1.71	0.72
42:DV:6:LYS:HB2	42:DV:38:LEU:HD21	1.69	0.72
1:AA:266:G:H5''	1:AA:268:C:H41	1.53	0.72
25:AY:56:C:H2'	25:AY:57:G:O4'	1.88	0.72
26:BA:1019:U:H3	26:BA:1142(A):A:H62	1.35	0.72
25:AY:76:A:N6	26:BA:2422:A:O4'	2.22	0.72
26:BA:2810:A:N6	26:BA:2891:G:O2'	2.21	0.72
1:CA:1055:A:N7	1:CA:1200:C:N4	2.37	0.72
25:CY:26:A:N1	25:CY:44:G:O6	2.23	0.72
26:DA:2683:C:O2	35:DO:70:LYS:NZ	2.23	0.72
1:AA:1183:A:O2'	1:AA:1184:G:OP1	2.06	0.72
1:AA:347:G:O2'	1:AA:348:G:OP1	2.08	0.72
26:BA:739:G:OP1	61:BA:5196:HOH:O	2.06	0.72
1:CA:324:G:N7	61:CA:4089:HOH:O	2.23	0.72
25:CY:5:G:H1	25:CY:68:C:H42	1.36	0.72
25:AY:62:C:H2'	25:AY:63:G:H8	1.55	0.72
47:B0:10:THR:HG22	47:B0:12:ASN:H	1.54	0.72
5:CE:102:ALA:O	5:CE:107:ARG:NH1	2.22	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:DA:2166:G:H3'	26:DA:2167:U:H5''	1.70	0.72
1:CA:1009:G:N2	1:CA:1021:G:H1'	2.04	0.72
1:CA:977:A:N6	1:CA:1224:G:OP1	2.21	0.72
2:AB:16:HIS:CD2	2:AB:17:PHE:H	2.07	0.72
9:AI:128:ARG:NH2	24:AX:33:U:OP2	2.23	0.72
26:BA:1714:G:H1	26:BA:1745(A):C:H42	1.38	0.72
9:CI:53:VAL:O	9:CI:55:ALA:N	2.22	0.72
26:DA:1670:C:OP1	61:DA:3752:HOH:O	2.06	0.72
25:CY:71:G:H4'	26:DA:1851:U:H4'	1.71	0.72
28:DD:28:GLU:OE1	61:DD:416:HOH:O	2.06	0.72
1:AA:1445:C:O2	1:AA:1457:G:N2	2.20	0.72
13:CM:58:GLU:O	13:CM:62:ASN:ND2	2.14	0.72
26:DA:1604:C:OP2	61:DA:4546:HOH:O	2.08	0.72
1:AA:1442:G:O2'	1:AA:1442(A):G:OP1	2.07	0.71
2:AB:185:ILE:HG22	2:AB:199:TYR:HB2	1.70	0.71
1:CA:1162:C:N3	1:CA:1174:G:N2	2.34	0.71
48:B1:86:SER:OG	48:B1:89:GLU:OE1	2.07	0.71
26:DA:2134:A:N3	26:DA:2159:G:O2'	2.21	0.71
1:AA:1086:U:H3	1:AA:1099:G:H22	1.37	0.71
26:BA:957:A:H5'	37:BQ:76:LYS:HG3	1.72	0.71
26:DA:1890:A:OP2	61:DA:4472:HOH:O	2.08	0.71
25:CY:15:G:N2	25:CY:48:C:N4	2.38	0.71
3:AC:6:HIS:HD2	3:AC:8:ILE:H	1.37	0.71
10:AJ:37:PRO:HA	10:AJ:72:VAL:HG12	1.73	0.71
17:AQ:3:LYS:HD2	17:AQ:60:ILE:HD11	1.71	0.71
25:AY:25:C:O2'	25:AY:26:A:O5'	2.09	0.71
1:CA:1054:C:C4	23:CW:34:G:H1'	2.25	0.71
10:CJ:5:ARG:N	61:CJ:5101:HOH:O	2.22	0.71
23:CW:29:G:H1	23:CW:41:C:N4	1.87	0.71
26:DA:370:G:N7	61:DA:3786:HOH:O	2.23	0.71
46:DZ:144:LEU:HD11	46:DZ:172:ALA:HB1	1.72	0.71
26:BA:528:A:H2'	26:BA:529:A:H5''	1.72	0.71
36:BP:116:GLY:O	36:BP:137:LYS:NZ	2.22	0.71
44:BX:53:LYS:HB3	44:BX:82:GLN:HB3	1.73	0.71
2:AB:77:ALA:HB2	2:AB:211:ILE:HD13	1.72	0.71
26:BA:2124:G:H1	26:BA:2174:C:H42	1.37	0.71
1:CA:406:G:H5'	4:CD:5:ILE:HD11	1.73	0.71
26:BA:2130:U:H4'	26:BA:2133:G:H4'	1.72	0.71
17:CQ:66:SER:O	17:CQ:70:ARG:NH1	2.24	0.71
23:CW:27:G:H1	23:CW:43:C:H42	1.37	0.71
5:AE:110:LEU:HD13	5:AE:118:ILE:HG21	1.73	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CB:155:LEU:HD21	2:CB:159:PRO:HG3	1.71	0.71
12:CL:24:VAL:HG13	12:CL:98:TYR:CE1	2.24	0.71
61:DA:4209:HOH:O	29:DE:135:HIS:NE2	2.24	0.71
30:DF:33:LEU:HD13	30:DF:112:MET:HE2	1.72	0.71
46:DZ:92:SER:O	46:DZ:130:PRO:HG2	1.91	0.71
9:AI:46:ALA:HB2	9:AI:74:ILE:HG23	1.72	0.70
26:BA:1022:G:H22	26:BA:1142(A):A:H2	1.39	0.70
26:BA:1815:A:OP2	28:BD:54:ARG:NH2	2.22	0.70
40:BT:95:ARG:HG2	40:BT:95:ARG:HH11	1.54	0.70
26:DA:643:A:N1	26:DA:2369:A:O2'	2.22	0.70
26:DA:731:C:OP1	61:DA:4348:HOH:O	2.08	0.70
31:DG:63:ILE:HA	31:DG:143:GLU:HG3	1.72	0.70
46:DZ:145:GLU:H	46:DZ:148:ASP:HB2	1.57	0.70
1:AA:972:C:OP1	61:AA:4173:HOH:O	2.09	0.70
26:BA:2239:G:OP2	61:BA:4335:HOH:O	2.08	0.70
30:BF:185:ASP:HA	30:BF:188:ARG:HD3	1.70	0.70
40:BT:16:ARG:NH2	40:BT:83:ILE:O	2.24	0.70
1:CA:986:A:O2'	19:CS:55:LYS:O	2.08	0.70
38:BR:67:LEU:HD13	38:BR:76:VAL:HG21	1.72	0.70
26:DA:1637:A:OP2	61:DA:4569:HOH:O	2.09	0.70
1:AA:1492:A:O2'	1:AA:1493:A:O5'	2.08	0.70
1:AA:406:G:H5'	4:AD:5:ILE:HD11	1.73	0.70
26:BA:1310:G:OP2	54:B7:9:ARG:NH1	2.25	0.70
1:CA:771:G:N7	61:CA:4042:HOH:O	2.24	0.70
46:DZ:119:GLU:O	46:DZ:122:ARG:NH1	2.24	0.70
12:AL:70:ILE:HG12	12:AL:100:ILE:HD12	1.74	0.70
23:AW:6:G:H1	23:AW:67:C:H42	1.32	0.70
1:CA:1256:A:H61	1:CA:1278:U:H1'	1.56	0.70
10:CJ:52:GLY:O	14:CN:41:ARG:NH2	2.21	0.70
1:CA:1128:C:H1'	1:CA:1147:C:H42	1.56	0.70
2:CB:87:ARG:NH2	2:CB:220:ASP:OD1	2.24	0.70
25:CY:51:U:O2	25:CY:63:G:N2	2.23	0.70
26:BA:2102:U:O2	26:BA:2187:G:N2	2.25	0.70
26:BA:2108:C:H2'	26:BA:2109:U:H6	1.57	0.70
31:BG:41:GLN:NE2	31:BG:154:GLY:O	2.24	0.70
1:AA:134:A:H61	16:AP:25:ARG:HH12	1.39	0.70
26:BA:2102:U:H3	26:BA:2187:G:H1	1.40	0.70
26:DA:2820:A:OP2	38:DR:2:ARG:NH2	2.24	0.70
1:AA:1027:C:O2	1:AA:1034:G:C2	2.45	0.70
1:AA:1076:C:H5'	1:AA:1076:C:H6	1.57	0.70
23:AW:47:U:H5'	23:AW:47:U:H6	1.57	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:BA:729:G:OP2	28:BD:13:ARG:NH1	2.24	0.70
7:CG:113:GLU:HG2	7:CG:119:ARG:HG2	1.73	0.70
26:DA:2138:C:N4	26:DA:2153:G:N1	2.27	0.70
18:AR:26:LEU:HD21	18:AR:39:VAL:HG13	1.74	0.69
26:DA:987:G:O2'	26:DA:1000:A:N3	2.23	0.69
1:AA:96:U:HO2'	1:AA:97:G:H8	1.40	0.69
1:AA:656:C:O2'	15:AO:28:GLN:NE2	2.25	0.69
26:BA:1250:G:OP2	36:BP:21:ARG:NH1	2.26	0.69
6:CF:81:ILE:HD11	28:DD:125:ILE:HB	1.73	0.69
48:D1:59:THR:O	48:D1:91:LYS:NZ	2.24	0.69
36:BP:59:LEU:HD21	55:B8:10:ALA:HA	1.75	0.69
26:BA:2285:C:OP2	53:B6:6:ARG:NH1	2.25	0.69
26:DA:2504:U:OP2	61:DA:4169:HOH:O	2.11	0.69
44:DX:53:LYS:HB3	44:DX:82:GLN:HB3	1.74	0.69
44:DX:8:ILE:O	49:D2:36:ARG:NH2	2.25	0.69
1:AA:1414:U:H3	1:AA:1486:G:H1	1.40	0.69
28:BD:147:LEU:HD13	28:BD:155:LEU:HD21	1.73	0.69
1:CA:76:C:N3	1:CA:93:G:N2	2.34	0.69
26:DA:1011:G:OP2	41:DU:66:ASN:ND2	2.24	0.69
54:B7:24:THR:HG22	54:B7:27:GLY:H	1.57	0.69
1:CA:664:G:OP1	18:CR:64:ARG:NH2	2.26	0.69
26:DA:993:G:OP1	41:DU:50:ARG:NH2	2.25	0.69
35:DO:80:ASP:OD1	40:DT:64:ARG:NH2	2.25	0.69
28:BD:148:GLU:HB2	28:BD:151:LYS:HD2	1.75	0.69
4:AD:23:GLY:HA3	4:AD:112:VAL:HG12	1.74	0.69
3:CC:18:TRP:O	3:CC:21:ARG:NH1	2.23	0.69
30:DF:184:TYR:CE2	30:DF:188:ARG:HD2	2.28	0.69
1:CA:200:G:H1	1:CA:217:C:H42	1.40	0.69
26:DA:2323:G:O6	26:DA:2332:U:N3	2.18	0.69
1:AA:78:G:N1	1:AA:91:C:N4	2.40	0.69
2:AB:16:HIS:HB3	2:AB:210:SER:HB2	1.73	0.69
27:BB:106:G:H5'	46:BZ:31:ARG:HG2	1.75	0.69
10:CJ:49:VAL:HG23	14:CN:41:ARG:HD2	1.75	0.69
26:DA:2060:A:N3	61:DA:4112:HOH:O	2.25	0.69
26:DA:2206:G:H3'	26:DA:2207:G:H8	1.57	0.69
39:DS:93:LYS:HD2	39:DS:95:HIS:HB2	1.74	0.69
1:AA:427:U:OP1	4:AD:13:ARG:NH2	2.26	0.69
26:BA:527:C:OP1	61:BA:4682:HOH:O	2.11	0.69
37:BQ:21:THR:HG21	37:BQ:101:ARG:HD3	1.75	0.69
46:BZ:145:GLU:O	46:BZ:148:ASP:N	2.26	0.69
1:CA:1119:C:H2'	1:CA:1120:G:C8	2.28	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:20:GLU:HG2	2:AB:191:ASP:HB3	1.74	0.68
26:BA:1352:U:OP1	61:BA:4087:HOH:O	2.11	0.68
1:CA:560:U:OP2	61:CA:4161:HOH:O	2.11	0.68
26:DA:882:G:N2	26:DA:894:C:O2	2.18	0.68
26:BA:1140:C:O3'	34:BN:25:ARG:NH1	2.27	0.68
1:CA:1314:C:OP2	19:CS:4:SER:OG	2.08	0.68
31:DG:161:THR:HG22	31:DG:163:ALA:H	1.59	0.68
5:CE:20:GLN:NE2	5:CE:21:ALA:O	2.26	0.68
31:DG:41:GLN:HB3	31:DG:43:LEU:HD22	1.76	0.68
1:CA:1129:C:OP1	9:CI:16:ARG:NH1	2.26	0.68
26:DA:1223:G:N2	26:DA:1226:A:OP2	2.23	0.68
29:DE:72:VAL:HG13	29:DE:73:GLU:O	1.93	0.68
1:AA:1182:G:H4'	1:AA:1183:A:H5'	1.74	0.68
26:BA:2612:C:OP2	52:B5:2:ALA:N	2.27	0.68
1:CA:1004:A:H8	1:CA:1005:A:H4'	1.58	0.68
5:CE:7:GLU:OE1	5:CE:37:ARG:NH2	2.26	0.68
26:DA:880:G:H22	26:DA:898:C:H1'	1.59	0.68
26:DA:89:G:H3'	26:DA:90:U:H5''	1.76	0.68
1:AA:538:G:H5''	12:AL:114:LYS:HB2	1.73	0.68
26:BA:1843:C:H5'	28:BD:253:GLN:NE2	2.09	0.68
26:DA:2127:G:O6	26:DA:2161:C:N3	2.26	0.68
26:DA:2139:C:N4	26:DA:2152:G:N1	2.16	0.68
26:BA:1045:A:OP1	26:BA:1045:A:H4'	1.92	0.68
10:CJ:17:ASP:OD1	10:CJ:70:ARG:NH1	2.26	0.68
16:CP:22:THR:HA	16:CP:33:ILE:HG13	1.76	0.68
24:CX:8:4SU:O5'	24:CX:8:4SU:H6	1.93	0.68
26:DA:194:G:N7	61:DA:4296:HOH:O	2.26	0.68
33:DI:4:ILE:HG12	33:DI:18:VAL:HG22	1.76	0.68
43:DW:18:ARG:NH1	43:DW:76:VAL:O	2.27	0.68
3:AC:3:ASN:OD1	3:AC:3:ASN:N	2.26	0.68
26:BA:2110:G:O2'	26:BA:2120:G:OP2	2.12	0.68
26:DA:2165:G:H22	26:DA:2172:U:H5	1.40	0.68
1:AA:235:C:H5'	17:AQ:70:ARG:HG2	1.76	0.68
1:CA:1442:G:O2'	1:CA:1442(A):G:OP1	2.11	0.68
1:CA:952:U:O2'	1:CA:965:A:N6	2.27	0.68
15:CO:4:THR:OG1	15:CO:7:GLU:OE1	2.10	0.68
26:DA:1647:G:OP1	61:DA:4215:HOH:O	2.12	0.68
30:DF:157:VAL:HB	30:DF:194:MET:HG2	1.76	0.68
1:AA:1027:C:N3	1:AA:1034:G:C6	2.63	0.67
23:AW:66:U:H2'	23:AW:67:C:C6	2.29	0.67
26:BA:271(L):U:OP1	33:BI:50:ARG:NH1	2.26	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:446:G:H1	1:CA:488:C:H42	1.39	0.67
26:DA:857:C:OP2	47:D0:77:ARG:NH2	2.26	0.67
51:B4:55:ARG:HB2	51:B4:56:VAL:O	1.94	0.67
26:BA:2312:U:H5'	31:BG:88:ILE:HD11	1.75	0.67
1:CA:1277:C:HO2'	1:CA:1279:A:H8	1.42	0.67
15:CO:22:THR:OG1	15:CO:23:GLY:N	2.24	0.67
25:CY:25:C:H2'	25:CY:26:A:C8	2.30	0.67
1:CA:1026:G:H5'	1:CA:1027:C:O5'	1.94	0.67
1:CA:1133:G:H1	1:CA:1141:C:N4	1.92	0.67
2:AB:91:PRO:HG2	2:AB:155:LEU:HD23	1.75	0.67
30:BF:53:THR:HG23	30:BF:55:GLY:H	1.58	0.67
2:CB:88:ALA:HB2	2:CB:219:VAL:HG13	1.76	0.67
49:D2:29:LYS:HE2	49:D2:57:ILE:HG21	1.74	0.67
26:DA:1449:A:HO2'	26:DA:1529:G:N2	1.92	0.67
1:AA:324:G:N7	61:AA:4166:HOH:O	2.27	0.67
5:AE:95:ALA:HB1	5:AE:96:PRO:HD2	1.77	0.67
25:AY:66:U:H2'	25:AY:67:C:C6	2.29	0.67
26:BA:692:C:O2'	28:BD:38:LYS:NZ	2.26	0.67
1:AA:1075:C:OP1	2:AB:179:LYS:NZ	2.24	0.67
5:AE:100:VAL:O	5:AE:107:ARG:NH2	2.27	0.67
26:BA:1783:A:N7	61:BA:5061:HOH:O	2.26	0.67
46:BZ:11:GLU:O	46:BZ:36:LYS:NZ	2.23	0.67
23:CW:43:C:H2'	23:CW:44:G:C8	2.29	0.67
51:D4:24:THR:OG1	51:D4:25:TYR:N	2.24	0.67
26:BA:662:G:H5''	36:BP:16:ARG:HG2	1.75	0.67
1:AA:1103:C:OP1	2:AB:96:ARG:NH2	2.28	0.67
24:AX:5:G:N2	24:AX:68:C:N3	2.40	0.67
25:AY:22:G:H2'	25:AY:23:A:C8	2.29	0.67
26:BA:994:C:OP1	41:BU:53:ARG:NH2	2.28	0.67
1:CA:999:C:N3	1:CA:1042:G:N2	2.38	0.67
10:CJ:35:SER:HB3	10:CJ:73:ASP:HB2	1.77	0.67
26:DA:2886:G:N7	61:DA:4141:HOH:O	2.26	0.67
26:DA:307:G:N1	26:DA:310:A:OP2	2.26	0.67
28:DD:28:GLU:OE2	61:DD:417:HOH:O	2.13	0.67
31:DG:41:GLN:NE2	31:DG:154:GLY:O	2.27	0.67
1:CA:1492:A:O2'	1:CA:1493:A:O5'	2.13	0.67
13:CM:80:ARG:HH22	19:CS:69:HIS:CE1	2.12	0.67
26:BA:2759:G:N7	61:BA:4124:HOH:O	2.28	0.67
29:BE:149:ARG:O	61:BE:406:HOH:O	2.12	0.67
1:CA:316:G:OP2	1:CA:351:G:O2'	2.12	0.67
26:DA:2639:A:OP2	61:DA:3839:HOH:O	2.12	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:DA:600:G:O6	61:DA:4398:HOH:O	2.11	0.67
30:DF:178:PRO:HB3	30:DF:198:ALA:HA	1.77	0.67
1:AA:1238:A:OP2	61:AA:4160:HOH:O	2.12	0.66
1:CA:1125:U:O2'	1:CA:1126:U:H2'	1.95	0.66
1:CA:664:G:P	18:CR:64:ARG:HH22	2.18	0.66
3:CC:34:LEU:HG	3:CC:38:ARG:HH12	1.59	0.66
9:CI:46:ALA:HB2	9:CI:74:ILE:HG23	1.77	0.66
23:CW:51:U:H3	23:CW:63:G:H1	1.41	0.66
26:DA:1993:U:OP2	61:DA:4714:HOH:O	2.13	0.66
26:DA:692:C:O2'	28:DD:38:LYS:NZ	2.28	0.66
1:AA:437:U:H5'	4:AD:155:LEU:HD21	1.75	0.66
26:BA:1238:G:OP2	61:BA:5012:HOH:O	2.14	0.66
26:BA:568:U:O2'	61:BA:5168:HOH:O	2.13	0.66
26:DA:2499:C:OP2	61:DA:4653:HOH:O	2.12	0.66
26:DA:2805:G:H2'	26:DA:2807:G:C8	2.30	0.66
13:CM:3:ARG:NH2	13:CM:9:ILE:O	2.28	0.66
26:DA:1019:U:H3	26:DA:1142(A):A:H62	1.41	0.66
1:AA:410:G:OP1	4:AD:30:LYS:NZ	2.23	0.66
25:AY:9:A:H5''	25:AY:46:7MG:HN22	1.60	0.66
37:BQ:111:GLU:OE1	37:BQ:133:ARG:NH2	2.26	0.66
26:BA:84:A:H5'	45:BY:8:LYS:HG2	1.76	0.66
3:CC:6:HIS:HD2	3:CC:8:ILE:H	1.42	0.66
26:DA:2148:G:H2'	26:DA:2149:G:H8	1.60	0.66
26:DA:20:C:OP1	41:DU:22:LYS:NZ	2.25	0.66
24:AX:8:4SU:O2	24:AX:21:A:H2	1.79	0.66
25:AY:35:A:H2'	25:AY:36:A:C8	2.30	0.66
26:BA:278:A:H2'	26:BA:279:C:C6	2.30	0.66
25:CY:2:C:H2'	25:CY:3:C:H6	1.61	0.66
26:DA:2552:U:H2'	26:DA:2554:U:OP2	1.95	0.66
26:DA:307:G:H21	26:DA:330:A:H62	1.44	0.66
26:DA:770:G:OP2	61:DA:4267:HOH:O	2.12	0.66
36:DP:39:LYS:HB2	36:DP:45:LEU:HG	1.77	0.66
26:BA:250:G:OP2	55:B8:13:ARG:NH2	2.28	0.66
30:BF:53:THR:HG22	30:BF:56:GLU:HG3	1.78	0.66
1:CA:972:C:OP1	61:CA:4167:HOH:O	2.13	0.66
13:CM:6:GLY:H	13:CM:67:GLU:HG3	1.61	0.66
32:DH:46:GLU:HB2	32:DH:49:VAL:HG12	1.76	0.66
41:DU:83:LEU:HD12	41:DU:88:ILE:HD12	1.78	0.66
1:AA:1278:U:H5'	1:AA:1279:A:O4'	1.96	0.66
9:AI:71:SER:HA	9:AI:74:ILE:HD12	1.78	0.66
10:AJ:61:GLU:OE2	14:AN:45:ARG:NE	2.29	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CB:125:PRO:O	2:CB:127:ILE:N	2.27	0.66
18:CR:52:PRO:HB2	18:CR:54:ARG:HG2	1.77	0.66
1:AA:165:C:H2'	1:AA:166:G:C8	2.31	0.66
1:AA:567:G:N3	61:AA:4131:HOH:O	2.28	0.66
25:AY:9:A:O2'	25:AY:10:G:N7	2.28	0.66
26:BA:624:C:O2'	26:BA:657:U:OP1	2.12	0.66
1:CA:1352:C:OP1	21:CU:3:LYS:NZ	2.19	0.66
2:CB:122:PHE:HD1	2:CB:123:ALA:H	1.43	0.66
52:D5:16:ARG:NH1	52:D5:17:ASP:OD1	2.29	0.66
5:AE:50:GLU:HB2	5:AE:53:LEU:HD13	1.77	0.66
20:AT:43:LEU:HD13	20:AT:51:GLU:HB3	1.78	0.66
40:DT:108:ARG:HG2	40:DT:111:ARG:HH12	1.60	0.66
6:AF:97:PHE:N	18:AR:30:ASP:OD1	2.29	0.66
26:DA:2171:A:N3	26:DA:2172:U:N3	2.44	0.66
27:DB:4:C:H42	27:DB:117:G:H1	1.45	0.66
2:AB:16:HIS:CD2	2:AB:17:PHE:N	2.64	0.65
7:AG:111:ARG:NH1	7:AG:113:GLU:OE2	2.27	0.65
3:CC:137:ALA:HA	3:CC:140:ARG:HH12	1.61	0.65
10:CJ:78:ASN:O	10:CJ:80:LYS:N	2.28	0.65
25:CY:28:G:N2	25:CY:43:C:H1'	2.10	0.65
26:DA:740:U:OP2	61:DA:4223:HOH:O	2.13	0.65
4:AD:140:VAL:HG11	4:AD:146:ILE:HD11	1.78	0.65
5:AE:122:GLU:O	5:AE:126:ARG:NH1	2.29	0.65
26:BA:84:A:H5''	45:BY:8:LYS:HE3	1.77	0.65
1:CA:673:G:H2'	1:CA:674:G:C8	2.31	0.65
3:CC:15:THR:HG21	3:CC:181:ASN:HA	1.78	0.65
51:D4:62:ARG:O	51:D4:64:GLY:N	2.29	0.65
26:DA:2336:A:H61	47:D0:43:THR:HG22	1.60	0.65
31:DG:15:VAL:HG22	31:DG:175:LEU:HB3	1.78	0.65
9:AI:53:VAL:HG11	9:AI:92:TYR:CZ	2.31	0.65
20:AT:9:ASN:O	20:AT:10:LEU:HB2	1.95	0.65
46:BZ:108:PRO:HB3	46:BZ:117:LEU:HD13	1.79	0.65
1:CA:460:G:O6	1:CA:470:C:H5''	1.96	0.65
2:CB:178:ARG:HH22	8:CH:68:ARG:HH22	1.43	0.65
26:DA:2492:U:OP1	61:DA:4150:HOH:O	2.15	0.65
26:DA:1140:C:O3'	34:DN:25:ARG:NH1	2.29	0.65
26:BA:744:G:OP1	61:BA:4704:HOH:O	2.14	0.65
37:BQ:110:THR:HG23	37:BQ:113:GLN:HB2	1.78	0.65
1:CA:1015:A:N3	1:CA:1218:C:O2'	2.24	0.65
1:CA:974:A:OP2	14:CN:41:ARG:NH1	2.29	0.65
26:DA:1246:A:OP1	30:DF:38:ARG:NH1	2.30	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:DA:2260:C:OP1	61:DA:4688:HOH:O	2.14	0.65
26:DA:422:A:OP2	61:DA:3787:HOH:O	2.15	0.65
26:BA:1267:U:OP1	61:BA:5106:HOH:O	2.14	0.65
40:BT:118:ARG:HH11	40:BT:118:ARG:HG3	1.60	0.65
1:CA:396:G:O2'	1:CA:398:C:OP1	2.05	0.65
29:DE:72:VAL:HG22	29:DE:73:GLU:HG3	1.78	0.65
10:AJ:5:ARG:NE	10:AJ:73:ASP:OD1	2.30	0.65
27:BB:66:A:H61	27:BB:108:U:H2'	1.62	0.65
26:DA:2404:C:O3'	36:DP:77:ARG:NH2	2.26	0.65
31:DG:36:LYS:HG2	31:DG:160:VAL:HB	1.78	0.65
51:B4:63:TYR:N	51:B4:64:GLY:HA2	2.12	0.65
1:CA:1402:C:N4	22:CV:18:G:OP2	2.28	0.65
27:DB:5:C:H42	27:DB:116:G:H1	1.43	0.65
1:AA:1028:C:H42	1:AA:1033:G:H1	1.45	0.65
2:AB:69:LEU:HB3	2:AB:162:ILE:HG22	1.77	0.65
8:CH:29:SER:HB2	8:CH:32:LYS:HG3	1.78	0.65
30:DF:101:LEU:O	30:DF:106:ARG:NH1	2.29	0.65
30:DF:140:LEU:HD21	30:DF:170:LEU:HD11	1.79	0.65
36:DP:42:SER:O	61:DP:304:HOH:O	2.14	0.65
26:BA:2079:U:OP1	48:B1:21:ARG:NH2	2.29	0.65
26:BA:1314:C:OP1	61:BA:4653:HOH:O	2.14	0.65
29:BE:105:THR:OG1	29:BE:199:ARG:NH2	2.29	0.65
1:CA:1011:G:N2	1:CA:1019:C:H1'	2.12	0.65
1:CA:1132:C:H2'	1:CA:1133:G:H8	1.61	0.65
8:CH:45:ILE:HD13	8:CH:61:VAL:HG13	1.79	0.65
26:DA:2355:C:H4'	47:D0:24:LYS:HD3	1.79	0.65
26:DA:1642:G:N7	61:DA:4099:HOH:O	2.28	0.65
1:AA:1502:A:H2	1:AA:1505:G:N1	1.91	0.64
4:AD:64:LEU:HA	4:AD:67:ILE:HD12	1.77	0.64
1:AA:166:G:H2'	1:AA:167:G:C8	2.32	0.64
26:BA:2287:A:N6	26:BA:2344:U:H3	1.93	0.64
26:BA:568:U:H5'	26:BA:945:A:N1	2.12	0.64
2:AB:16:HIS:HE1	2:AB:214:ILE:HD11	1.63	0.64
26:BA:1113:U:H2'	26:BA:1114:G:H8	1.62	0.64
26:BA:1300:U:H4'	26:BA:1301:A:C5'	2.27	0.64
26:BA:2608:G:N7	61:BA:4411:HOH:O	2.29	0.64
33:BI:130:TYR:HB3	33:BI:138:ILE:HB	1.78	0.64
1:CA:35:G:O2'	12:CL:118:SER:O	2.15	0.64
13:CM:37:THR:O	13:CM:55:ARG:NH1	2.29	0.64
26:DA:299:A:N1	26:DA:322:A:O2'	2.25	0.64
31:DG:80:PHE:O	31:DG:82:LEU:N	2.30	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:AI:3:GLN:OE1	9:AI:20:ARG:NH2	2.27	0.64
47:B0:27:GLU:HG3	47:B0:68:GLU:HA	1.80	0.64
26:BA:1434:A:H61	26:BA:1558:A:H62	1.44	0.64
26:BA:2131:G:H5''	26:BA:2132:U:H3'	1.80	0.64
26:BA:956:G:OP2	37:BQ:14:ARG:NH2	2.25	0.64
1:CA:1024:G:C2'	1:CA:1025:U:H5''	2.27	0.64
1:CA:187:C:O2'	20:CT:89:ARG:NH2	2.28	0.64
13:CM:23:TYR:HB3	13:CM:67:GLU:HA	1.79	0.64
25:AY:19:G:N1	25:AY:56:C:N4	2.45	0.64
26:BA:1557:C:OP2	26:BA:1558:A:O2'	2.10	0.64
26:BA:607:U:OP1	30:BF:102:PRO:HA	1.98	0.64
30:BF:157:VAL:HB	30:BF:194:MET:HG2	1.79	0.64
1:CA:96:U:O2'	1:CA:97:G:H5'	1.97	0.64
12:CL:117:ARG:HB3	12:CL:122:THR:HB	1.80	0.64
1:CA:377:G:OP1	16:CP:3:LYS:HD2	1.98	0.64
20:CT:16:HIS:O	20:CT:19:SER:OG	2.13	0.64
26:DA:2624:G:N7	61:DA:4478:HOH:O	2.29	0.64
41:DU:76:TYR:OH	41:DU:92:ARG:NH1	2.30	0.64
4:AD:154:ASN:HA	4:AD:159:ARG:HH21	1.63	0.64
26:BA:887:A:O2'	26:BA:888:C:OP2	2.13	0.64
13:CM:107:ALA:HB3	13:CM:111:LYS:HD2	1.79	0.64
25:CY:12:U:O4	25:CY:23:A:N1	2.31	0.64
1:CA:1118:C:C2	1:CA:1119:C:H5	2.16	0.64
1:CA:1348:U:H2'	1:CA:1349:A:H8	1.63	0.64
37:DQ:18:LYS:O	37:DQ:98:LYS:NZ	2.26	0.64
39:DS:84:GLN:H	39:DS:111:GLU:HB2	1.62	0.64
1:CA:1032:G:H2'	1:CA:1033:G:C8	2.33	0.64
22:CV:16:A:H61	24:CX:36:U:H3	1.46	0.64
31:DG:5:VAL:HG22	31:DG:8:LYS:H	1.62	0.64
2:AB:83:MET:HB3	2:AB:234:PRO:HG2	1.80	0.64
26:BA:1047:G:H2'	26:BA:1110:G:H1	1.62	0.64
26:BA:187:G:OP2	61:BA:4468:HOH:O	2.14	0.64
26:DA:2161:C:H2'	26:DA:2162:G:C8	2.33	0.64
37:DQ:85:LYS:HG2	47:D0:7:LEU:HB3	1.80	0.64
28:BD:69:ARG:NH2	28:BD:128:GLY:O	2.30	0.64
35:BO:37:ASP:OD1	35:BO:109:LYS:NZ	2.30	0.64
26:DA:568:U:H5'	26:DA:945:A:N1	2.13	0.64
40:DT:95:ARG:HG2	40:DT:95:ARG:HH11	1.62	0.64
1:AA:11:G:O2'	1:AA:506:G:N2	2.31	0.63
25:AY:26:A:N6	25:AY:44:G:N1	2.43	0.63
53:B6:6:ARG:NH1	53:B6:26:ASN:HB2	2.12	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:BH:149:ARG:NH1	32:BH:167:GLU:OE2	2.32	0.63
1:CA:1318:A:OP1	19:CS:3:ARG:NH2	2.31	0.63
26:DA:918:A:N3	27:DB:80:U:O2'	2.28	0.63
31:DG:33:ARG:NH2	31:DG:162:THR:HG21	2.13	0.63
1:AA:922:G:H4'	5:AE:20:GLN:HA	1.79	0.63
11:AK:98:LEU:O	11:AK:101:SER:OG	2.16	0.63
26:BA:700:G:O2'	26:BA:1632:A:N3	2.29	0.63
26:BA:2328:A:H2'	26:BA:2329:G:C8	2.33	0.63
26:BA:526:A:OP1	61:BA:4682:HOH:O	2.15	0.63
1:CA:1157:A:H4'	1:CA:1158:C:O5'	1.98	0.63
1:CA:148:G:H2'	1:CA:149:A:H8	1.63	0.63
48:D1:51:VAL:HG11	48:D1:74:VAL:HG21	1.80	0.63
26:DA:2893:G:H5'	26:DA:2893:G:H8	1.63	0.63
2:AB:178:ARG:HG2	8:AH:72:PRO:HA	1.78	0.63
2:AB:178:ARG:HH21	8:AH:74:PRO:HB3	1.62	0.63
11:AK:79:SER:HA	11:AK:104:GLN:HB2	1.80	0.63
26:BA:2632:A:HO2'	26:BA:2811:G:HO2'	1.43	0.63
27:BB:105:A:OP1	46:BZ:72:ARG:NH1	2.30	0.63
1:CA:683:G:O6	61:CA:4143:HOH:O	2.14	0.63
3:CC:12:LEU:HD23	3:CC:16:ARG:HB3	1.80	0.63
26:DA:1022:G:H22	26:DA:1142(A):A:H2	1.42	0.63
26:DA:248:G:OP1	61:DA:4415:HOH:O	2.16	0.63
1:AA:1157:A:H4'	1:AA:1158:C:O5'	1.98	0.63
12:AL:49:ASN:ND2	12:AL:92:ASP:OD2	2.25	0.63
55:B8:23:VAL:HG11	55:B8:47:LYS:HD3	1.80	0.63
26:BA:2022:U:OP1	61:BA:4666:HOH:O	2.15	0.63
1:CA:991:U:O2'	1:CA:992:U:O5'	2.14	0.63
26:DA:2143:C:H2'	26:DA:2144:U:O4'	1.98	0.63
1:AA:1030(D):A:H2'	1:AA:1031:G:O4'	1.99	0.63
25:AY:55:PSU:C2	25:AY:57:G:H5'	2.34	0.63
26:BA:625:G:O6	36:BP:107:LYS:NZ	2.31	0.63
1:CA:406:G:H21	4:CD:119:GLN:HE22	1.46	0.63
3:CC:152:ILE:HG23	3:CC:199:LYS:HB2	1.80	0.63
21:CU:5:ASP:O	21:CU:11:GLY:HA3	1.98	0.63
29:DE:111:ARG:HG3	29:DE:160:TYR:CD2	2.33	0.63
1:CA:266:G:H5''	1:CA:268:C:H41	1.64	0.63
12:CL:32:PHE:HB3	12:CL:84:LEU:HD11	1.81	0.63
26:DA:662:G:OP1	61:DA:4188:HOH:O	2.15	0.63
31:DG:113:ARG:NH1	31:DG:141:PHE:O	2.32	0.63
1:AA:557:G:OP1	61:AA:4076:HOH:O	2.16	0.63
55:B8:62:LEU:HB3	55:B8:65:GLU:HG3	1.80	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:CC:125:GLU:HG3	3:CC:190:ARG:O	1.99	0.63
1:CA:1347:G:H5''	9:CI:107:ARG:HB3	1.81	0.63
26:DA:2148:G:H2'	26:DA:2149:G:C8	2.34	0.63
26:DA:2537:U:H2'	26:DA:2538:C:C6	2.33	0.63
26:DA:852:G:H2'	26:DA:853:G:H8	1.63	0.63
26:DA:2839:G:H5'	38:DR:46:GLY:HA2	1.79	0.63
1:AA:1003:G:C2	1:AA:1004:A:H1'	2.34	0.63
1:AA:352:C:OP2	61:AA:4116:HOH:O	2.15	0.63
2:AB:127:ILE:HD12	2:AB:130:ARG:HD3	1.80	0.63
5:AE:74:GLY:HA3	5:AE:116:THR:HG22	1.80	0.63
5:AE:92:LYS:HB3	5:AE:119:LEU:HB2	1.81	0.63
11:AK:99:GLN:HG2	11:AK:105:VAL:HG21	1.79	0.63
26:BA:1371:G:O6	61:BA:4345:HOH:O	2.12	0.63
1:CA:1256:A:N6	1:CA:1278:U:H1'	2.13	0.63
25:CY:27:G:O6	25:CY:43:C:N3	2.32	0.63
32:DH:159:GLU:HG3	32:DH:169:VAL:HG11	1.80	0.63
1:AA:1047:G:H5''	14:AN:4:LYS:HD2	1.81	0.62
1:AA:346:G:C4	1:AA:347:G:H1'	2.33	0.62
26:BA:1364:G:OP2	48:B1:3:LYS:HG3	1.99	0.62
26:BA:1174:A:H4'	26:BA:1175:U:OP1	1.98	0.62
28:BD:12:SER:HB3	28:BD:208:LYS:HB3	1.80	0.62
29:BE:121:ASN:ND2	61:BE:411:HOH:O	2.22	0.62
2:CB:18:GLY:HA2	2:CB:42:ILE:HG13	1.81	0.62
3:CC:22:TRP:CG	3:CC:59:ARG:HD2	2.34	0.62
25:CY:50:U:O2	25:CY:64:A:N1	2.32	0.62
49:D2:65:ASN:OD1	49:D2:69:ARG:NH1	2.32	0.62
26:DA:1803:A:O2'	28:DD:259:THR:HG21	1.98	0.62
26:DA:2183:C:H2'	26:DA:2184:G:H8	1.63	0.62
31:DG:113:ARG:NH1	31:DG:139:LEU:O	2.32	0.62
1:AA:1030(A):G:O2'	1:AA:1030(C):G:N7	2.27	0.62
1:AA:157:G:H1	1:AA:164:U:H3	1.47	0.62
33:BI:92:VAL:HG11	33:BI:144:VAL:HG11	1.82	0.62
46:BZ:117:LEU:HD21	46:BZ:144:LEU:HD13	1.80	0.62
1:CA:1029:C:N4	1:CA:1032:G:H1	1.96	0.62
1:CA:1076:C:H6	1:CA:1076:C:H5'	1.62	0.62
1:CA:1129:C:H2'	1:CA:1139:G:N7	2.13	0.62
13:CM:122:LYS:HD3	13:CM:123:ALA:H	1.64	0.62
26:DA:2273:A:H2'	26:DA:2274:A:C8	2.33	0.62
1:AA:1347:G:H5''	9:AI:107:ARG:HB3	1.81	0.62
26:BA:2689:U:H4'	26:BA:2690:C:H5'	1.82	0.62
38:BR:97:VAL:HG22	38:BR:114:VAL:HG13	1.82	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:473:G:H2'	1:CA:474:G:H8	1.62	0.62
2:CB:19:HIS:HB2	2:CB:204:ASN:HB2	1.80	0.62
15:CO:11:VAL:HG21	15:CO:34:LEU:HD22	1.81	0.62
23:CW:47:U:O2'	23:CW:48:C:OP1	2.16	0.62
1:AA:56:U:H2'	1:AA:57:G:C8	2.34	0.62
7:AG:37:ASN:ND2	9:AI:39:GLY:O	2.32	0.62
15:AO:22:THR:OG1	15:AO:23:GLY:N	2.31	0.62
26:BA:2830:G:O6	61:BA:5189:HOH:O	2.13	0.62
26:BA:1143:A:OP1	34:BN:25:ARG:NH2	2.32	0.62
26:DA:1842:G:O2'	28:DD:253:GLN:NE2	2.32	0.62
38:DR:97:VAL:HG22	38:DR:114:VAL:HG13	1.80	0.62
1:CA:1244:C:H42	1:CA:1293:G:H1	1.47	0.62
1:CA:983:A:N1	1:CA:1222:G:N2	2.47	0.62
1:CA:1054:C:N4	23:CW:34:G:H1'	2.14	0.62
26:DA:880:G:N2	26:DA:898:C:H1'	2.14	0.62
1:AA:202:U:O2'	1:AA:203:U:O5'	2.16	0.62
1:AA:277:C:H5''	17:AQ:68:ARG:NH2	2.15	0.62
25:AY:22:G:N7	25:AY:46:7MG:O6	2.32	0.62
3:CC:20:SER:HB2	3:CC:40:ARG:HH12	1.65	0.62
12:CL:60:LEU:N	12:CL:64:TYR:O	2.25	0.62
23:CW:19:G:N2	23:CW:56:C:N3	2.45	0.62
1:AA:406:G:OP2	61:AA:4123:HOH:O	2.15	0.62
3:AC:12:LEU:HD23	3:AC:16:ARG:HB3	1.81	0.62
26:BA:2893:G:O2'	26:BA:2894:G:OP2	2.14	0.62
4:CD:175:SER:HB3	4:CD:186:LEU:HD11	1.81	0.62
15:CO:5:LYS:H	15:CO:5:LYS:HD3	1.64	0.62
25:CY:9:A:O2'	25:CY:10:G:N7	2.32	0.62
27:DB:106:G:H5'	46:DZ:31:ARG:HG2	1.82	0.62
8:AH:121:ASP:OD1	8:AH:125:ARG:NH2	2.32	0.62
23:AW:56:C:H5	26:BA:897:C:O4'	1.83	0.62
26:BA:2572:A:N7	29:BE:144:ARG:HD2	2.15	0.62
34:BN:15:LEU:HD12	34:BN:137:LYS:HG2	1.82	0.62
1:CA:1067:A:N3	1:CA:1068:G:H1'	2.15	0.62
1:CA:959:A:O2'	1:CA:984:C:O2'	2.17	0.62
2:CB:50:GLU:HG3	2:CB:200:ILE:O	1.98	0.62
13:CM:4:ILE:HG23	13:CM:22:ILE:HD11	1.82	0.62
1:AA:92:C:H2'	1:AA:93:G:C8	2.35	0.62
1:CA:1151:A:O2'	1:CA:1152:A:H8	1.82	0.62
13:CM:121:LYS:H	13:CM:121:LYS:NZ	1.97	0.62
1:AA:1007:C:H2'	1:AA:1008:C:H5''	1.81	0.62
2:AB:231:GLU:HB3	2:AB:232:PRO:CD	2.30	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:AR:38:GLU:HA	18:AR:41:LYS:HD3	1.82	0.62
30:BF:101:LEU:O	30:BF:106:ARG:NH1	2.32	0.62
1:CA:1126:U:H3	10:CJ:40:LEU:HD11	1.65	0.62
26:DA:882:G:N1	26:DA:894:C:N3	2.46	0.62
26:DA:900:A:H2'	26:DA:901:A:H8	1.65	0.62
31:DG:179:PRO:HB2	51:D4:42:PHE:HE1	1.64	0.62
9:AI:53:VAL:HG11	9:AI:92:TYR:CE1	2.35	0.61
26:BA:732:C:OP2	61:BA:4004:HOH:O	2.16	0.61
1:CA:977:A:O2'	1:CA:981:U:N3	2.33	0.61
26:DA:509:C:OP1	61:DA:4324:HOH:O	2.16	0.61
28:DD:132:PRO:HD3	28:DD:190:TYR:CZ	2.35	0.61
1:AA:1027:C:C2	1:AA:1034:G:N1	2.67	0.61
1:AA:953:G:H5'	1:AA:965:A:H61	1.65	0.61
2:AB:17:PHE:HD2	2:AB:44:LEU:HD21	1.65	0.61
24:AX:6:G:H1	24:AX:67:C:N4	1.97	0.61
26:BA:2168:G:C6	26:BA:2171:A:H8	2.18	0.61
27:BB:45:A:OP2	31:BG:96:ARG:NH2	2.28	0.61
1:CA:345:C:OP2	40:DT:39:ARG:NH2	2.30	0.61
25:CY:8:4SU:HN3	25:CY:14:A:N6	1.91	0.61
26:DA:373:U:H2'	26:DA:374:A:H8	1.65	0.61
27:DB:24:G:N7	27:DB:56:G:H2'	2.15	0.61
27:DB:24:G:N3	27:DB:26:A:N6	2.48	0.61
28:DD:206:LEU:HD22	28:DD:211:ARG:HG2	1.81	0.61
1:AA:976:G:H5'	1:AA:1358:U:O2'	1.99	0.61
26:BA:2049:G:N7	61:BA:5165:HOH:O	2.31	0.61
26:DA:1261:C:OP2	43:DW:83:LYS:NZ	2.33	0.61
26:DA:2022:U:O2'	26:DA:2617:C:H5'	2.00	0.61
29:DE:52:LEU:O	29:DE:76:ARG:N	2.25	0.61
1:AA:677:U:H3	1:AA:713:G:H22	1.47	0.61
2:AB:74:LYS:NZ	2:AB:205:ASP:OD2	2.33	0.61
15:AO:79:ARG:O	15:AO:83:GLU:HB2	1.99	0.61
26:BA:1800:C:OP2	28:BD:183:ARG:NH2	2.32	0.61
1:CA:757:U:H2'	1:CA:758:G:O4'	1.99	0.61
25:CY:26:A:N1	25:CY:44:G:C6	2.69	0.61
36:DP:99:LEU:O	36:DP:103:ALA:N	2.32	0.61
1:AA:1005:A:H1'	1:AA:1036:G:H22	1.65	0.61
1:AA:1070:U:H2'	1:AA:1071:C:C6	2.36	0.61
1:AA:148:G:H2'	1:AA:149:A:H8	1.66	0.61
8:AH:51:VAL:HG11	8:AH:60:ARG:HH12	1.66	0.61
26:BA:1816:G:O6	28:BD:35:LYS:NZ	2.28	0.61
26:BA:2206:G:H5'	26:BA:2207:G:N7	2.14	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:BE:111:ARG:HG3	29:BE:160:TYR:CD2	2.34	0.61
1:CA:1120:G:O6	1:CA:1154:G:N2	2.33	0.61
2:CB:185:ILE:HG22	2:CB:199:TYR:HB2	1.83	0.61
2:CB:55:PHE:HA	2:CB:58:ILE:HB	1.82	0.61
3:CC:52:LEU:HD21	3:CC:55:VAL:HG23	1.80	0.61
12:CL:24:VAL:HG11	12:CL:27:LEU:HD22	1.81	0.61
50:D3:12:PRO:HB2	50:D3:20:LYS:HG2	1.81	0.61
26:DA:2074:U:H2'	26:DA:2075:U:C6	2.36	0.61
26:DA:2431:U:OP1	61:DA:3906:HOH:O	2.16	0.61
1:AA:1027:C:H2'	1:AA:1028:C:C5	2.35	0.61
1:AA:189:G:H1	1:AA:189(K):U:H3	1.48	0.61
26:BA:1385:G:O2'	26:BA:1396:U:O2	2.14	0.61
1:CA:985:C:N3	1:CA:1220:G:N2	2.46	0.61
3:CC:18:TRP:H	3:CC:18:TRP:HE3	1.47	0.61
3:CC:179:ARG:NH1	3:CC:206:GLU:OE1	2.33	0.61
1:CA:1148:U:H1'	9:CI:66:ARG:HH12	1.66	0.61
50:D3:6:VAL:HG13	50:D3:56:VAL:HG22	1.81	0.61
44:DX:46:ALA:O	49:D2:30:ARG:NH2	2.33	0.61
46:DZ:117:LEU:HD12	46:DZ:174:VAL:HG22	1.80	0.61
26:BA:2350:C:OP2	61:BA:4049:HOH:O	2.16	0.61
41:BU:76:TYR:OH	41:BU:92:ARG:NH1	2.33	0.61
50:D3:5:LYS:NZ	50:D3:34:GLU:OE2	2.18	0.61
1:AA:1435:G:H2'	1:AA:1436:U:C6	2.35	0.61
3:AC:39:ILE:HG23	3:AC:91:LEU:HD11	1.83	0.61
26:BA:2714:G:OP1	61:BA:4546:HOH:O	2.16	0.61
1:CA:952:U:H2'	1:CA:953:G:C8	2.36	0.61
10:CJ:27:ALA:HA	10:CJ:81:THR:HG22	1.83	0.61
25:CY:5:G:H1	25:CY:68:C:N4	1.99	0.61
26:DA:1220:A:OP2	41:DU:19:LYS:NZ	2.29	0.61
26:DA:958:U:OP2	37:DQ:14:ARG:NH1	2.33	0.61
26:DA:952:G:OP1	37:DQ:16:ARG:NH2	2.33	0.61
38:DR:33:ARG:NH1	38:DR:115:GLU:OE2	2.29	0.61
26:DA:301:G:OP2	45:DY:84:ARG:NH2	2.33	0.61
1:AA:166:G:H2'	1:AA:167:G:H8	1.65	0.61
1:AA:562:C:H1'	12:AL:15:ARG:HB3	1.82	0.61
37:BQ:85:LYS:HG2	47:B0:7:LEU:HB3	1.83	0.61
1:CA:1317:C:O2	19:CS:37:ARG:NH1	2.33	0.61
1:CA:692:U:O2'	1:CA:694:A:N7	2.31	0.61
1:CA:920:U:H2'	1:CA:921:U:C6	2.35	0.61
11:CK:34:ASP:HB3	11:CK:40:ILE:HD11	1.83	0.61
16:CP:51:VAL:HG12	16:CP:53:VAL:H	1.64	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:DA:1939:U:OP1	26:DA:2604:U:O2'	2.19	0.61
26:DA:526:A:OP1	61:DA:4194:HOH:O	2.16	0.61
27:DB:110:G:H2'	27:DB:111:G:C8	2.36	0.61
1:AA:1025:U:O2'	1:AA:1026:G:O4'	2.19	0.61
26:BA:528:A:C2'	26:BA:529:A:H5''	2.31	0.61
43:BW:14:PRO:HG2	43:BW:78:GLU:HG2	1.82	0.61
1:CA:1067:A:O2'	1:CA:1068:G:OP2	2.17	0.61
1:CA:957:U:H2'	1:CA:959:A:OP2	2.01	0.61
26:DA:2126:A:N3	26:DA:2127:G:H1'	2.16	0.61
40:DT:85:LYS:NZ	40:DT:87:ASP:OD2	2.28	0.61
2:AB:55:PHE:HA	2:AB:58:ILE:HB	1.83	0.60
26:BA:2791:C:H2'	26:BA:2792:G:C8	2.36	0.60
1:CA:646:U:H2'	1:CA:647:C:C6	2.36	0.60
2:CB:47:THR:O	2:CB:51:LEU:N	2.32	0.60
9:CI:16:ARG:HB2	9:CI:64:THR:HB	1.82	0.60
26:DA:1005:C:H2'	26:DA:1006:C:C6	2.36	0.60
26:DA:2046:G:H5'	52:D5:19:ARG:HA	1.83	0.60
26:DA:2708:G:H1'	38:DR:71:GLN:HE22	1.65	0.60
13:AM:80:ARG:HH22	19:AS:69:HIS:HE1	1.48	0.60
26:BA:1204:A:H2	26:BA:1241:A:H62	1.49	0.60
30:BF:143:ALA:HB1	30:BF:148:LEU:HB2	1.82	0.60
39:BS:56:LEU:HD12	39:BS:69:VAL:HG12	1.82	0.60
29:BE:9:VAL:HB	40:BT:3:ARG:HG2	1.82	0.60
1:CA:1376:U:H2'	1:CA:1377:A:C8	2.36	0.60
26:DA:1816:G:O6	28:DD:35:LYS:NZ	2.25	0.60
2:AB:80:ILE:HD11	2:AB:212:GLN:HA	1.82	0.60
19:AS:3:ARG:NH1	19:AS:8:GLY:O	2.35	0.60
48:B1:51:VAL:HG11	48:B1:74:VAL:HG21	1.84	0.60
27:BB:33:G:H5'	31:BG:2:PRO:HD3	1.83	0.60
1:CA:1412:C:H2'	1:CA:1413:A:C8	2.36	0.60
1:CA:148:G:H2'	1:CA:149:A:C8	2.37	0.60
38:DR:56:LYS:NZ	38:DR:90:ARG:O	2.33	0.60
46:DZ:7:ALA:HB3	46:DZ:61:LEU:HD12	1.81	0.60
1:AA:413:G:N2	1:AA:428:G:H1'	2.16	0.60
12:AL:24:VAL:HG12	12:AL:27:LEU:HB2	1.83	0.60
17:AQ:67:LYS:HA	17:AQ:70:ARG:HH12	1.66	0.60
51:B4:57:GLU:HB3	51:B4:58:ARG:HA	1.83	0.60
29:BE:29:GLY:HA3	61:BE:408:HOH:O	2.01	0.60
31:BG:47:LYS:HG3	31:BG:48:GLU:H	1.66	0.60
45:BY:92:ASN:N	45:BY:93:GLY:HA2	2.16	0.60
9:CI:23:ASN:ND2	9:CI:60:ASP:OD2	2.33	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:DA:1449:A:HO2'	26:DA:1529:G:H21	1.45	0.60
26:DA:1739:U:HO2'	26:DA:1740:G:H8	1.49	0.60
26:DA:954:G:H5''	37:DQ:13:GLN:HB3	1.83	0.60
1:AA:865:A:H2	1:AA:918:A:H4'	1.67	0.60
3:AC:150:LYS:HG3	3:AC:169:ALA:HB2	1.84	0.60
25:AY:59:U:H3'	25:AY:60:U:C6	2.35	0.60
28:BD:71:ASP:HB3	28:BD:103:ARG:NH2	2.16	0.60
36:BP:26:GLY:O	61:BP:311:HOH:O	2.16	0.60
1:CA:1151:A:O4'	10:CJ:39:PRO:HB2	2.02	0.60
1:CA:1120:G:C6	1:CA:1154:G:N2	2.69	0.60
1:CA:1157:A:H5'	1:CA:1158:C:C6	2.35	0.60
11:CK:98:LEU:O	11:CK:101:SER:OG	2.19	0.60
46:DZ:159:PRO:HA	46:DZ:161:VAL:HG12	1.84	0.60
2:AB:201:ILE:HG21	2:AB:214:ILE:HG21	1.82	0.60
1:CA:9:G:H2'	1:CA:10:A:H8	1.66	0.60
48:D1:23:LYS:HB3	48:D1:29:GLY:HA3	1.84	0.60
26:DA:2400:G:O3'	53:D6:18:ARG:NH1	2.34	0.60
46:DZ:53:ILE:HG22	46:DZ:71:VAL:O	2.02	0.60
1:AA:1026:G:O6	1:AA:1034:G:N2	2.32	0.60
4:AD:108:LEU:HD13	4:AD:174:LEU:HD13	1.83	0.60
25:AY:19:G:H1	25:AY:56:C:N4	2.00	0.60
51:B4:53:GLU:O	51:B4:55:ARG:N	2.34	0.60
26:BA:2870:C:H2'	26:BA:2871:C:O4'	2.02	0.60
1:CA:1075:C:H2'	1:CA:1076:C:H5''	1.84	0.60
1:CA:1273:G:H3'	1:CA:1274:G:H8	1.67	0.60
26:DA:1007:C:OP1	34:DN:35:ARG:NH1	2.34	0.60
26:DA:1226:A:OP1	42:DV:84:LYS:HE2	2.01	0.60
1:AA:662:G:H2'	1:AA:663:A:C8	2.37	0.60
19:AS:28:LYS:HZ2	19:AS:28:LYS:HB3	1.66	0.60
26:BA:2033:A:OP1	61:BA:4308:HOH:O	2.17	0.60
26:BA:2447:G:OP2	61:BA:4563:HOH:O	2.16	0.60
1:CA:662:G:H2'	1:CA:663:A:H8	1.67	0.60
26:DA:2291:U:H2'	26:DA:2292:C:C6	2.37	0.60
26:DA:2747:G:H1	26:DA:2754:U:H2'	1.66	0.60
26:DA:774:A:N6	61:DA:3733:HOH:O	2.35	0.60
26:DA:1693:U:O2'	28:DD:14:ARG:NH2	2.35	0.60
26:BA:880:G:N2	26:BA:898:C:O2	2.35	0.60
23:AW:56:C:P	26:BA:897:C:H5'	2.42	0.60
32:BH:25:LYS:HG2	32:BH:34:GLU:HG2	1.84	0.60
1:CA:1118:C:OP1	9:CI:104:ARG:NH1	2.34	0.60
18:CR:60:ALA:O	18:CR:64:ARG:HG3	2.02	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:DA:2808:U:C2'	26:DA:2809:A:H5'	2.32	0.60
32:DH:20:ALA:HB1	32:DH:21:PRO:HD2	1.84	0.60
36:DP:38:GLN:O	36:DP:39:LYS:HB3	2.02	0.60
26:BA:1048:A:OP2	26:BA:1109:C:N4	2.30	0.60
1:CA:542:G:OP1	4:CD:10:ARG:NH2	2.27	0.60
1:CA:1505:G:HO2'	22:CV:13:A:H2	1.49	0.60
26:DA:2136:C:O2'	26:DA:2137:C:H6	1.85	0.60
26:DA:2499:C:N3	61:DA:3930:HOH:O	2.31	0.60
26:DA:1247:A:OP1	30:DF:95:ARG:NH2	2.32	0.60
36:DP:59:LEU:HD21	55:D8:10:ALA:HA	1.82	0.60
17:AQ:66:SER:O	17:AQ:70:ARG:NH1	2.35	0.59
26:BA:1418:G:OP2	61:BA:4580:HOH:O	2.16	0.59
26:BA:2155:G:H2'	26:BA:2156:G:O4'	2.01	0.59
26:BA:2206:G:H3'	26:BA:2207:G:C8	2.37	0.59
26:BA:2871:C:N3	61:BA:4781:HOH:O	2.31	0.59
28:BD:132:PRO:HG2	28:BD:135:PHE:CD2	2.37	0.59
40:BT:118:ARG:HH22	40:BT:125:ARG:HH12	1.50	0.59
46:BZ:139:VAL:HG22	46:BZ:155:LEU:HD11	1.84	0.59
5:CE:102:ALA:HB1	5:CE:106:PRO:HG2	1.84	0.59
14:CN:6:LEU:HB3	14:CN:23:ARG:HH21	1.67	0.59
26:DA:247:G:H4'	26:DA:386:G:C5	2.36	0.59
26:DA:2638:G:P	29:DE:82:ARG:HH22	2.25	0.59
30:DF:116:ASP:OD2	36:DP:1:MET:N	2.24	0.59
1:AA:1070:U:H2'	1:AA:1071:C:H6	1.67	0.59
17:AQ:26:GLN:HG2	17:AQ:37:LYS:HG2	1.84	0.59
26:BA:1173:G:O2'	26:BA:1174:A:O5'	2.20	0.59
26:BA:898:C:H2'	26:BA:899:A:C8	2.37	0.59
31:BG:5:VAL:HG22	31:BG:8:LYS:H	1.67	0.59
32:BH:56:SER:HB3	32:BH:61:HIS:ND1	2.17	0.59
22:CV:14:A:C4	25:CY:34:G:C6	2.90	0.59
26:DA:1434:A:H61	26:DA:1558:A:H62	1.49	0.59
26:DA:2846:G:N7	61:DA:4073:HOH:O	2.32	0.59
31:DG:151:ALA:HB3	31:DG:153:ARG:HH11	1.66	0.59
42:DV:76:LYS:HB2	42:DV:81:TYR:HB3	1.83	0.59
1:AA:1292:U:P	7:AG:41:ARG:HH22	2.25	0.59
1:AA:200:G:H1	1:AA:217:C:H42	1.51	0.59
31:BG:15:VAL:HG21	31:BG:176:LEU:HD23	1.82	0.59
46:BZ:150:LEU:O	46:BZ:171:ILE:HG13	2.03	0.59
1:CA:113:G:OP1	61:CA:4148:HOH:O	2.17	0.59
1:CA:1279:A:O2'	1:CA:1281:U:OP2	2.17	0.59
1:CA:539:A:H2'	1:CA:540:G:C8	2.37	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:596:C:O2	1:CA:644:G:N2	2.17	0.59
3:CC:134:ILE:HD11	3:CC:153:VAL:HG21	1.83	0.59
13:CM:65:LYS:N	51:D4:50:VAL:HG21	2.18	0.59
14:CN:32:SER:OG	14:CN:32:SER:O	2.19	0.59
23:CW:14:A:H61	23:CW:21:A:H2	1.49	0.59
23:CW:61:C:O2'	23:CW:62:C:O5'	2.14	0.59
37:DQ:85:LYS:HB2	47:D0:7:LEU:HD12	1.83	0.59
26:DA:1800:C:OP2	28:DD:183:ARG:NH2	2.35	0.59
1:CA:1495:U:O2'	26:DA:1919:A:N1	2.31	0.59
36:DP:85:LEU:HA	36:DP:88:LEU:HD12	1.85	0.59
46:DZ:105:VAL:N	46:DZ:139:VAL:O	2.35	0.59
3:AC:19:GLU:HB3	3:AC:40:ARG:HH22	1.67	0.59
1:AA:428:G:OP2	4:AD:10:ARG:NH1	2.35	0.59
25:AY:59:U:H3'	25:AY:60:U:H6	1.68	0.59
26:BA:2103:C:N4	26:BA:2186:G:H1	1.98	0.59
1:CA:769:G:H4'	1:CA:1513:A:H4'	1.85	0.59
1:CA:254:G:OP1	17:CQ:66:SER:OG	2.17	0.59
1:CA:538:G:H5''	12:CL:114:LYS:HB2	1.82	0.59
51:D4:33:VAL:HG12	51:D4:35:VAL:H	1.66	0.59
26:DA:1446:C:H42	26:DA:1465:G:H1	1.50	0.59
30:DF:185:ASP:HA	30:DF:188:ARG:HD3	1.84	0.59
34:DN:58:ASP:OD1	34:DN:58:ASP:N	2.34	0.59
46:DZ:108:PRO:HG3	46:DZ:141:VAL:HB	1.84	0.59
1:AA:189(A):C:H42	1:AA:189(J):G:H1	1.51	0.59
1:AA:736:C:H2'	1:AA:737:A:C8	2.37	0.59
3:AC:8:ILE:HD13	3:AC:184:TYR:HB3	1.84	0.59
3:AC:82:GLU:HG2	3:AC:85:ARG:NH2	2.17	0.59
3:AC:6:HIS:CD2	3:AC:8:ILE:H	2.20	0.59
26:BA:271(M):G:H4'	26:BA:271(N):U:OP1	2.01	0.59
26:DA:2023:G:H5'	26:DA:2617:C:H4'	1.83	0.59
3:AC:114:PRO:O	3:AC:118:GLN:NE2	2.35	0.59
9:AI:21:PRO:HA	9:AI:59:PHE:HA	1.85	0.59
15:AO:18:PHE:HB2	15:AO:19:PRO:HD2	1.85	0.59
23:AW:22:G:O2'	23:AW:23:A:OP1	2.18	0.59
50:B3:23:LEU:HD13	50:B3:50:VAL:HG11	1.85	0.59
26:BA:1025:G:C4	26:BA:1135:C:H1'	2.37	0.59
26:BA:1040:C:H2'	26:BA:1041:C:O4'	2.01	0.59
26:BA:1649:G:O2'	38:BR:107:ASP:OD2	2.17	0.59
26:DA:2002:G:OP2	38:DR:9:LYS:NZ	2.35	0.59
26:DA:2140:C:H1'	26:DA:2152:G:N2	2.18	0.59
1:AA:1002:G:H3'	1:AA:1003:G:C8	2.38	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:AS:32:LYS:HA	19:AS:50:ALA:HB3	1.84	0.59
26:BA:652(E):G:O6	26:BA:652(T):C:N4	2.30	0.59
39:BS:15:ARG:O	39:BS:19:LYS:HG2	2.03	0.59
23:CW:11:C:H42	23:CW:24:G:H1	1.50	0.59
25:CY:18:G:N2	25:CY:55:PSU:C4	2.71	0.59
50:D3:7:LYS:NZ	50:D3:32:GLN:O	2.29	0.59
26:DA:2176:A:H2'	26:DA:2177:C:C6	2.37	0.59
37:DQ:31:ASP:OD1	37:DQ:134:ARG:NH1	2.32	0.59
25:AY:58:A:H3'	25:AY:58:A:P	2.43	0.59
26:BA:1405:U:H2'	26:BA:1406:U:C6	2.38	0.59
1:CA:1305:G:O2'	1:CA:1331:G:N2	2.36	0.59
26:DA:271(R):G:H5''	48:D1:97:LEU:HD21	1.84	0.59
31:DG:101:ILE:HD13	51:D4:25:TYR:HB2	1.84	0.59
26:DA:2062:A:OP1	61:DA:3829:HOH:O	2.17	0.59
1:AA:1239:A:H62	1:AA:1299:A:N6	2.01	0.59
23:AW:5:G:H2'	23:AW:6:G:H8	1.67	0.59
1:CA:1010:G:C2	1:CA:1011:G:C8	2.91	0.59
1:CA:1182:G:H4'	1:CA:1183:A:H3'	1.84	0.59
9:CI:9:ARG:O	9:CI:104:ARG:HG3	2.02	0.59
26:DA:2173:A:H2'	26:DA:2174:C:O4'	2.03	0.59
1:AA:1030(D):A:H62	1:AA:1031:G:H21	1.49	0.59
19:AS:30:LEU:HD11	19:AS:50:ALA:HB2	1.85	0.59
26:BA:1913:A:H4'	26:BA:1914:C:H5''	1.83	0.59
26:BA:322:A:OP1	30:BF:168:ARG:HD2	2.03	0.59
15:CO:18:PHE:HB2	15:CO:19:PRO:HD2	1.85	0.59
26:DA:2112:G:C5	26:DA:2113:U:H1'	2.37	0.59
26:DA:249:C:O2	55:D8:12:LYS:NZ	2.29	0.59
31:DG:64:THR:HB	31:DG:94:LEU:HD21	1.85	0.59
46:DZ:55:HIS:HE1	46:DZ:135:GLU:HG3	1.68	0.59
21:AU:5:ASP:OD2	61:AU:101:HOH:O	2.17	0.58
26:BA:2789:C:O2	26:BA:2894:G:N2	2.35	0.58
1:CA:1220:G:O3'	19:CS:36:ARG:HD3	2.03	0.58
1:CA:1510:U:H2'	1:CA:1511:G:C8	2.37	0.58
4:CD:15:GLU:OE2	4:CD:66:ARG:NH1	2.36	0.58
8:CH:4:ASP:OD1	8:CH:7:ALA:N	2.23	0.58
26:DA:2151:G:H2'	26:DA:2152:G:H8	1.67	0.58
26:DA:848:G:N3	26:DA:933:A:H1'	2.18	0.58
45:DY:5:MET:HE1	45:DY:32:PRO:HA	1.84	0.58
1:AA:1202:G:O4'	14:AN:29:ARG:NH1	2.35	0.58
1:AA:17:U:H2'	1:AA:18:C:C6	2.38	0.58
2:AB:162:ILE:O	2:AB:185:ILE:HG12	2.03	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:AT:45:GLN:HB2	20:AT:91:LEU:HD13	1.85	0.58
26:BA:526:A:O2'	26:BA:2043:C:O2	2.20	0.58
26:BA:636:G:OP1	36:BP:132:LYS:HE2	2.02	0.58
4:CD:64:LEU:HB2	4:CD:198:VAL:HG11	1.84	0.58
1:CA:1338:G:H21	24:CX:41:C:H1'	1.68	0.58
26:DA:2849:U:OP2	40:DT:95:ARG:NH1	2.37	0.58
37:DQ:111:GLU:O	37:DQ:115:MET:HG2	2.02	0.58
25:AY:53:G:C5	25:AY:54:5MU:H72	2.38	0.58
53:B6:6:ARG:NE	53:B6:24:GLU:OE1	2.22	0.58
1:CA:1204:A:OP1	14:CN:3:ARG:NH1	2.36	0.58
17:CQ:57:VAL:HG12	17:CQ:76:LEU:HA	1.84	0.58
37:DQ:48:GLU:OE1	37:DQ:51:ARG:NH2	2.33	0.58
39:DS:14:VAL:O	39:DS:18:ILE:HG12	2.03	0.58
1:AA:46:G:O6	61:AA:4200:HOH:O	2.15	0.58
23:AW:66:U:H2'	23:AW:67:C:H6	1.66	0.58
26:BA:1021:A:H62	26:BA:1141:U:H3	1.51	0.58
1:CA:504:C:OP1	61:CA:4008:HOH:O	2.17	0.58
12:CL:70:ILE:HD13	12:CL:77:LEU:HD12	1.85	0.58
35:DO:115:VAL:HG13	35:DO:121:VAL:HG21	1.86	0.58
9:AI:99:LEU:HB3	9:AI:101:PHE:CE1	2.38	0.58
23:AW:47:U:O2'	23:AW:48:C:OP1	2.20	0.58
26:BA:2336:A:H61	47:B0:43:THR:CG2	2.16	0.58
26:BA:2485:G:OP1	37:BQ:46:GLN:NE2	2.35	0.58
2:CB:77:ALA:HA	2:CB:80:ILE:HG22	1.84	0.58
5:CE:31:LEU:HD22	5:CE:43:LEU:HD11	1.85	0.58
24:CX:50:U:H3	24:CX:64:G:H1	1.51	0.58
26:DA:2365:G:O6	55:D8:43:GLN:NE2	2.36	0.58
30:DF:21:ALA:HB3	30:DF:22:ALA:HA	1.84	0.58
1:AA:1302:U:C5	13:AM:17:VAL:HG21	2.38	0.58
26:BA:184:C:H2'	26:BA:185:U:C6	2.38	0.58
1:CA:420:U:O2'	1:CA:423:G:O6	2.18	0.58
1:CA:48:C:OP2	61:CA:4100:HOH:O	2.16	0.58
26:DA:900:A:H2'	26:DA:901:A:C8	2.39	0.58
32:DH:3:ARG:NH1	32:DH:3:ARG:HB3	2.18	0.58
32:DH:73:ALA:O	32:DH:76:VAL:HG12	2.03	0.58
1:AA:1125:U:H1'	1:AA:1126:U:H2'	1.86	0.58
1:AA:473:G:H2'	1:AA:474:G:C8	2.39	0.58
46:BZ:24:LEU:HB2	46:BZ:41:LEU:HD23	1.85	0.58
6:CF:24:GLU:HG3	6:CF:28:ARG:NH1	2.19	0.58
2:CB:178:ARG:HE	8:CH:74:PRO:HG3	1.68	0.58
26:DA:2137:C:H2'	26:DA:2138:C:C6	2.38	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:DA:1952:A:OP1	35:DO:42:SER:OG	2.21	0.58
26:BA:2144:U:O2'	26:BA:2145:C:H2'	2.04	0.58
26:BA:2659:G:O2'	32:BH:175:LYS:NZ	2.37	0.58
26:BA:871:U:OP1	37:BQ:5:ARG:HD3	2.04	0.58
1:CA:1010:G:N2	1:CA:1020:U:H1'	2.19	0.58
1:CA:1302:U:OP2	13:CM:21:TYR:OH	2.14	0.58
1:CA:473:G:H2'	1:CA:474:G:C8	2.39	0.58
15:CO:3:ILE:H	15:CO:3:ILE:HD13	1.67	0.58
15:CO:69:TYR:O	15:CO:73:GLU:HG2	2.04	0.58
26:DA:1300:U:H4'	26:DA:1301:A:H5''	1.86	0.58
26:DA:2438:U:O2'	26:DA:2440:C:OP1	2.20	0.58
26:DA:2318:G:H21	39:DS:3:ARG:HD2	1.69	0.58
46:DZ:117:LEU:HA	46:DZ:174:VAL:HA	1.86	0.58
1:AA:473:G:H2'	1:AA:474:G:H8	1.69	0.58
2:AB:16:HIS:HB3	2:AB:210:SER:CB	2.33	0.58
4:AD:111:ALA:HB2	4:AD:120:LEU:HD12	1.86	0.58
23:AW:28:G:H2'	23:AW:29:G:H8	1.67	0.58
26:BA:801:G:O6	30:BF:53:THR:OG1	2.20	0.58
38:BR:56:LYS:NZ	38:BR:90:ARG:O	2.36	0.58
26:DA:1253:A:N6	61:DA:3721:HOH:O	2.33	0.58
26:DA:2646:C:OP2	26:DA:2732:G:O2'	2.15	0.58
26:DA:997:G:OP1	41:DU:92:ARG:HG2	2.04	0.58
1:AA:347:G:H2'	1:AA:348:G:O4'	2.03	0.58
1:AA:727:G:N2	1:AA:730:G:OP2	2.36	0.58
12:AL:24:VAL:HG11	12:AL:27:LEU:HD22	1.86	0.58
13:AM:40:ASN:O	13:AM:43:THR:OG1	2.21	0.58
20:AT:87:LYS:O	20:AT:91:LEU:HG	2.03	0.58
26:BA:303:U:O4	61:BA:4677:HOH:O	2.13	0.58
1:CA:1277:C:O2'	1:CA:1279:A:H8	1.86	0.58
1:CA:1422:G:O3'	35:DO:49:ARG:NH1	2.33	0.58
1:CA:971:G:OP2	1:CA:1231:G:N2	2.26	0.58
9:CI:5:TYR:O	9:CI:87:GLN:NE2	2.37	0.58
25:CY:40:C:C2'	25:CY:41:C:H5'	2.34	0.58
48:D1:76:ARG:HH11	48:D1:97:LEU:HD22	1.67	0.58
50:B3:18:ASP:N	50:B3:18:ASP:OD1	2.37	0.57
33:BI:129:THR:HG22	33:BI:139:GLN:NE2	2.17	0.57
26:BA:566:U:H5''	36:BP:29:LYS:HE3	1.86	0.57
46:BZ:138:GLU:H	46:BZ:156:LYS:HD3	1.69	0.57
1:CA:1153:C:H42	1:CA:1154:G:N2	2.01	0.57
1:CA:995:C:O2	14:CN:4:LYS:NZ	2.28	0.57
26:DA:465:G:OP1	54:D7:12:ARG:NH2	2.37	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AG:113:GLU:HG2	7:AG:119:ARG:HG2	1.86	0.57
9:AI:117:HIS:HB2	9:AI:121:ARG:HG3	1.85	0.57
25:AY:38:A:H2'	25:AY:39:PSU:O4'	2.04	0.57
26:BA:1166:C:H2'	26:BA:1167:U:C6	2.39	0.57
26:BA:2430:A:N3	26:BA:2430:A:H2'	2.18	0.57
27:BB:75:G:H8	27:BB:75:G:H5''	1.69	0.57
1:CA:34:C:H2'	1:CA:35:G:H8	1.69	0.57
9:CI:21:PRO:HA	9:CI:59:PHE:HA	1.85	0.57
16:CP:43:LYS:HA	16:CP:48:TRP:HB3	1.86	0.57
19:CS:64:GLU:O	19:CS:67:VAL:HG23	2.04	0.57
23:AW:5:G:H2'	23:AW:6:G:C8	2.39	0.57
33:BI:140:LEU:HD22	33:BI:142:VAL:HG13	1.86	0.57
38:DR:33:ARG:NH2	52:D5:57:VAL:O	2.29	0.57
26:DA:2110:G:OP1	26:DA:2118:U:N3	2.33	0.57
26:DA:399:G:OP2	61:DA:4406:HOH:O	2.17	0.57
26:DA:322:A:OP2	30:DF:169:ASN:HB2	2.04	0.57
1:AA:224:C:H2'	1:AA:225:C:C6	2.38	0.57
1:AA:757:U:H2'	1:AA:758:G:O4'	2.04	0.57
2:AB:16:HIS:HD2	2:AB:17:PHE:N	2.00	0.57
5:AE:78:HIS:HD1	8:AH:104:ARG:HD2	1.68	0.57
10:AJ:5:ARG:O	10:AJ:98:ILE:HA	2.05	0.57
25:AY:63:G:H2'	25:AY:64:A:O4'	2.04	0.57
26:BA:893:C:H2'	26:BA:894:C:C6	2.39	0.57
41:BU:89:GLU:HG3	42:BV:50:PRO:HB3	1.86	0.57
1:CA:1026:G:O6	1:CA:1036:G:N2	2.37	0.57
5:CE:137:GLU:HG2	5:CE:140:ARG:HH11	1.68	0.57
1:CA:975:A:N1	10:CJ:48:THR:HB	2.19	0.57
15:CO:82:ILE:HB	15:CO:87:ILE:HB	1.87	0.57
26:DA:1359:A:H61	26:DA:1372:U:H3	1.52	0.57
26:DA:1448:G:H4'	26:DA:1542:A:OP1	2.05	0.57
26:DA:2630:G:H2'	26:DA:2631:G:C8	2.39	0.57
28:DD:132:PRO:HG2	28:DD:135:PHE:CD2	2.40	0.57
1:AA:1392:G:N2	1:AA:1502:A:H8	2.01	0.57
1:AA:191:G:H21	20:AT:103:GLY:HA2	1.69	0.57
26:BA:2334:G:H5'	39:BS:9:ARG:HG2	1.85	0.57
31:BG:170:ARG:NH2	31:BG:182:LYS:O	2.37	0.57
1:CA:942:G:H21	9:CI:124:GLN:NE2	2.01	0.57
47:D0:10:THR:HG22	47:D0:12:ASN:H	1.70	0.57
26:DA:1264:G:OP1	52:D5:19:ARG:NH2	2.35	0.57
26:DA:1593:G:H2'	26:DA:1594:G:C8	2.40	0.57
26:DA:1853:A:H2'	26:DA:1854:A:C8	2.40	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:DA:531:C:H4'	26:DA:532:A:H5''	1.86	0.57
26:DA:903:C:H2'	26:DA:904:C:C6	2.40	0.57
27:DB:3:C:H2'	27:DB:4:C:C6	2.40	0.57
48:B1:3:LYS:HB2	48:B1:61:ARG:HH12	1.69	0.57
49:B2:65:ASN:OD1	49:B2:69:ARG:NH1	2.35	0.57
27:BB:14:U:OP2	27:BB:70:C:O2'	2.20	0.57
1:CA:1099:G:OP2	2:CB:144:ARG:NH2	2.34	0.57
2:CB:63:MET:HG3	2:CB:225:ALA:HB1	1.86	0.57
10:CJ:64:GLU:OE2	10:CJ:66:ARG:NH1	2.37	0.57
26:DA:1209:G:O2'	26:DA:1237:A:N1	2.32	0.57
13:AM:3:ARG:HG3	13:AM:4:ILE:H	1.70	0.57
26:BA:2001:A:OP1	38:BR:9:LYS:NZ	2.36	0.57
26:BA:30:G:OP2	41:BU:5:LYS:NZ	2.29	0.57
26:BA:878:A:H61	26:BA:899:A:H1'	1.70	0.57
31:BG:144:ILE:HA	31:BG:148:MET:HE1	1.87	0.57
32:BH:113:VAL:HG11	32:BH:151:ILE:HD13	1.86	0.57
4:CD:173:TRP:HB3	4:CD:187:ARG:HE	1.70	0.57
15:CO:55:GLY:HA2	15:CO:58:MET:HE2	1.86	0.57
25:CY:2:C:H2'	25:CY:3:C:C6	2.39	0.57
27:DB:41:U:H5	31:DG:70:VAL:H	1.51	0.57
46:DZ:7:ALA:O	46:DZ:62:PRO:HD3	2.05	0.57
26:BA:2207:G:O2'	26:BA:2208:A:OP1	2.21	0.57
26:BA:579:G:H2'	26:BA:580:C:C6	2.40	0.57
1:CA:992:U:H3	1:CA:1044:A:H62	1.53	0.57
26:DA:1013:C:H2'	26:DA:1014:U:H6	1.69	0.57
26:DA:1857:G:O2'	26:DA:1885:A:N6	2.35	0.57
26:DA:658:C:H2'	26:DA:659:C:C6	2.40	0.57
1:AA:1510:U:H2'	1:AA:1511:G:C8	2.40	0.57
1:AA:69:G:H2'	1:AA:70:G:C8	2.39	0.57
1:AA:993:G:H2'	1:AA:995:C:H41	1.69	0.57
26:BA:576:U:H2'	26:BA:577:G:C8	2.39	0.57
30:BF:24:LEU:HD23	30:BF:115:ALA:HA	1.87	0.57
31:BG:161:THR:HG22	31:BG:163:ALA:H	1.70	0.57
45:BY:54:LYS:H	45:BY:56:PRO:HD3	1.70	0.57
1:CA:1000:U:N3	1:CA:1041:A:N6	2.22	0.57
6:CF:25:ILE:HD13	6:CF:82:ARG:HE	1.70	0.57
11:CK:48:ILE:O	11:CK:50:TYR:N	2.37	0.57
14:CN:24:CYS:O	14:CN:28:GLY:N	2.30	0.57
24:CX:67:C:H2'	24:CX:68:C:H5'	1.86	0.57
25:CY:27:G:N1	25:CY:43:C:O2	2.38	0.57
26:DA:197:A:O2'	61:DA:3732:HOH:O	2.16	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:DP:44:GLY:CA	36:DP:45:LEU:HB2	2.33	0.57
38:DR:67:LEU:HD13	38:DR:76:VAL:HG21	1.86	0.57
14:AN:3:ARG:HH21	14:AN:3:ARG:HB3	1.70	0.57
1:AA:450:G:OP1	16:AP:43:LYS:NZ	2.37	0.57
25:AY:59:U:H5'	25:AY:60:U:H5	1.70	0.57
37:BQ:135:ASP:OD2	46:BZ:49:ARG:NH2	2.38	0.57
1:CA:1086:U:H3	1:CA:1099:G:H22	1.53	0.57
2:CB:178:ARG:NE	8:CH:74:PRO:HG3	2.20	0.57
32:DH:80:SER:OG	32:DH:81:GLU:OE1	2.17	0.57
26:DA:2875:C:O2'	40:DT:2:ASN:OD1	2.21	0.57
46:DZ:45:ASP:OD1	46:DZ:49:ARG:NH1	2.31	0.57
1:AA:1166:G:N2	1:AA:1170:A:OP2	2.38	0.56
26:BA:880:G:H2'	26:BA:881:G:H8	1.69	0.56
26:BA:1799:G:O2'	28:BD:181:GLU:OE2	2.22	0.56
40:BT:112:ARG:HG3	40:BT:115:ARG:HH21	1.70	0.56
44:BX:43:VAL:HG21	44:BX:81:VAL:HG11	1.86	0.56
1:CA:1321:C:H4'	13:CM:87:TYR:CE2	2.40	0.56
19:CS:28:LYS:HB2	19:CS:29:ARG:HA	1.87	0.56
26:DA:2808:U:H2'	26:DA:2809:A:H5'	1.87	0.56
44:DX:31:HIS:CD2	44:DX:33:LYS:H	2.22	0.56
1:AA:977:A:N6	1:AA:1224:G:OP1	2.29	0.56
7:AG:22:LEU:HD11	7:AG:101:LEU:HD21	1.85	0.56
46:BZ:45:ASP:OD2	46:BZ:49:ARG:NH1	2.38	0.56
1:CA:953:G:H5'	1:CA:965:A:N6	2.20	0.56
3:CC:11:ARG:HB3	3:CC:15:THR:HB	1.87	0.56
25:CY:9:A:OP2	25:CY:13:C:N4	2.38	0.56
26:DA:1864:U:OP1	26:DA:2410:G:O2'	2.17	0.56
40:DT:53:ARG:HH11	40:DT:53:ARG:HB3	1.70	0.56
46:DZ:69:THR:HG22	46:DZ:90:VAL:HA	1.88	0.56
1:CA:1154:G:N7	1:CA:1155:G:C8	2.73	0.56
3:CC:126:ARG:HB3	3:CC:128:PHE:CE1	2.40	0.56
13:AM:23:TYR:HB3	13:AM:67:GLU:HA	1.87	0.56
1:AA:333:G:H4'	20:AT:16:HIS:CE1	2.41	0.56
46:BZ:137:ILE:HA	46:BZ:156:LYS:NZ	2.20	0.56
1:CA:1502:A:H2	1:CA:1505:G:N1	1.99	0.56
1:CA:426:G:OP1	4:CD:36:ARG:HD2	2.05	0.56
8:CH:51:VAL:HG21	8:CH:60:ARG:HB2	1.87	0.56
23:CW:30:G:H1	23:CW:40:C:H42	1.51	0.56
26:DA:2167:U:H2'	26:DA:2168:G:H21	1.68	0.56
26:DA:866:A:H2	26:DA:867:C:C4	2.23	0.56
33:DI:110:ASP:N	33:DI:130:TYR:OH	2.34	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:952:U:H2'	1:AA:953:G:C8	2.41	0.56
2:AB:17:PHE:HB2	2:AB:44:LEU:HD21	1.88	0.56
4:AD:155:LEU:HD22	4:AD:157:LEU:H	1.70	0.56
24:AX:8:4SU:H6	24:AX:8:4SU:O5'	2.05	0.56
26:BA:1252:G:OP1	41:BU:36:ARG:NH2	2.39	0.56
26:BA:453:C:O2	26:BA:457:A:O2'	2.22	0.56
44:BX:5:TYR:CZ	49:B2:30:ARG:HB2	2.40	0.56
1:CA:222:U:H2'	1:CA:223:U:C6	2.39	0.56
20:CT:63:ILE:HD13	20:CT:80:ARG:HB3	1.88	0.56
26:DA:1405:U:H2'	26:DA:1406:U:C6	2.40	0.56
27:DB:110:G:H2'	27:DB:111:G:H8	1.70	0.56
46:DZ:141:VAL:HG12	46:DZ:144:LEU:HD12	1.87	0.56
1:AA:96:U:O2'	1:AA:97:G:H8	1.88	0.56
13:AM:84:ILE:HD12	19:AS:74:PHE:HE2	1.70	0.56
46:BZ:111:VAL:HG21	46:BZ:117:LEU:HB2	1.88	0.56
9:CI:49:PRO:HG2	9:CI:81:ILE:HG23	1.87	0.56
26:DA:1579:A:H2'	26:DA:1580:A:C8	2.41	0.56
26:DA:1805:U:O2	28:DD:50:THR:HB	2.05	0.56
26:DA:534:U:H2'	26:DA:535:C:C6	2.41	0.56
1:AA:58:C:O2'	1:AA:388:G:N7	2.33	0.56
5:AE:6:PHE:HB2	5:AE:34:VAL:HG22	1.88	0.56
31:BG:16:ARG:HB2	31:BG:17:PRO:HD3	1.88	0.56
26:BA:2708:G:H1'	38:BR:71:GLN:HE22	1.70	0.56
46:BZ:121:HIS:HB2	46:BZ:171:ILE:HG22	1.88	0.56
1:CA:1392:G:N2	1:CA:1502:A:H8	2.03	0.56
1:CA:9:G:H2'	1:CA:10:A:C8	2.41	0.56
8:CH:12:ARG:HD2	8:CH:26:VAL:HG12	1.88	0.56
12:CL:24:VAL:HG12	12:CL:27:LEU:HB2	1.88	0.56
26:DA:1507:A:O2'	26:DA:1508:A:O5'	2.20	0.56
26:DA:1639:U:H2'	26:DA:1640:C:H5''	1.88	0.56
26:DA:323:G:O2'	26:DA:1205:U:N3	2.35	0.56
31:DG:16:ARG:O	31:DG:20:ILE:HG13	2.05	0.56
1:AA:976:G:N2	1:AA:1363:C:OP2	2.38	0.56
1:AA:671:G:H5'	6:AF:77:ARG:HH22	1.70	0.56
26:BA:171:G:O2'	26:BA:172:C:H5'	2.06	0.56
26:BA:2022:U:O2'	26:BA:2617:C:H5'	2.06	0.56
26:BA:2869:G:H2'	26:BA:2870:C:O4'	2.04	0.56
26:BA:588:U:H2'	26:BA:589:C:C6	2.41	0.56
26:BA:668:G:H5'	26:BA:669:G:OP2	2.06	0.56
30:BF:161:GLU:HG2	30:BF:164:ARG:NH2	2.20	0.56
31:BG:41:GLN:HG3	31:BG:60:LEU:HD21	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:DA:125:G:O2'	54:D7:48:LYS:NZ	2.36	0.56
26:DA:1787:A:N3	61:DA:3727:HOH:O	2.33	0.56
26:DA:2167:U:O2'	26:DA:2168:G:O4'	2.23	0.56
26:DA:2327:A:H2'	26:DA:2328:A:C8	2.41	0.56
26:DA:245:G:O6	55:D8:8:LYS:NZ	2.31	0.56
26:DA:912:C:OP1	37:DQ:8:LYS:NZ	2.25	0.56
45:DY:99:CYS:HB2	45:DY:106:LEU:HD21	1.88	0.56
1:AA:1060:C:C5	3:AC:2:GLY:HA3	2.41	0.56
1:AA:103:C:O2'	1:AA:172:A:N1	2.34	0.56
20:AT:9:ASN:HD22	20:AT:10:LEU:H	1.53	0.56
26:BA:2023:G:H5'	26:BA:2617:C:H4'	1.88	0.56
26:BA:71:A:OP2	26:BA:71:A:H3'	2.06	0.56
44:BX:35:THR:HG22	44:BX:38:GLU:HB2	1.87	0.56
16:CP:53:VAL:O	16:CP:57:ARG:HB2	2.06	0.56
21:CU:7:ARG:HD2	21:CU:21:TYR:HE2	1.69	0.56
28:DD:4:LYS:HB3	28:DD:18:VAL:HG23	1.88	0.56
37:DQ:1:MET:N	37:DQ:1:MET:SD	2.66	0.56
45:DY:20:TYR:CE1	45:DY:43:ASN:HA	2.41	0.56
26:BA:2151:G:H2'	26:BA:2152:G:C8	2.41	0.56
26:BA:2124:G:H1	26:BA:2174:C:N4	2.04	0.56
31:BG:77:ILE:HG22	31:BG:80:PHE:H	1.69	0.56
36:BP:89:ALA:O	36:BP:121:LYS:NZ	2.27	0.56
44:BX:31:HIS:CD2	44:BX:33:LYS:H	2.24	0.56
2:CB:219:VAL:HA	2:CB:222:ILE:HG12	1.88	0.56
8:CH:39:LEU:HD12	8:CH:44:PHE:HB2	1.88	0.56
10:CJ:47:PHE:N	10:CJ:63:PHE:O	2.33	0.56
1:CA:1047:G:H5''	14:CN:4:LYS:HD2	1.87	0.56
26:DA:2138:C:H2'	26:DA:2139:C:H5''	1.87	0.56
1:AA:139:G:N2	1:AA:224:C:O2	2.35	0.56
4:AD:173:TRP:CZ3	4:AD:174:LEU:HG	2.41	0.56
26:BA:2646:C:OP2	26:BA:2732:G:O2'	2.19	0.56
26:BA:784:A:H5'	26:BA:785:G:OP1	2.06	0.56
26:DA:1265:A:OP2	61:DA:4004:HOH:O	2.18	0.56
32:DH:113:VAL:HG11	32:DH:151:ILE:HD13	1.87	0.56
34:DN:4:TYR:HB2	41:DU:101:ARG:NH1	2.21	0.56
1:AA:736:C:H2'	1:AA:737:A:H8	1.71	0.55
10:AJ:11:PHE:HE1	10:AJ:67:THR:HG22	1.71	0.55
1:CA:1120:G:C6	1:CA:1121:U:C4	2.94	0.55
1:CA:1286:A:H2'	1:CA:1287:A:H4'	1.88	0.55
51:D4:59:PHE:HA	51:D4:60:GLN:C	2.27	0.55
30:DF:21:ALA:CB	30:DF:22:ALA:HA	2.37	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1392:G:H21	1:AA:1502:A:H8	1.54	0.55
2:AB:178:ARG:HH22	8:AH:68:ARG:HH12	1.53	0.55
4:AD:175:SER:HB3	4:AD:186:LEU:HD11	1.88	0.55
13:AM:87:TYR:O	13:AM:91:ARG:HG2	2.06	0.55
15:AO:39:LEU:HD13	15:AO:56:LEU:HB2	1.87	0.55
26:BA:1309:G:O6	61:BA:4912:HOH:O	2.17	0.55
26:BA:592:G:O6	61:BA:4937:HOH:O	2.16	0.55
33:BI:27:ARG:HD2	48:B1:71:TYR:CE1	2.41	0.55
1:CA:442:C:H42	1:CA:492:G:H1	1.53	0.55
2:CB:8:LYS:HG3	2:CB:9:GLU:HG3	1.87	0.55
1:CA:450:G:OP1	16:CP:43:LYS:NZ	2.38	0.55
24:CX:40:C:H2'	24:CX:41:C:H6	1.71	0.55
26:DA:1039:G:O6	26:DA:1116:C:N4	2.37	0.55
26:DA:1527:G:HO2'	26:DA:1544:A:H62	1.53	0.55
2:AB:231:GLU:HB3	2:AB:232:PRO:HD3	1.88	0.55
7:AG:16:LEU:HD11	9:AI:45:ALA:HB2	1.87	0.55
12:AL:24:VAL:HG13	12:AL:98:TYR:CE1	2.41	0.55
25:AY:19:G:H3'	25:AY:20:U:C6	2.41	0.55
26:BA:2238:G:H2'	26:BA:2238:G:N3	2.20	0.55
26:BA:2662:A:H2'	26:BA:2663:G:O4'	2.07	0.55
5:CE:50:GLU:HB2	5:CE:53:LEU:HD12	1.88	0.55
19:CS:28:LYS:HB2	19:CS:29:ARG:CA	2.36	0.55
24:CX:31:G:H3'	24:CX:32:5MC:HM51	1.88	0.55
26:DA:140:G:N2	26:DA:1596:A:H4'	2.21	0.55
26:DA:2135:A:H2'	26:DA:2136:C:C6	2.41	0.55
34:DN:17:ASP:HB2	34:DN:137:LYS:HZ1	1.71	0.55
1:AA:442:C:H42	1:AA:492:G:H1	1.53	0.55
11:AK:34:ASP:OD1	11:AK:38:ASN:N	2.40	0.55
20:AT:9:ASN:ND2	20:AT:10:LEU:H	2.05	0.55
26:BA:2791:C:H2'	26:BA:2792:G:H8	1.71	0.55
30:BF:158:THR:O	30:BF:164:ARG:NH1	2.38	0.55
1:CA:1065:U:OP2	1:CA:1190:G:N2	2.39	0.55
3:CC:6:HIS:CD2	3:CC:8:ILE:H	2.23	0.55
9:CI:125:TYR:HD1	9:CI:126:SER:N	2.03	0.55
23:CW:39:PSU:H2'	23:CW:40:C:C6	2.41	0.55
9:CI:128:ARG:NH2	24:CX:33:U:OP2	2.40	0.55
13:CM:65:LYS:HA	51:D4:50:VAL:HG11	1.87	0.55
26:DA:1378:A:OP1	54:D7:10:ARG:NH2	2.39	0.55
26:DA:2169:A:H2'	26:DA:2170:A:C8	2.41	0.55
33:DI:38:LEU:HB2	33:DI:40:THR:HG22	1.89	0.55
1:AA:1445:C:N3	1:AA:1457:G:N1	2.37	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AF:50:TYR:OH	18:AR:74:ARG:O	2.18	0.55
26:BA:222:A:H5''	26:BA:421:U:OP1	2.07	0.55
1:CA:1154:G:N7	1:CA:1155:G:N9	2.55	0.55
3:CC:33:LEU:HD21	14:CN:53:LEU:HD23	1.88	0.55
9:CI:9:ARG:HG2	9:CI:14:VAL:HG12	1.88	0.55
26:DA:1239:G:H2'	26:DA:1240:U:O4'	2.06	0.55
26:DA:2400:G:H2'	26:DA:2401:U:H6	1.70	0.55
26:DA:320:A:OP2	30:DF:137:LYS:NZ	2.33	0.55
26:DA:859:G:N2	26:DA:917:A:OP2	2.39	0.55
26:DA:2882:A:H5'	38:DR:96:ARG:HG3	1.87	0.55
46:DZ:111:VAL:HG21	46:DZ:117:LEU:HB2	1.88	0.55
1:AA:123:C:OP1	1:AA:311:C:O2'	2.20	0.55
55:B8:62:LEU:HB3	55:B8:65:GLU:CG	2.36	0.55
26:BA:2110:G:C2	26:BA:2120:G:H1'	2.42	0.55
26:BA:2171:A:H1'	26:BA:2172:U:O4'	2.07	0.55
27:BB:91:C:H5'	37:BQ:18:LYS:HA	1.87	0.55
44:BX:2:LYS:NZ	44:BX:38:GLU:OE2	2.30	0.55
1:CA:129(A):G:C6	1:CA:189(E):U:H4'	2.41	0.55
2:CB:48:MET:HA	2:CB:51:LEU:HB2	1.89	0.55
3:CC:22:TRP:CD2	3:CC:59:ARG:HD2	2.41	0.55
11:CK:24:SER:OG	11:CK:25:TYR:N	2.38	0.55
26:DA:848:G:C2	26:DA:933:A:H1'	2.42	0.55
26:DA:84:A:H5''	45:DY:8:LYS:HE3	1.88	0.55
36:DP:121:LYS:HG2	36:DP:122:PRO:HD2	1.89	0.55
26:DA:833:U:O2	36:DP:55:ARG:NH2	2.37	0.55
1:AA:1305:G:N2	1:AA:1331:G:H1'	2.21	0.55
1:AA:353:A:H5'	1:AA:353:A:H8	1.72	0.55
18:AR:31:LEU:HD23	18:AR:31:LEU:H	1.72	0.55
20:AT:65:LYS:HA	20:AT:68:LYS:HD3	1.88	0.55
26:BA:330:A:H2	26:BA:1210:A:HO2'	1.54	0.55
26:BA:1566:A:OP1	28:BD:211:ARG:NH1	2.40	0.55
33:BI:106:GLY:HA2	33:BI:107:VAL:O	2.06	0.55
33:BI:72:LEU:C	33:BI:74:ASN:H	2.10	0.55
1:CA:1002:G:H1	1:CA:1038:C:H42	0.70	0.55
1:CA:1069:C:O2'	1:CA:1192:C:H1'	2.07	0.55
1:CA:235:C:H5'	17:CQ:70:ARG:HG2	1.88	0.55
10:CJ:55:LYS:HG3	10:CJ:56:HIS:CD2	2.42	0.55
51:D4:46:GLN:C	51:D4:48:ARG:H	2.10	0.55
26:DA:1530:C:HO2'	26:DA:1531:C:P	2.29	0.55
26:DA:330:A:H2	26:DA:1210:A:HO2'	1.54	0.55
27:DB:24:G:H4'	27:DB:25:A:C8	2.41	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:DA:1803:A:H4'	28:DD:259:THR:HG23	1.89	0.55
8:AH:51:VAL:HG11	8:AH:60:ARG:NH1	2.20	0.55
3:AC:13:GLY:HA3	14:AN:57:ARG:HH21	1.72	0.55
24:AX:64:G:H4'	37:BQ:10:ARG:HH21	1.71	0.55
26:BA:898:C:H2'	26:BA:899:A:H8	1.70	0.55
1:CA:1376:U:H2'	1:CA:1377:A:H8	1.70	0.55
1:CA:328:C:H4'	1:CA:329:A:H5'	1.89	0.55
1:CA:947:G:O3'	13:CM:109:THR:OG1	2.25	0.55
2:CB:45:GLN:O	2:CB:49:GLU:HB2	2.06	0.55
31:DG:179:PRO:HB2	51:D4:42:PHE:CE1	2.41	0.55
26:DA:1796:U:H2'	26:DA:1797:C:C6	2.42	0.55
1:AA:1255:G:N7	10:AJ:43:ARG:NH2	2.55	0.55
1:AA:1290:G:H2'	1:AA:1291:G:H8	1.71	0.55
2:AB:16:HIS:O	2:AB:17:PHE:HD1	1.89	0.55
25:AY:50:U:N3	25:AY:64:A:C2	2.69	0.55
26:BA:2141:G:H1	26:BA:2149:G:N2	2.02	0.55
26:BA:2336:A:H61	47:B0:43:THR:HG22	1.71	0.55
36:BP:36:LYS:O	61:BP:306:HOH:O	2.18	0.55
1:CA:1023:G:C4	1:CA:1024:G:C8	2.94	0.55
1:CA:1035:A:H2'	1:CA:1036:G:H8	1.71	0.55
1:CA:1104:G:H4'	2:CB:111:ARG:NH1	2.22	0.55
4:CD:196:LEU:O	4:CD:198:VAL:N	2.36	0.55
26:DA:900:A:O2'	26:DA:901:A:OP1	2.24	0.55
30:DF:150:GLY:HA2	30:DF:172:TRP:CD2	2.41	0.55
34:DN:128:HIS:O	34:DN:131:GLN:NE2	2.40	0.55
2:AB:155:LEU:HD21	2:AB:159:PRO:HG3	1.88	0.55
6:AF:69:GLU:O	6:AF:72:VAL:HG12	2.06	0.55
35:BO:63:VAL:HG12	35:BO:106:LEU:HD11	1.88	0.55
7:CG:78:ARG:HB2	7:CG:156:TRP:HZ3	1.72	0.55
7:CG:91:VAL:HB	7:CG:96:GLN:HG2	1.88	0.55
26:DA:2349:G:OP1	61:DA:3781:HOH:O	2.18	0.55
36:DP:84:ASN:CG	36:DP:117:GLU:HB2	2.27	0.55
41:DU:85:LYS:HB2	41:DU:116:ALA:HB1	1.89	0.55
1:AA:109:A:OP1	61:AA:4215:HOH:O	2.18	0.54
9:AI:24:GLY:HA2	9:AI:59:PHE:O	2.07	0.54
13:AM:3:ARG:HG2	13:AM:8:GLU:HA	1.89	0.54
25:AY:33:U:H2'	25:AY:35:A:OP2	2.07	0.54
26:BA:1371:G:H2'	26:BA:1372:U:H5	1.70	0.54
4:CD:58:LEU:HD22	4:CD:62:GLN:HG2	1.89	0.54
25:CY:29:G:H1	25:CY:41:C:N4	2.05	0.54
26:DA:1467:C:C5	26:DA:1546:C:H2'	2.42	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:DA:223:A:O2'	26:DA:420:C:O2	2.25	0.54
46:DZ:163:LEU:HG	46:DZ:165:VAL:HG22	1.88	0.54
2:AB:109:SER:HA	2:AB:112:VAL:HG13	1.87	0.54
1:AA:1179:A:O3'	9:AI:103:THR:HB	2.06	0.54
26:BA:1253:A:OP1	61:BA:4931:HOH:O	2.18	0.54
26:BA:2532:G:O2'	26:BA:2657:A:N1	2.39	0.54
26:BA:1693:U:O2'	28:BD:14:ARG:NH2	2.40	0.54
1:CA:419:C:OP1	1:CA:513:C:O2'	2.23	0.54
4:CD:98:GLU:HG2	4:CD:189:PRO:HG2	1.89	0.54
9:CI:28:VAL:HG22	9:CI:63:ILE:HB	1.90	0.54
15:CO:5:LYS:N	15:CO:5:LYS:HD3	2.23	0.54
16:CP:8:ARG:HG3	16:CP:17:TYR:CE1	2.42	0.54
25:CY:39:PSU:C2	25:CY:40:C:C2	2.95	0.54
48:D1:54:ALA:HB1	48:D1:83:GLU:HG3	1.88	0.54
26:DA:1014:U:H2'	26:DA:1015:G:H8	1.72	0.54
26:DA:1300:U:H4'	26:DA:1301:A:C5'	2.37	0.54
26:DA:191:A:N1	61:DA:4228:HOH:O	2.34	0.54
26:DA:2150:U:H2'	26:DA:2151:G:C8	2.41	0.54
26:DA:2155:G:H2'	26:DA:2156:G:H5'	1.89	0.54
30:DF:150:GLY:HA2	30:DF:172:TRP:CE3	2.42	0.54
26:DA:637:A:H2'	36:DP:117:GLU:OE2	2.08	0.54
39:DS:93:LYS:HD3	39:DS:94:TYR:N	2.22	0.54
1:AA:1007:C:N3	1:AA:1022:G:O6	2.41	0.54
1:AA:1074:G:O2'	1:AA:1101:A:N1	2.31	0.54
1:AA:1149:C:H2'	1:AA:1150:U:C6	2.42	0.54
1:AA:501:C:H2'	1:AA:502:G:C8	2.43	0.54
2:AB:20:GLU:HA	2:AB:21:ARG:NH2	2.22	0.54
5:AE:33:VAL:HG21	5:AE:109:ILE:HA	1.89	0.54
7:AG:152:ALA:HB1	7:AG:155:ARG:HH21	1.72	0.54
26:BA:1047:G:HO2'	26:BA:1048:A:H8	1.55	0.54
26:BA:2180:U:H2'	26:BA:2181:G:O4'	2.08	0.54
26:BA:226:G:H21	26:BA:228:A:H62	1.54	0.54
26:BA:404:C:H4'	26:BA:405:U:H5'	1.89	0.54
26:BA:69:C:O2	26:BA:73:A:O2'	2.23	0.54
39:BS:34:HIS:ND1	39:BS:53:SER:OG	2.36	0.54
43:BW:25:ARG:NH2	43:BW:74:ALA:O	2.35	0.54
46:BZ:4:ARG:NE	46:BZ:60:GLU:OE1	2.28	0.54
26:DA:2612:C:OP2	52:D5:2:ALA:N	2.41	0.54
26:DA:2136:C:O2'	26:DA:2137:C:O5'	2.25	0.54
26:DA:276:A:H5''	26:DA:277:C:H5'	1.88	0.54
31:DG:23:PHE:HB2	31:DG:25:TYR:CZ	2.42	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:AY:51:U:H3	25:AY:63:G:H1	1.55	0.54
26:BA:1113:U:H2'	26:BA:1114:G:C8	2.41	0.54
26:BA:2129:C:H2'	26:BA:2130:U:C6	2.42	0.54
26:BA:2445:G:OP1	30:BF:74:ARG:NH2	2.38	0.54
29:BE:55:ASN:HB3	29:BE:58:ARG:HG3	1.88	0.54
1:CA:1378:C:H5	1:CA:1379:G:C4	2.25	0.54
1:CA:859:A:OP2	1:CA:869:G:N1	2.34	0.54
3:CC:20:SER:OG	3:CC:22:TRP:NE1	2.40	0.54
4:CD:60:GLU:HG2	4:CD:202:LEU:HB2	1.90	0.54
26:DA:2733:A:N1	29:DE:203:LYS:HA	2.23	0.54
26:DA:300:A:P	45:DY:86:ARG:HH22	2.30	0.54
26:DA:796:C:H2'	26:DA:797:C:C6	2.42	0.54
40:DT:24:PRO:HA	40:DT:49:VAL:HG22	1.89	0.54
1:AA:1033:G:H2'	1:AA:1034:G:H8	1.72	0.54
1:AA:1189:C:OP1	10:AJ:51:ARG:NH2	2.24	0.54
1:AA:848:C:H2'	1:AA:849:C:C6	2.43	0.54
2:AB:105:PHE:CE1	2:AB:155:LEU:HD12	2.43	0.54
3:AC:104:GLN:HE21	3:AC:105:GLU:N	2.05	0.54
5:AE:91:LEU:HB3	5:AE:118:ILE:HD11	1.89	0.54
5:AE:140:ARG:O	5:AE:143:ARG:NH2	2.41	0.54
15:AO:56:LEU:O	15:AO:60:VAL:HG23	2.06	0.54
26:BA:1721:G:H3'	26:BA:1722:A:H5''	1.88	0.54
26:BA:2116:G:N1	26:BA:2162:G:OP1	2.41	0.54
26:DA:641:C:H42	26:DA:647:G:H1	1.56	0.54
32:DH:56:SER:OG	32:DH:57:ASP:N	2.41	0.54
1:AA:923:A:O2'	1:AA:1399:C:OP2	2.23	0.54
3:AC:150:LYS:HB2	3:AC:173:VAL:HG21	1.88	0.54
5:AE:105:VAL:HB	5:AE:106:PRO:HD3	1.90	0.54
1:AA:1292:U:H5'	9:AI:38:GLN:NE2	2.22	0.54
25:AY:67:C:H2'	25:AY:68:C:O4'	2.08	0.54
26:BA:1971:A:N1	61:BA:4352:HOH:O	2.33	0.54
29:BE:174:ASP:OD1	29:BE:175:VAL:N	2.40	0.54
36:BP:100:LEU:HD12	36:BP:112:LEU:HD11	1.90	0.54
23:AW:52:G:H4'	37:BQ:56:ARG:NH2	2.22	0.54
1:CA:1301:U:O2'	1:CA:1302:U:H5'	2.08	0.54
1:CA:701:C:OP1	1:CA:702:A:O2'	2.14	0.54
2:CB:61:LEU:HD23	2:CB:68:ILE:HD11	1.89	0.54
4:CD:57:ARG:HH22	5:CE:107:ARG:HD3	1.72	0.54
6:CF:46:ARG:HG3	6:CF:47:ARG:N	2.21	0.54
10:CJ:49:VAL:HG23	14:CN:41:ARG:HB2	1.88	0.54
18:CR:61:LYS:O	18:CR:65:ILE:HG12	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:DA:1183:G:H5'	50:D3:30:ARG:HH12	1.73	0.54
33:DI:14:ASP:OD1	33:DI:15:VAL:N	2.38	0.54
1:AA:171:A:H2'	1:AA:172:A:C8	2.42	0.54
1:AA:45:U:H2'	1:AA:46:G:C8	2.42	0.54
11:AK:84:VAL:HG11	11:AK:91:ARG:HD2	1.88	0.54
19:AS:67:VAL:HG21	51:B4:59:PHE:HB3	1.88	0.54
24:AX:19:G:H4'	24:AX:20:U:OP2	2.06	0.54
26:BA:2327:A:H2'	26:BA:2328:A:C8	2.42	0.54
26:BA:443:A:H1'	26:BA:1201:C:O4'	2.07	0.54
1:CA:1003:G:N2	1:CA:1025:U:O4	2.40	0.54
3:CC:6:HIS:CG	14:CN:49:HIS:HB3	2.43	0.54
24:CX:58:A:H4'	24:CX:59:A:OP1	2.08	0.54
26:DA:2206:G:H3'	26:DA:2207:G:N7	2.23	0.54
26:DA:252:G:P	36:DP:50:ARG:HH12	2.31	0.54
26:DA:855:G:H2'	26:DA:856:C:C6	2.43	0.54
1:AA:1347:G:N2	1:AA:1373:G:H2'	2.23	0.54
1:AA:159:G:O2'	1:AA:161:A:N7	2.30	0.54
1:AA:524:G:H2'	1:AA:525:C:C6	2.43	0.54
1:AA:539:A:H2'	1:AA:540:G:C8	2.43	0.54
1:AA:934:C:OP1	61:AA:4110:HOH:O	2.18	0.54
4:AD:188:LEU:H	4:AD:188:LEU:HD23	1.73	0.54
20:AT:86:ARG:O	20:AT:90:GLN:NE2	2.40	0.54
51:B4:54:GLY:C	51:B4:56:VAL:HA	2.28	0.54
26:BA:2243:U:OP1	61:BA:4017:HOH:O	2.17	0.54
26:BA:271(E):U:H2'	26:BA:271(F):C:C6	2.43	0.54
26:BA:784:A:C6	28:BD:229:VAL:HG11	2.43	0.54
1:CA:399:G:H2'	1:CA:400:C:C6	2.43	0.54
1:CA:441:A:H3'	1:CA:442:C:C6	2.43	0.54
1:CA:723:U:HO2'	1:CA:724:G:C5'	2.21	0.54
3:CC:29:TYR:OH	14:CN:54:PRO:O	2.20	0.54
26:DA:1153:C:H2'	26:DA:1154:G:O4'	2.07	0.54
26:DA:2591:C:OP1	28:DD:239:ARG:HD2	2.08	0.54
26:DA:879:G:H3'	26:DA:880:G:H8	1.72	0.54
26:DA:971:C:OP2	61:DA:4647:HOH:O	2.18	0.54
28:DD:3:VAL:HG13	28:DD:17:THR:HB	1.89	0.54
31:DG:48:GLU:O	31:DG:51:ARG:HG3	2.07	0.54
42:DV:35:LEU:HB2	42:DV:57:VAL:HG23	1.90	0.54
1:AA:222:U:H2'	1:AA:223:U:C6	2.43	0.54
1:AA:316:G:OP2	1:AA:351:G:O2'	2.25	0.54
3:AC:11:ARG:NH2	3:AC:177:THR:O	2.41	0.54
3:AC:58:GLU:HB3	10:AJ:92:THR:HG21	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:AW:9:A:O2'	23:AW:10:G:N7	2.40	0.54
26:BA:1174:A:H1'	26:BA:1175:U:H5''	1.89	0.54
26:BA:1796:U:H2'	26:BA:1797:C:C6	2.43	0.54
26:BA:272:G:O2'	26:BA:421:U:OP2	2.22	0.54
26:BA:887:A:H4'	26:BA:888:C:C5	2.43	0.54
1:CA:1084:G:H5'	1:CA:1102:A:OP2	2.08	0.54
1:CA:1490:C:H2'	1:CA:1491:G:H8	1.72	0.54
3:CC:157:ILE:HD12	3:CC:164:ARG:HB3	1.90	0.54
3:CC:55:VAL:HG22	3:CC:68:VAL:HG22	1.88	0.54
1:CA:428:G:OP2	4:CD:10:ARG:NH1	2.41	0.54
26:DA:1013:C:H2'	26:DA:1014:U:C6	2.43	0.54
26:DA:391:G:O2'	26:DA:410:G:OP1	2.19	0.54
1:AA:1077:G:N2	1:AA:1080:A:OP2	2.41	0.54
1:AA:26:A:N6	1:AA:558:G:O2'	2.39	0.54
1:AA:880:C:OP1	12:AL:8:ASN:ND2	2.39	0.54
25:AY:6:G:O6	25:AY:7:A:N6	2.40	0.54
26:BA:1470:G:N2	26:BA:1520:G:OP2	2.34	0.54
26:BA:2630:G:H2'	26:BA:2631:G:C8	2.43	0.54
26:BA:271(H):G:O2'	26:BA:271(I):G:H8	1.90	0.54
36:BP:97:PRO:HD3	36:BP:126:VAL:O	2.08	0.54
1:CA:411:A:OP1	4:CD:30:LYS:NZ	2.40	0.54
1:CA:59:A:H5''	1:CA:60:A:H5''	1.89	0.54
2:CB:16:HIS:CB	2:CB:210:SER:HB2	2.28	0.54
13:CM:64:TRP:HB2	13:CM:66:LEU:HD21	1.89	0.54
26:DA:2182:G:H2'	26:DA:2183:C:C6	2.42	0.54
26:DA:2102:U:H3	26:DA:2187:G:H1	1.56	0.54
26:DA:2723:C:OP2	29:DE:109:LYS:NZ	2.41	0.54
1:AA:1005:A:H1'	1:AA:1036:G:N2	2.23	0.53
1:AA:940:C:OP1	7:AG:29:LYS:NZ	2.41	0.53
9:AI:17:VAL:HG11	9:AI:81:ILE:HA	1.90	0.53
25:AY:9:A:H5''	25:AY:46:7MG:N2	2.23	0.53
54:B7:24:THR:CG2	54:B7:27:GLY:H	2.20	0.53
26:BA:2693:A:H2'	26:BA:2694:G:H8	1.72	0.53
1:CA:1012:U:H2'	1:CA:1013:G:C8	2.43	0.53
1:CA:1206:G:O4'	3:CC:194:GLY:HA2	2.08	0.53
1:CA:299:G:H2'	1:CA:300:A:C8	2.43	0.53
1:CA:93:G:O2'	1:CA:96:U:H5'	2.08	0.53
2:CB:15:VAL:HG12	2:CB:16:HIS:H	1.73	0.53
4:CD:98:GLU:OE1	4:CD:103:ASN:ND2	2.31	0.53
5:CE:74:GLY:HA3	5:CE:116:THR:HG22	1.89	0.53
18:CR:58:LEU:HB3	18:CR:62:GLU:HG3	1.89	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:CS:49:ILE:HD13	19:CS:62:ILE:HD13	1.90	0.53
23:CW:66:U:C3'	23:CW:67:C:H5''	2.32	0.53
26:DA:203:C:OP2	61:DA:4309:HOH:O	2.19	0.53
26:DA:625:G:O6	36:DP:107:LYS:NZ	2.36	0.53
45:DY:28:LYS:HD2	45:DY:40:GLU:HG3	1.89	0.53
1:AA:159:G:N2	1:AA:162:A:OP2	2.37	0.53
37:BQ:85:LYS:HB2	47:B0:7:LEU:HD12	1.91	0.53
26:BA:1406:U:H2'	26:BA:1407:C:C6	2.44	0.53
26:BA:2142:C:H2'	26:BA:2143:C:C6	2.43	0.53
1:CA:1011:G:C6	1:CA:1012:U:C2	2.97	0.53
1:CA:1251:A:H2'	1:CA:1252:A:C8	2.43	0.53
1:CA:1305:G:N2	1:CA:1331:G:H1'	2.23	0.53
1:CA:986:A:H1'	19:CS:55:LYS:HA	1.90	0.53
13:CM:13:LYS:HA	13:CM:44:ARG:HH11	1.72	0.53
26:DA:500:G:N1	26:DA:503:A:OP2	2.40	0.53
29:DE:174:ASP:OD1	29:DE:175:VAL:N	2.40	0.53
33:DI:27:ARG:HD2	48:D1:71:TYR:CE1	2.43	0.53
1:AA:1191:A:H5''	3:AC:4:LYS:NZ	2.23	0.53
2:AB:204:ASN:OD1	2:AB:206:ASP:N	2.29	0.53
10:AJ:13:HIS:O	10:AJ:17:ASP:HB2	2.09	0.53
12:AL:32:PHE:HB3	12:AL:84:LEU:HD11	1.89	0.53
19:AS:65:ASN:ND2	19:AS:66:MET:HG2	2.23	0.53
38:BR:44:LEU:HD22	38:BR:48:VAL:HG23	1.90	0.53
1:CA:890:G:O2'	1:CA:906:G:O6	2.20	0.53
2:CB:95:GLN:HG3	2:CB:148:TYR:HA	1.90	0.53
4:CD:61:LYS:HD2	4:CD:206:PHE:CE2	2.43	0.53
5:CE:92:LYS:HB3	5:CE:119:LEU:HB2	1.90	0.53
1:CA:523:A:H61	12:CL:92:ASP:HB2	1.74	0.53
26:DA:1021:A:H3'	26:DA:1021:A:H8	1.72	0.53
26:DA:957:A:H5'	37:DQ:76:LYS:HG3	1.90	0.53
27:DB:90:A:C5	27:DB:91:C:H1'	2.44	0.53
36:DP:121:LYS:O	36:DP:123:LEU:N	2.40	0.53
1:AA:452:A:H4'	16:AP:72:ARG:NH1	2.24	0.53
17:AQ:95:TYR:HA	17:AQ:98:LEU:HD22	1.89	0.53
13:AM:80:ARG:HH22	19:AS:69:HIS:CE1	2.25	0.53
51:B4:15:ILE:O	51:B4:33:VAL:N	2.39	0.53
26:BA:2115:G:H21	26:BA:2171:A:H61	1.57	0.53
26:BA:910:A:H62	37:BQ:12:GLN:HA	1.73	0.53
28:BD:132:PRO:HD3	28:BD:190:TYR:CZ	2.44	0.53
1:CA:1272:G:C2	1:CA:1273:G:H1'	2.43	0.53
1:CA:382:A:H2'	1:CA:383:A:C8	2.43	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CB:186:ALA:O	2:CB:201:ILE:N	2.40	0.53
3:CC:125:GLU:OE2	3:CC:125:GLU:N	2.36	0.53
7:CG:26:PHE:CE1	7:CG:30:ILE:HD11	2.44	0.53
8:CH:86:ILE:HG13	8:CH:133:LEU:HD22	1.91	0.53
23:CW:27:G:H1	23:CW:43:C:N4	2.03	0.53
23:CW:8:4SU:H1'	23:CW:48:C:H1'	1.89	0.53
51:D4:59:PHE:HA	51:D4:61:ARG:N	2.23	0.53
26:DA:1007:C:P	34:DN:37:LYS:HZ1	2.31	0.53
26:DA:1203:G:O2'	26:DA:1242:A:N6	2.39	0.53
29:DE:36:ARG:HD3	29:DE:85:ASN:HD21	1.73	0.53
1:AA:198:G:O6	1:AA:219:C:N4	2.42	0.53
1:AA:346:G:OP1	40:BT:41:ARG:NH2	2.41	0.53
1:AA:715:A:H2'	1:AA:716:A:C8	2.44	0.53
26:BA:2537:U:H2'	26:BA:2538:C:C6	2.44	0.53
26:BA:2557:G:H2'	26:BA:2558:C:C6	2.44	0.53
33:BI:61:ARG:HA	33:BI:61:ARG:HH11	1.73	0.53
36:BP:42:SER:O	61:BP:305:HOH:O	2.18	0.53
1:CA:543:C:OP1	4:CD:14:ARG:NE	2.36	0.53
2:CB:230:VAL:HG22	2:CB:231:GLU:H	1.74	0.53
3:CC:155:GLY:HA3	3:CC:196:LEU:HD13	1.90	0.53
13:CM:22:ILE:HG23	13:CM:67:GLU:HG2	1.91	0.53
47:D0:27:GLU:HG3	47:D0:68:GLU:HA	1.91	0.53
26:DA:1266:G:O5'	43:DW:15:ARG:NH2	2.41	0.53
26:DA:2070:G:OP2	61:DA:4495:HOH:O	2.18	0.53
27:DB:95:C:H2'	27:DB:96:U:C6	2.44	0.53
39:DS:67:ARG:HG3	39:DS:104:GLY:HA3	1.90	0.53
1:AA:1112:C:O2	3:AC:179:ARG:HG3	2.09	0.53
1:AA:69:G:H2'	1:AA:70:G:H8	1.74	0.53
1:AA:848:C:H2'	1:AA:849:C:H6	1.74	0.53
3:AC:19:GLU:HB3	3:AC:40:ARG:NH2	2.23	0.53
3:AC:36:ASP:O	3:AC:40:ARG:HG3	2.09	0.53
23:AW:18:G:H4'	23:AW:60:U:C5	2.43	0.53
25:AY:49:C:H42	25:AY:65:G:H1	0.68	0.53
26:BA:2693:A:H2'	26:BA:2694:G:C8	2.44	0.53
29:BE:31:CYS:HB3	29:BE:49:LEU:HG	1.90	0.53
26:BA:548:A:H61	42:BV:19:LYS:H	1.56	0.53
1:CA:1347:G:N2	1:CA:1373:G:H2'	2.24	0.53
26:DA:922:U:H2'	26:DA:923:C:C6	2.43	0.53
31:DG:106:LEU:HA	31:DG:110:ALA:HB3	1.90	0.53
35:DO:16:ALA:HB2	35:DO:52:VAL:HG21	1.91	0.53
1:AA:1064:G:H4'	1:AA:1065:U:OP1	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:BA:1778:U:H2'	26:BA:1784:A:N6	2.23	0.53
26:BA:2116:G:H2'	26:BA:2117:A:C6	2.44	0.53
26:BA:2137:C:H2'	26:BA:2138:C:C6	2.43	0.53
26:BA:2690:C:OP1	38:BR:17:ARG:NH1	2.33	0.53
1:CA:1120:G:C6	1:CA:1154:G:C2	2.96	0.53
1:CA:895:G:N7	61:CA:4069:HOH:O	2.34	0.53
2:CB:46:LYS:O	2:CB:50:GLU:N	2.42	0.53
26:DA:1364:G:OP2	48:D1:3:LYS:HG3	2.09	0.53
26:DA:1423:G:OP1	26:DA:1492:G:O2'	2.26	0.53
26:DA:1658:C:OP1	61:DA:4209:HOH:O	2.18	0.53
26:DA:2177:C:H2'	26:DA:2178:C:O4'	2.08	0.53
26:DA:2630:G:H2'	26:DA:2631:G:H8	1.74	0.53
26:DA:644:A:H4'	26:DA:645:C:C5	2.43	0.53
42:DV:24:LYS:HG3	42:DV:64:HIS:HD2	1.73	0.53
1:AA:1062:U:H2'	1:AA:1063:C:C6	2.44	0.53
1:AA:946:A:H2'	1:AA:947:G:C8	2.43	0.53
4:AD:15:GLU:CG	4:AD:63:LYS:HB3	2.39	0.53
12:AL:39:VAL:HG11	12:AL:41:ARG:NH1	2.24	0.53
23:AW:1:G:H2'	23:AW:2:C:C6	2.44	0.53
23:AW:9:A:H1'	23:AW:45:U:O2'	2.09	0.53
26:BA:2115:G:N2	26:BA:2171:A:H61	2.06	0.53
46:BZ:126:VAL:HG11	46:BZ:161:VAL:HG23	1.89	0.53
2:CB:16:HIS:CG	2:CB:17:PHE:H	2.27	0.53
3:CC:8:ILE:HD13	3:CC:184:TYR:HB3	1.90	0.53
8:CH:30:ARG:O	8:CH:34:GLU:HG2	2.08	0.53
23:CW:75:C:H2'	23:CW:76:31M:C4	2.39	0.53
26:DA:875:G:O2'	46:DZ:151:HIS:HE1	1.92	0.53
39:DS:11:LYS:O	39:DS:15:ARG:HG3	2.08	0.53
1:AA:270:A:H2'	1:AA:271:C:C6	2.44	0.53
1:AA:520:A:N1	1:AA:536:C:H1'	2.23	0.53
6:AF:9:VAL:HB	6:AF:87:ARG:HB2	1.90	0.53
24:AX:7:G:H1	24:AX:66:C:H42	1.56	0.53
29:BE:12:THR:HG22	29:BE:13:ARG:H	1.73	0.53
26:DA:1379:A:H4'	26:DA:1380:G:OP2	2.07	0.53
26:DA:1420:U:O2'	26:DA:1421:G:OP1	2.25	0.53
26:DA:144:C:H2'	26:DA:145:G:H8	1.73	0.53
39:DS:87:PHE:CZ	39:DS:102:ALA:HB2	2.44	0.53
1:AA:262:A:H2'	1:AA:263:A:C8	2.44	0.53
1:AA:97:G:O2'	1:AA:98:G:H5''	2.09	0.53
26:BA:639:U:H2'	26:BA:640:C:C6	2.44	0.53
33:BI:40:THR:O	33:BI:44:LEU:HB2	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:BZ:111:VAL:HG12	46:BZ:112:ARG:H	1.73	0.53
1:CA:1122:U:C4	1:CA:1123:A:N7	2.76	0.53
1:CA:1125:U:C3'	1:CA:1126:U:H5''	2.38	0.53
17:CQ:12:SER:HB3	17:CQ:20:THR:HB	1.89	0.53
26:DA:1532:C:N4	26:DA:1537:G:O6	2.20	0.53
26:DA:2112:G:N7	26:DA:2169:A:N6	2.57	0.53
46:DZ:53:ILE:HD13	46:DZ:99:TYR:HB2	1.91	0.53
1:AA:942:G:H21	9:AI:124:GLN:NE2	2.08	0.52
49:B2:11:GLU:O	49:B2:15:LYS:HG3	2.09	0.52
26:BA:252:G:OP1	36:BP:50:ARG:NH1	2.42	0.52
28:BD:10:THR:OG1	28:BD:13:ARG:HB2	2.08	0.52
1:CA:1125:U:O2	10:CJ:38:ILE:HG21	2.09	0.52
1:CA:620:C:C2	4:CD:135:LEU:HG	2.43	0.52
2:CB:91:PRO:HD3	2:CB:154:LEU:HD12	1.91	0.52
3:CC:54:ARG:HH11	3:CC:54:ARG:HB3	1.74	0.52
4:CD:119:GLN:HG2	4:CD:123:HIS:CD2	2.45	0.52
1:CA:437:U:H5'	4:CD:155:LEU:HD21	1.91	0.52
16:CP:52:ASP:O	16:CP:54:GLU:N	2.33	0.52
26:DA:857:C:H4'	47:D0:23:VAL:HG21	1.91	0.52
26:DA:1415:U:O2'	26:DA:1417:C:OP1	2.25	0.52
26:DA:2646:C:H2'	26:DA:2647:U:O4'	2.09	0.52
26:DA:878:A:N6	26:DA:899:A:O2'	2.43	0.52
28:DD:85:ASP:OD2	28:DD:88:ARG:NH1	2.40	0.52
26:DA:2684:U:O2'	35:DO:68:GLU:OE1	2.28	0.52
29:DE:27:LEU:HD22	40:DT:1:MET:HE1	1.90	0.52
1:AA:167:G:H2'	1:AA:168:G:H8	1.75	0.52
24:AX:56:C:O5'	24:AX:56:C:H6	1.92	0.52
25:AY:67:C:H2'	25:AY:68:C:C6	2.44	0.52
26:BA:330:A:H2	26:BA:1210:A:O2'	1.92	0.52
26:BA:1359:A:H2'	26:BA:1360:A:H5'	1.91	0.52
32:BH:159:GLU:HG3	32:BH:169:VAL:HG11	1.91	0.52
1:CA:1119:C:N3	1:CA:1154:G:O6	2.42	0.52
1:CA:1125:U:C2	10:CJ:38:ILE:HD13	2.44	0.52
1:CA:1260:C:O5'	1:CA:1284:C:H4'	2.09	0.52
1:CA:164:U:H2'	1:CA:165:C:C6	2.44	0.52
26:DA:1790:C:H5''	26:DA:1791:A:OP1	2.09	0.52
26:DA:2180:U:H2'	26:DA:2181:G:O4'	2.09	0.52
1:AA:1027:C:N3	1:AA:1028:C:N4	2.57	0.52
1:AA:67:C:H2'	1:AA:68:G:C8	2.44	0.52
3:AC:152:ILE:HB	3:AC:199:LYS:HB2	1.91	0.52
3:AC:22:TRP:CZ2	14:AN:54:PRO:HG3	2.44	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:AD:155:LEU:HB3	4:AD:158:ILE:CD1	2.39	0.52
17:AQ:56:VAL:HB	17:AQ:78:GLU:HB3	1.91	0.52
50:B3:50:VAL:HB	50:B3:53:LEU:HD12	1.90	0.52
34:BN:21:LYS:HE3	34:BN:140:VAL:OXT	2.09	0.52
1:CA:1278:U:H5'	1:CA:1279:A:O4'	2.08	0.52
1:CA:625:G:H2'	1:CA:626:U:H6	1.74	0.52
3:CC:3:ASN:N	3:CC:3:ASN:OD1	2.42	0.52
30:DF:120:GLU:HB2	30:DF:122:LYS:HG2	1.90	0.52
34:DN:67:LEU:O	34:DN:88:GLU:HG3	2.10	0.52
40:DT:11:GLU:O	40:DT:15:VAL:HG23	2.10	0.52
26:DA:1188:U:H4'	42:DV:79:VAL:HG22	1.91	0.52
1:AA:1053:G:C3'	1:AA:1054:C:H5'	2.39	0.52
10:AJ:62:HIS:HB3	14:AN:59:ALA:HB3	1.92	0.52
12:AL:24:VAL:HG13	12:AL:98:TYR:HE1	1.73	0.52
31:BG:179:PRO:HG3	51:B4:43:TYR:OH	2.10	0.52
26:BA:1429:G:H2'	26:BA:1430:C:C6	2.44	0.52
26:BA:1482:G:O6	26:BA:1507:A:N6	2.42	0.52
27:BB:7:G:H5''	27:BB:7:G:H8	1.75	0.52
28:BD:108:PRO:HB3	28:BD:143:HIS:CE1	2.45	0.52
26:BA:1843:C:H5'	28:BD:253:GLN:HE22	1.74	0.52
32:BH:56:SER:OG	32:BH:57:ASP:N	2.42	0.52
37:BQ:54:MET:HG3	37:BQ:117:ALA:HB1	1.92	0.52
1:CA:1158:C:O3'	2:CB:133:LYS:NZ	2.43	0.52
1:CA:1103:C:OP1	2:CB:96:ARG:NH2	2.42	0.52
3:CC:111:LEU:HD22	3:CC:146:ALA:HB2	1.92	0.52
8:CH:20:TYR:HA	8:CH:65:TYR:CZ	2.44	0.52
55:D8:6:THR:HG22	55:D8:63:PRO:HD2	1.92	0.52
26:DA:1021:A:C8	26:DA:1021:A:H3'	2.45	0.52
26:DA:2176:A:H2'	26:DA:2177:C:C5	2.44	0.52
26:DA:2803:C:H2'	26:DA:2804:C:H6	1.74	0.52
28:DD:276:LYS:H	28:DD:276:LYS:HD3	1.74	0.52
26:DA:2748:A:H5'	32:DH:4:ILE:HD12	1.92	0.52
33:DI:40:THR:O	33:DI:44:LEU:HB2	2.09	0.52
44:DX:44:GLU:O	44:DX:48:LYS:N	2.42	0.52
44:DX:11:PRO:HB3	44:DX:92:LEU:HD11	1.90	0.52
6:AF:19:LEU:HD11	6:AF:59:TYR:CE2	2.45	0.52
23:AW:1:G:O6	23:AW:72:C:N3	2.42	0.52
36:BP:49:ARG:NH1	55:B8:61:LEU:HD23	2.24	0.52
26:BA:2136:C:N4	26:BA:2155:G:N1	2.32	0.52
26:BA:1187:G:H5''	42:BV:81:TYR:CE1	2.43	0.52
1:CA:1243:C:H42	1:CA:1294:G:H1	1.58	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:1490:C:H2'	1:CA:1491:G:C8	2.44	0.52
3:CC:125:GLU:O	3:CC:127:ARG:NH1	2.41	0.52
26:DA:77:C:O2'	49:D2:14:ARG:NH2	2.42	0.52
50:D3:13:ILE:O	61:D3:3101:HOH:O	2.19	0.52
26:DA:1839:G:C8	26:DA:1927:A:H1'	2.44	0.52
36:DP:95:VAL:HG13	36:DP:125:VAL:HA	1.91	0.52
1:AA:1131:G:H2'	1:AA:1132:C:H6	1.74	0.52
1:AA:1320:C:OP1	19:AS:70:LYS:HE3	2.09	0.52
1:AA:1376:U:H2'	1:AA:1377:A:C8	2.43	0.52
1:AA:1530:G:H2'	1:AA:1531:A:O4'	2.09	0.52
1:AA:685:G:N2	1:AA:704:A:OP2	2.33	0.52
4:AD:79:PHE:HE1	4:AD:204:ILE:HD13	1.75	0.52
7:AG:49:ILE:O	7:AG:53:LYS:HG3	2.10	0.52
24:AX:4:G:H2'	24:AX:5:G:C8	2.44	0.52
26:BA:141:A:H8	26:BA:1408:C:HO2'	1.54	0.52
26:BA:957:A:N1	26:BA:2458:G:H4'	2.25	0.52
1:AA:1464:G:OP2	40:BT:111:ARG:NH2	2.43	0.52
1:CA:1469:G:N7	61:CA:4124:HOH:O	2.34	0.52
1:CA:876:G:O5'	8:CH:14:ARG:NH1	2.43	0.52
2:CB:141:GLU:O	2:CB:145:LEU:HG	2.09	0.52
8:CH:13:ILE:O	8:CH:17:THR:HG23	2.10	0.52
15:CO:39:LEU:HD13	15:CO:56:LEU:HB2	1.91	0.52
25:CY:61:C:H2'	25:CY:62:C:C6	2.45	0.52
26:DA:1899:G:O2'	26:DA:1900:A:OP2	2.24	0.52
26:DA:821:A:N1	61:DA:4093:HOH:O	2.34	0.52
41:DU:81:HIS:HB3	41:DU:117:GLN:HE22	1.74	0.52
1:AA:838:G:H2'	1:AA:839:U:H2'	1.92	0.52
4:AD:107:ARG:HH22	4:AD:194:LEU:HD21	1.74	0.52
6:AF:22:GLU:OE2	6:AF:82:ARG:HG2	2.10	0.52
26:BA:1803:A:O2'	28:BD:259:THR:HG21	2.09	0.52
26:BA:2243:U:H2'	26:BA:2244:U:C6	2.45	0.52
39:BS:106:ARG:O	39:BS:109:GLY:N	2.40	0.52
1:CA:1075:C:C2'	1:CA:1076:C:H5''	2.40	0.52
1:CA:1154:G:N7	1:CA:1155:G:C4	2.78	0.52
1:CA:189(L):G:H2'	1:CA:190:U:H6	1.74	0.52
1:CA:296:U:O2'	1:CA:556:C:O2	2.27	0.52
2:CB:53:ARG:NH1	2:CB:53:ARG:HB3	2.25	0.52
5:CE:6:PHE:HB2	5:CE:34:VAL:HG22	1.91	0.52
8:CH:49:GLU:HG2	8:CH:62:TYR:HE1	1.75	0.52
17:CQ:5:VAL:HG22	17:CQ:60:ILE:HG12	1.91	0.52
20:CT:43:LEU:O	20:CT:47:GLY:N	2.42	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:D0:17:GLN:O	47:D0:19:LYS:NZ	2.38	0.52
26:DA:2171:A:C4	26:DA:2172:U:C4	2.98	0.52
31:DG:17:PRO:HA	31:DG:20:ILE:HD12	1.92	0.52
1:AA:346:G:H3'	1:AA:347:G:H4'	1.92	0.52
1:AA:649:G:H2'	1:AA:650:G:H8	1.74	0.52
2:AB:47:THR:HA	2:AB:202:PRO:HG2	1.91	0.52
4:AD:155:LEU:HB3	4:AD:158:ILE:HD11	1.92	0.52
11:AK:15:ALA:HA	11:AK:76:GLY:O	2.09	0.52
26:BA:2051:A:H5'	26:BA:2578:G:O4'	2.10	0.52
26:BA:2747:G:O6	26:BA:2755:C:H5''	2.10	0.52
1:CA:1070:U:H2'	1:CA:1071:C:H6	1.75	0.52
3:CC:126:ARG:HB3	3:CC:128:PHE:HE1	1.75	0.52
5:CE:140:ARG:O	5:CE:143:ARG:NH2	2.43	0.52
9:CI:15:ALA:HB2	9:CI:65:VAL:HG23	1.91	0.52
26:DA:2203:U:H2'	26:DA:2205:C:C6	2.45	0.52
26:DA:2785:C:OP1	29:DE:41:LYS:NZ	2.34	0.52
26:DA:657:U:H2'	26:DA:658:C:C6	2.44	0.52
31:DG:68:PRO:HB3	31:DG:92:VAL:HB	1.92	0.52
36:DP:44:GLY:HA3	36:DP:45:LEU:HB2	1.92	0.52
1:AA:428:G:H4'	1:AA:429:U:O5'	2.10	0.52
20:AT:14:LYS:HG3	20:AT:17:ARG:NH2	2.25	0.52
25:AY:5:G:H1'	25:AY:69:G:N2	2.25	0.52
26:BA:1177:A:H3'	26:BA:1178:C:C6	2.44	0.52
26:BA:2404:C:O3'	36:BP:77:ARG:NH2	2.43	0.52
40:BT:118:ARG:HG3	40:BT:118:ARG:NH1	2.22	0.52
1:CA:768:A:OP2	61:CA:4019:HOH:O	2.19	0.52
7:CG:50:ILE:HD11	7:CG:58:PRO:HA	1.92	0.52
20:CT:10:LEU:HB3	20:CT:12:ALA:H	1.74	0.52
23:CW:19:G:H1	23:CW:56:C:N4	2.04	0.52
26:DA:1033:U:OP1	56:D9:9:ARG:NH2	2.43	0.52
26:DA:942:G:OP2	36:DP:39:LYS:NZ	2.42	0.52
40:DT:16:ARG:NH2	40:DT:83:ILE:O	2.42	0.52
1:AA:1131:G:H2'	1:AA:1132:C:C6	2.45	0.52
7:AG:12:LEU:H	7:AG:12:LEU:HD12	1.74	0.52
32:BH:88:LEU:HD13	32:BH:130:ARG:HG2	1.92	0.52
39:BS:11:LYS:O	39:BS:15:ARG:HG3	2.09	0.52
39:BS:46:VAL:HG12	39:BS:48:LEU:HD12	1.91	0.52
1:CA:1004:A:H3'	1:CA:1005:A:C5'	2.38	0.52
1:CA:1006:C:OP1	1:CA:1037:C:O2'	2.27	0.52
1:CA:551:U:H2'	1:CA:552:U:C6	2.44	0.52
2:CB:76:GLN:HB2	2:CB:208:ILE:HG12	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:261:U:OP2	20:CT:79:ARG:NH2	2.43	0.52
26:DA:171:G:H2'	26:DA:172:C:H6	1.75	0.52
26:DA:373:U:H2'	26:DA:374:A:C8	2.44	0.52
26:DA:81:G:N7	61:DA:4166:HOH:O	2.33	0.52
26:DA:2590:A:OP2	28:DD:238:GLY:HA2	2.10	0.52
30:DF:20:LEU:HD12	30:DF:125:LEU:HD13	1.91	0.52
36:DP:29:LYS:HG3	36:DP:30:THR:H	1.75	0.52
43:DW:45:TYR:CZ	43:DW:49:LYS:HE3	2.45	0.52
1:AA:664:G:N2	1:AA:741:G:H1	2.00	0.51
3:AC:18:TRP:HE3	3:AC:18:TRP:H	1.56	0.51
8:AH:39:LEU:HB3	8:AH:45:ILE:HG12	1.92	0.51
8:AH:73:ASP:OD1	8:AH:75:ARG:HD3	2.10	0.51
19:AS:65:ASN:HD22	19:AS:66:MET:N	2.09	0.51
26:BA:1858:G:N2	26:BA:1883:G:H2'	2.24	0.51
29:BE:143:ASN:HD22	29:BE:147:PRO:HD3	1.76	0.51
33:BI:93:THR:HG22	33:BI:119:PRO:HB3	1.91	0.51
1:CA:1218:C:H2'	1:CA:1219:U:C6	2.45	0.51
1:CA:1304:G:C6	1:CA:1305:G:N1	2.78	0.51
9:CI:55:ALA:HA	9:CI:58:HIS:CD2	2.45	0.51
15:CO:8:LYS:O	15:CO:12:ILE:HG13	2.10	0.51
26:DA:2299:G:H2'	26:DA:2300:G:H8	1.75	0.51
29:DE:12:THR:HG22	40:DT:58:ASN:OD1	2.10	0.51
41:DU:58:ARG:HA	41:DU:61:TRP:CE3	2.45	0.51
1:AA:1036:G:H5'	1:AA:1037:C:OP2	2.09	0.51
1:AA:78:G:C2	1:AA:91:C:N3	2.78	0.51
13:AM:122:LYS:HD3	13:AM:123:ALA:H	1.74	0.51
25:AY:7:A:N1	25:AY:66:U:O2	2.42	0.51
49:B2:2:LYS:O	49:B2:6:VAL:HG23	2.09	0.51
26:BA:1593:G:H2'	26:BA:1594:G:C8	2.45	0.51
26:BA:2361:A:OP1	55:B8:27:THR:OG1	2.13	0.51
26:BA:793:A:OP2	26:BA:2071:A:O2'	2.27	0.51
29:BE:47:VAL:HG23	29:BE:84:PHE:O	2.10	0.51
1:CA:1118:C:C2	1:CA:1119:C:C5	2.96	0.51
1:CA:1327:C:H5''	21:CU:20:LYS:HB3	1.93	0.51
1:CA:17:U:H2'	1:CA:18:C:C6	2.44	0.51
8:CH:67:PRO:O	8:CH:69:ARG:HG3	2.10	0.51
1:CA:1129:C:P	9:CI:16:ARG:HH12	2.33	0.51
9:CI:53:VAL:C	9:CI:55:ALA:H	2.10	0.51
26:DA:1006:C:OP2	61:DA:4190:HOH:O	2.19	0.51
26:DA:1803:A:HO2'	28:DD:259:THR:HG21	1.76	0.51
29:DE:50:GLY:HA3	29:DE:75:VAL:HG11	1.91	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:DG:39:ILE:HB	31:DG:92:VAL:HG13	1.92	0.51
32:DH:81:GLU:OE1	32:DH:81:GLU:N	2.44	0.51
1:AA:1032:G:H2'	1:AA:1033:G:C8	2.44	0.51
2:AB:100:GLY:N	2:AB:176:GLU:OE2	2.30	0.51
26:BA:2277:G:OP2	47:B0:10:THR:HG21	2.10	0.51
26:BA:8:A:H2'	26:BA:9:U:H6	1.74	0.51
1:CA:1226:C:H2'	13:CM:103:THR:HB	1.93	0.51
1:CA:1360:A:O5'	1:CA:1360:A:H8	1.93	0.51
1:CA:955:U:O2'	19:CS:83:HIS:HD2	1.93	0.51
2:CB:15:VAL:HG13	2:CB:209:ARG:HB3	1.92	0.51
2:CB:168:THR:OG1	2:CB:192:SER:HA	2.09	0.51
4:CD:38:TYR:CE1	4:CD:45:GLN:HG2	2.45	0.51
9:CI:85:LEU:HB3	9:CI:92:TYR:HD2	1.75	0.51
12:CL:28:LYS:N	12:CL:29:GLY:HA2	2.24	0.51
18:CR:47:THR:HG23	18:CR:49:LYS:HG3	1.92	0.51
26:DA:867:C:H2'	26:DA:868:U:H5'	1.92	0.51
26:DA:62:C:H42	26:DA:93:G:H1	1.57	0.51
44:DX:88:LYS:HG2	44:DX:93:GLU:HG3	1.92	0.51
1:AA:1035:A:H2	1:AA:1036:G:N7	2.09	0.51
10:AJ:38:ILE:HG13	10:AJ:71:LEU:O	2.10	0.51
50:B3:8:LEU:HD13	50:B3:31:LEU:HD23	1.90	0.51
26:BA:1164:G:H2'	26:BA:1165:U:C6	2.46	0.51
26:BA:1420:U:O2'	26:BA:1421:G:OP1	2.22	0.51
26:BA:2687:U:H2'	26:BA:2688:U:O4'	2.10	0.51
26:BA:602:G:O2'	26:BA:655:A:N6	2.43	0.51
26:BA:637:A:H4'	26:BA:638:G:O5'	2.11	0.51
1:CA:1004:A:H62	1:CA:1037:C:H3'	1.76	0.51
1:CA:1362:C:H2'	1:CA:1363:C:H5''	1.92	0.51
1:CA:179:A:H2'	1:CA:180:U:C6	2.46	0.51
1:CA:34:C:H2'	1:CA:35:G:C8	2.45	0.51
1:CA:352:C:N3	1:CA:356:A:N6	2.58	0.51
1:CA:784:C:H4'	26:DA:1837:C:OP1	2.10	0.51
3:CC:118:GLN:HA	3:CC:121:ALA:HB3	1.92	0.51
3:CC:187:ALA:O	3:CC:198:VAL:HG23	2.11	0.51
9:CI:96:LEU:O	9:CI:100:GLY:N	2.43	0.51
17:CQ:95:TYR:HA	17:CQ:98:LEU:HD13	1.91	0.51
13:CM:3:ARG:HA	51:D4:34:GLU:HG2	1.92	0.51
26:DA:2019:A:H4'	41:DU:34:LYS:HD2	1.92	0.51
23:CW:74:C:N4	26:DA:2507:C:O2'	2.44	0.51
26:DA:710:G:H1	26:DA:721:C:H42	1.56	0.51
26:DA:832:G:OP1	61:DA:4285:HOH:O	2.19	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:DE:52:LEU:HB2	29:DE:76:ARG:HB2	1.92	0.51
26:DA:607:U:OP1	30:DF:102:PRO:HA	2.10	0.51
26:DA:1155:A:H5''	41:DU:55:ARG:HD3	1.93	0.51
42:DV:10:LYS:HZ1	42:DV:23:GLU:HG3	1.74	0.51
1:AA:997:U:H3	1:AA:1044:A:H61	1.59	0.51
26:BA:45:C:OP2	26:BA:215:G:H2'	2.10	0.51
26:BA:34:C:H5''	26:BA:35:G:OP2	2.09	0.51
30:BF:53:THR:CG2	30:BF:55:GLY:H	2.24	0.51
1:CA:1050:G:H1'	1:CA:1214:C:O2	2.10	0.51
1:CA:1155:G:H2'	1:CA:1156:G:O4'	2.11	0.51
1:CA:448:A:P	1:CA:485:G:H22	2.33	0.51
19:CS:11:VAL:HB	19:CS:16:LEU:HD12	1.93	0.51
23:CW:47:U:H3'	23:CW:48:C:H5'	1.92	0.51
51:D4:7:PRO:HB2	51:D4:27:THR:HG21	1.93	0.51
26:DA:1593:G:H2'	26:DA:1594:G:H8	1.76	0.51
26:DA:621:A:OP2	36:DP:108:LYS:NZ	2.43	0.51
26:DA:652(T):C:H2'	26:DA:652(U):G:C8	2.46	0.51
30:DF:154:VAL:HG22	30:DF:191:ARG:HB2	1.92	0.51
45:DY:6:HIS:CD2	45:DY:6:HIS:H	2.28	0.51
1:AA:1002:G:N3	1:AA:1003:G:H1'	2.26	0.51
1:AA:1025:U:C2	1:AA:1036:G:O6	2.63	0.51
1:AA:1221:G:OP1	1:AA:1320:C:N4	2.43	0.51
2:AB:67:THR:N	2:AB:160:ASP:OD1	2.44	0.51
4:AD:162:LEU:HD13	4:AD:181:MET:HG2	1.91	0.51
9:AI:77:ILE:O	9:AI:81:ILE:HG22	2.10	0.51
18:AR:33:ASP:OD2	18:AR:36:ASN:HB2	2.11	0.51
26:BA:2123:G:N2	26:BA:2175:C:N3	2.48	0.51
26:BA:859:G:O2'	26:BA:916:G:O6	2.21	0.51
33:BI:72:LEU:O	33:BI:74:ASN:N	2.44	0.51
1:CA:1057:G:H2'	1:CA:1058:G:O4'	2.11	0.51
1:CA:1392:G:H21	1:CA:1502:A:H8	1.57	0.51
4:CD:65:ARG:HD3	4:CD:70:ILE:O	2.11	0.51
1:CA:1227:A:OP2	13:CM:111:LYS:HE3	2.09	0.51
31:DG:37:VAL:HG23	31:DG:99:MET:HG3	1.92	0.51
36:DP:82:GLY:HA2	36:DP:113:LYS:O	2.10	0.51
37:DQ:36:ALA:HA	37:DQ:129:THR:HG22	1.92	0.51
1:AA:1352:C:OP1	21:AU:3:LYS:NZ	2.40	0.51
1:AA:164:U:H2'	1:AA:165:C:C6	2.46	0.51
7:AG:27:ILE:HD12	7:AG:40:ALA:HA	1.91	0.51
23:AW:28:G:H2'	23:AW:29:G:C8	2.46	0.51
26:BA:1506:C:H2'	26:BA:1507:A:C8	2.36	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:BA:1790:C:H5''	26:BA:1791:A:OP1	2.11	0.51
26:BA:848:G:C4	26:BA:933:A:H8	2.29	0.51
33:BI:75:LEU:HD22	33:BI:105:HIS:ND1	2.25	0.51
34:BN:12:ARG:NH1	34:BN:50:ASP:OD2	2.43	0.51
1:CA:662:G:H2'	1:CA:663:A:C8	2.46	0.51
15:CO:64:ARG:HD3	15:CO:68:ARG:NH2	2.25	0.51
26:DA:2218:U:O4'	48:D1:52:ARG:NH2	2.44	0.51
26:DA:1023:U:OP2	61:DA:4648:HOH:O	2.20	0.51
26:DA:10:G:H2'	26:DA:11:G:H8	1.76	0.51
26:DA:1639:U:H4'	26:DA:2699:C:H4'	1.92	0.51
26:DA:1670:C:O2	29:DE:129:HIS:NE2	2.42	0.51
1:AA:954:G:H21	1:AA:1227:A:H62	1.59	0.51
1:AA:145:G:H1	1:AA:177:C:H42	1.59	0.51
24:AX:61:C:H2'	24:AX:62:C:H6	1.75	0.51
24:AX:76:A:O3'	61:AX:3101:HOH:O	2.19	0.51
26:BA:2691:C:O3'	26:BA:2871:C:H4'	2.10	0.51
26:BA:529:A:H62	26:BA:2041:U:H3	1.59	0.51
26:BA:271(K):U:C2	33:BI:50:ARG:HD3	2.46	0.51
1:CA:1004:A:C6	1:CA:1037:C:C2	2.98	0.51
1:CA:1062:U:H2'	1:CA:1063:C:C6	2.45	0.51
1:CA:375:U:O4	61:CA:4093:HOH:O	2.17	0.51
1:CA:950:U:H2'	1:CA:951:G:H8	1.76	0.51
7:CG:78:ARG:HG2	7:CG:79:ARG:HB2	1.93	0.51
1:CA:1457:G:H5''	20:CT:35:THR:HG21	1.93	0.51
26:DA:2364:C:OP1	47:D0:55:ARG:NH1	2.41	0.51
26:DA:82:G:N1	26:DA:103:A:OP2	2.37	0.51
26:DA:2769:C:H2'	26:DA:2770:G:O4'	2.11	0.51
28:DD:134:ARG:NH1	28:DD:188:GLU:OE2	2.44	0.51
28:DD:218:ARG:HB3	28:DD:219:PRO:HD2	1.93	0.51
32:DH:90:LYS:HD3	32:DH:159:GLU:HG2	1.92	0.51
1:AA:1004:A:N7	1:AA:1036:G:C2	2.79	0.51
1:AA:600:C:H2'	1:AA:601:C:C6	2.45	0.51
25:AY:19:G:H1	25:AY:56:C:H42	1.48	0.51
26:BA:467:G:OP1	54:B7:33:ARG:NH1	2.44	0.51
26:BA:952:G:OP1	37:BQ:16:ARG:NH2	2.44	0.51
1:CA:1120:G:N1	1:CA:1154:G:N3	2.59	0.51
1:CA:1169:A:H2'	1:CA:1170:A:C8	2.46	0.51
1:CA:1391:U:H2'	1:CA:1392:G:C8	2.45	0.51
1:CA:429:U:H3'	4:CD:9:CYS:SG	2.51	0.51
1:CA:69:G:H2'	1:CA:70:G:H8	1.76	0.51
1:CA:587:G:N1	1:CA:754:C:OP2	2.41	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:CC:53:ALA:HB3	3:CC:106:VAL:HG21	1.93	0.51
9:CI:8:GLY:HA3	9:CI:76:ALA:O	2.10	0.51
44:DX:5:TYR:CE1	49:D2:30:ARG:HB2	2.46	0.51
26:DA:1688:U:O2	26:DA:1700:A:H5'	2.11	0.51
26:DA:2121:G:O6	26:DA:2176:A:N6	2.44	0.51
26:DA:2357:U:OP1	47:D0:20:ARG:NH1	2.35	0.51
1:AA:460:G:O5'	1:AA:460:G:H8	1.93	0.51
8:AH:124:ALA:O	8:AH:128:GLY:N	2.43	0.51
20:AT:76:ALA:HA	20:AT:79:ARG:NH1	2.26	0.51
9:AI:128:ARG:NH1	24:AX:35:A:OP2	2.44	0.51
26:BA:1365:A:OP2	48:B1:3:LYS:HG2	2.10	0.51
26:BA:2168:G:C6	26:BA:2171:A:C8	2.99	0.51
1:CA:1358:U:H2'	1:CA:1359:C:O4'	2.11	0.51
1:CA:1513:A:H2'	1:CA:1514:C:C6	2.46	0.51
1:CA:533:A:O2'	1:CA:535:A:OP2	2.25	0.51
3:CC:130:VAL:O	3:CC:134:ILE:HD13	2.11	0.51
7:CG:22:LEU:HG	7:CG:62:PHE:HE2	1.74	0.51
26:DA:1028:A:N6	26:DA:1125:G:H2'	2.26	0.51
26:DA:2142:C:H2'	26:DA:2143:C:C6	2.46	0.51
26:DA:309:G:N3	26:DA:329:G:O2'	2.43	0.51
41:DU:104:GLN:OE1	41:DU:105:VAL:N	2.34	0.51
41:DU:52:ARG:HA	41:DU:55:ARG:HE	1.74	0.51
1:AA:1179:A:H2'	1:AA:1180:A:O4'	2.11	0.50
1:AA:749:C:H2'	1:AA:750:G:H8	1.76	0.50
4:AD:108:LEU:HD12	4:AD:176:LEU:HB2	1.93	0.50
17:AQ:12:SER:HB3	17:AQ:20:THR:HB	1.92	0.50
19:AS:3:ARG:HH21	19:AS:7:LYS:HE2	1.76	0.50
25:AY:40:C:H2'	25:AY:41:C:H6	1.76	0.50
25:AY:8:4SU:H4'	25:AY:48:C:H4'	1.93	0.50
26:BA:1817:G:OP1	28:BD:88:ARG:NH2	2.40	0.50
31:BG:43:LEU:HD11	31:BG:153:ARG:HG2	1.93	0.50
1:CA:719:C:N4	18:CR:71:LYS:HE2	2.26	0.50
1:CA:1014:A:H4'	19:CS:14:HIS:CE1	2.46	0.50
20:CT:56:MET:HG3	20:CT:57:ARG:N	2.27	0.50
25:CY:7:A:H61	25:CY:66:U:H3	0.60	0.50
26:DA:1671:U:HO2'	26:DA:1673:U:H5	1.57	0.50
26:DA:1916:A:H2'	26:DA:1917:U:O4'	2.12	0.50
31:DG:97:ASP:HA	31:DG:100:TRP:HD1	1.75	0.50
1:AA:1144:G:N2	1:AA:1146:A:H62	2.10	0.50
3:AC:35:GLU:OE2	3:AC:59:ARG:NH2	2.43	0.50
1:AA:377:G:OP1	16:AP:3:LYS:HD2	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:AX:61:C:H2'	24:AX:62:C:C6	2.46	0.50
48:B1:3:LYS:HB2	48:B1:61:ARG:NH1	2.26	0.50
56:B9:25:VAL:HB	56:B9:34:GLN:HB2	1.92	0.50
36:BP:88:LEU:HD11	36:BP:114:ILE:HD12	1.93	0.50
45:BY:87:LYS:HB3	45:BY:95:LYS:HD3	1.93	0.50
1:CA:160:A:H61	1:CA:347:G:H1'	1.76	0.50
1:CA:431:A:H2'	1:CA:432:A:C8	2.46	0.50
7:CG:111:ARG:NH1	7:CG:113:GLU:OE2	2.44	0.50
7:CG:28:ASN:HA	7:CG:31:MET:HE2	1.93	0.50
25:CY:11:C:N3	25:CY:24:G:O6	2.44	0.50
51:D4:62:ARG:HD3	51:D4:62:ARG:H	1.77	0.50
26:DA:376:C:OP1	61:DA:4418:HOH:O	2.19	0.50
26:DA:479:A:N3	26:DA:481:G:H5''	2.26	0.50
29:DE:116:VAL:HG13	29:DE:122:PHE:HB2	1.92	0.50
44:DX:43:VAL:HG21	44:DX:81:VAL:HG11	1.93	0.50
1:AA:1277:C:O2'	1:AA:1279:A:H1'	2.10	0.50
5:AE:36:ASP:OD2	5:AE:40:ARG:HB2	2.12	0.50
25:AY:62:C:H2'	25:AY:63:G:C8	2.40	0.50
26:BA:1274:A:N3	26:BA:1297:C:H1'	2.26	0.50
26:BA:1423:G:OP1	26:BA:1492:G:O2'	2.23	0.50
26:BA:1030:G:OP2	37:BQ:128:LYS:NZ	2.44	0.50
37:BQ:18:LYS:O	37:BQ:98:LYS:NZ	2.25	0.50
1:CA:1176:A:H2'	1:CA:1177:G:C8	2.47	0.50
4:CD:173:TRP:CZ3	4:CD:193:ASP:HB3	2.46	0.50
7:CG:26:PHE:HE2	7:CG:104:LEU:HD23	1.76	0.50
7:CG:22:LEU:HG	7:CG:62:PHE:CE2	2.46	0.50
53:D6:23:THR:OG1	53:D6:24:GLU:N	2.43	0.50
27:DB:17:C:H2'	27:DB:18:G:O4'	2.11	0.50
29:DE:2:LYS:HB2	29:DE:95:ILE:HD12	1.93	0.50
29:DE:7:VAL:HG12	29:DE:27:LEU:HB3	1.92	0.50
31:DG:70:VAL:HA	31:DG:90:LEU:HD23	1.92	0.50
45:DY:38:ILE:HD11	45:DY:66:PRO:HG3	1.92	0.50
1:AA:1176:A:H2'	1:AA:1177:G:C8	2.46	0.50
1:AA:619:U:C2	4:AD:135:LEU:HD22	2.45	0.50
26:BA:796:C:H2'	26:BA:797:C:C6	2.46	0.50
27:BB:2:C:H2'	27:BB:3:C:C6	2.46	0.50
33:BI:135:GLU:C	33:BI:137:PRO:HD3	2.31	0.50
45:BY:20:TYR:CE1	45:BY:43:ASN:HA	2.46	0.50
1:CA:1119:C:H2'	1:CA:1120:G:H8	1.75	0.50
1:CA:923:A:O2'	1:CA:1399:C:OP2	2.21	0.50
3:CC:8:ILE:HG23	3:CC:16:ARG:HG2	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:CP:68:ASP:O	16:CP:71:ARG:HG2	2.11	0.50
26:DA:2153:G:C2	26:DA:2154:G:C4	2.99	0.50
26:DA:2753:A:N3	56:D9:15:LYS:NZ	2.54	0.50
32:DH:56:SER:HB3	32:DH:61:HIS:ND1	2.26	0.50
38:DR:2:ARG:NH1	38:DR:5:LYS:O	2.44	0.50
1:AA:1067:A:O2'	1:AA:1068:G:OP2	2.21	0.50
1:AA:1521:G:N3	61:AA:4065:HOH:O	2.35	0.50
1:AA:78:G:H1	1:AA:91:C:N4	2.07	0.50
2:AB:60:ASP:O	2:AB:64:ARG:HB2	2.12	0.50
4:AD:147:ALA:HB2	4:AD:182:LYS:HA	1.94	0.50
9:AI:4:TYR:CD2	9:AI:88:TYR:HA	2.47	0.50
14:AN:23:ARG:NH1	14:AN:30:ALA:HB2	2.26	0.50
26:BA:2512:C:H2'	26:BA:2513:G:O4'	2.12	0.50
43:BW:79:GLY:HA3	43:BW:100:THR:HG22	1.93	0.50
1:CA:1001(A):G:H3'	1:CA:1002:G:O4'	2.11	0.50
1:CA:1030:C:N4	1:CA:1032:G:O6	2.44	0.50
1:CA:67:C:H2'	1:CA:68:G:C8	2.47	0.50
2:CB:233:SER:HB2	2:CB:234:PRO:HD2	1.93	0.50
8:CH:43:GLY:O	8:CH:64:LYS:NZ	2.42	0.50
10:CJ:55:LYS:HG3	10:CJ:56:HIS:H	1.75	0.50
26:DA:443:A:H1'	26:DA:1201:C:O4'	2.10	0.50
26:DA:286:C:H2'	26:DA:287:C:H6	1.77	0.50
27:DB:11:C:OP2	27:DB:12:C:N4	2.32	0.50
34:DN:4:TYR:HB2	41:DU:101:ARG:HH12	1.76	0.50
26:DA:2318:G:N2	39:DS:3:ARG:HH11	2.09	0.50
26:DA:483:A:O2'	45:DY:49:VAL:O	2.25	0.50
4:AD:15:GLU:HG2	4:AD:63:LYS:CB	2.41	0.50
11:AK:29:ILE:HG23	11:AK:44:SER:HB3	1.94	0.50
12:AL:28:LYS:HG3	12:AL:62:SER:HB2	1.94	0.50
18:AR:42:ARG:HH21	18:AR:42:ARG:HA	1.75	0.50
23:AW:58:A:O2'	23:AW:60:U:OP2	2.24	0.50
55:B8:6:THR:HG22	55:B8:63:PRO:HD2	1.93	0.50
26:BA:1045:A:H1'	26:BA:1047:G:N3	2.26	0.50
26:BA:1449:A:H5'	26:BA:1450:G:OP2	2.12	0.50
26:BA:1448:G:H4'	26:BA:1542:A:OP1	2.11	0.50
26:BA:456:C:H4'	61:BA:3946:HOH:O	2.11	0.50
39:BS:15:ARG:HE	39:BS:88:ASP:CG	2.14	0.50
3:CC:142:MET:HG3	3:CC:170:GLN:HB3	1.93	0.50
17:CQ:45:HIS:HA	17:CQ:69:LYS:HE3	1.94	0.50
23:CW:14:A:H2'	23:CW:15:G:O4'	2.11	0.50
25:CY:23:A:H8	25:CY:23:A:O5'	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:DA:1266:G:O4'	43:DW:15:ARG:NH2	2.45	0.50
26:DA:885:C:H2'	26:DA:886:C:H4'	1.94	0.50
33:DI:130:TYR:HB3	33:DI:138:ILE:HB	1.94	0.50
1:AA:1333:A:H2'	1:AA:1334:G:O4'	2.11	0.50
5:AE:78:HIS:HD1	8:AH:104:ARG:CD	2.24	0.50
14:AN:33:VAL:HA	14:AN:40:CYS:HA	1.94	0.50
10:AJ:49:VAL:HG23	14:AN:41:ARG:HB2	1.92	0.50
15:AO:8:LYS:O	15:AO:12:ILE:HG13	2.11	0.50
1:AA:376:G:P	16:AP:67:THR:HG21	2.51	0.50
25:AY:69:G:C2	25:AY:70:G:H1'	2.47	0.50
26:BA:1379:A:H4'	26:BA:1380:G:OP2	2.10	0.50
26:BA:1688:U:O2	26:BA:1700:A:H5'	2.12	0.50
23:AW:37:MIA:O2'	26:BA:1913:A:N1	2.44	0.50
1:CA:677:U:H3	1:CA:713:G:H22	1.58	0.50
20:CT:67:ALA:HB2	20:CT:77:ALA:HB2	1.92	0.50
21:CU:6:ARG:O	21:CU:12:LYS:NZ	2.37	0.50
23:CW:9:A:O2'	23:CW:10:G:N7	2.43	0.50
24:CX:6:G:H1	24:CX:67:C:H42	1.58	0.50
26:DA:2139:C:N4	26:DA:2153:G:C2	2.79	0.50
26:DA:854:G:H2'	26:DA:855:G:H8	1.76	0.50
31:DG:11:TYR:HB2	31:DG:176:LEU:HD21	1.93	0.50
36:DP:89:ALA:O	36:DP:121:LYS:NZ	2.39	0.50
39:DS:50:SER:O	39:DS:76:LYS:NZ	2.45	0.50
27:DB:75:G:H1'	46:DZ:27:VAL:HG11	1.94	0.50
1:AA:1132:C:H2'	1:AA:1133:G:H8	1.76	0.50
1:AA:1181:G:O2'	1:AA:1182:G:N7	2.45	0.50
1:AA:714:G:H2'	1:AA:715:A:C8	2.47	0.50
2:AB:93:VAL:HG21	2:AB:97:TRP:CD1	2.46	0.50
6:AF:36:ARG:HH11	6:AF:36:ARG:HB3	1.77	0.50
23:AW:49:C:H42	23:AW:65:G:H1	1.60	0.50
19:AS:68:GLY:H	51:B4:58:ARG:HH11	1.59	0.50
52:B5:11:THR:HG23	52:B5:15:ARG:HB3	1.93	0.50
26:BA:1866:C:H2'	26:BA:1876:A:O4'	2.11	0.50
26:BA:272(H):C:H42	26:BA:363(B):G:H1	1.58	0.50
26:BA:2319:G:H22	39:BS:3:ARG:NE	2.09	0.50
45:BY:6:HIS:CD2	45:BY:6:HIS:H	2.30	0.50
1:CA:1411:C:H2'	1:CA:1412:C:H6	1.76	0.50
1:CA:952:U:H2'	1:CA:953:G:H8	1.77	0.50
3:CC:136:GLN:O	3:CC:140:ARG:NH1	2.45	0.50
6:CF:37:VAL:HA	6:CF:65:VAL:HG12	1.93	0.50
26:DA:1021:A:H62	26:DA:1141:U:H3	1.59	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:DA:1187:G:H5'	42:DV:81:TYR:CE1	2.47	0.50
26:DA:11:G:H2'	26:DA:12:U:H5''	1.93	0.50
26:DA:1399:C:OP1	44:DX:25:LYS:NZ	2.40	0.50
26:DA:1894:C:H2'	26:DA:1895:C:H6	1.77	0.50
26:DA:586:A:N1	26:DA:809:G:O2'	2.35	0.50
39:DS:93:LYS:CD	39:DS:95:HIS:HB2	2.40	0.50
46:DZ:93:ASP:OD1	46:DZ:94:GLU:HG3	2.12	0.50
1:AA:1131:G:O2'	1:AA:1132:C:H5'	2.12	0.50
1:AA:279:A:C5	17:AQ:98:LEU:HD23	2.47	0.50
1:AA:673:G:H2'	1:AA:674:G:C8	2.47	0.50
9:AI:110:GLU:OE2	9:AI:113:LYS:NZ	2.45	0.50
1:AA:1249:C:O2'	9:AI:73:GLN:NE2	2.45	0.50
16:AP:4:ILE:HB	16:AP:66:PRO:HA	1.94	0.50
23:AW:11:C:H42	23:AW:24:G:H1	1.58	0.50
25:AY:33:U:C3'	25:AY:34:G:H5''	2.41	0.50
26:BA:2441:C:OP2	26:BA:2586:C:O2'	2.26	0.50
26:BA:2712:U:H2'	26:BA:2714:G:H5''	1.93	0.50
30:BF:64:ILE:HD11	30:BF:75:HIS:HB2	1.94	0.50
40:BT:29:ARG:HG3	40:BT:46:GLU:HB2	1.93	0.50
26:BA:548:A:N6	42:BV:19:LYS:H	2.09	0.50
44:BX:61:GLY:HA3	44:BX:73:ARG:O	2.11	0.50
1:CA:1244:C:N4	1:CA:1293:G:H1	2.10	0.50
1:CA:1435:G:H2'	1:CA:1436:U:C6	2.46	0.50
1:CA:933:G:N2	1:CA:935:A:O4'	2.45	0.50
1:CA:936:C:H2'	1:CA:937:A:O4'	2.10	0.50
1:CA:950:U:H2'	1:CA:951:G:C8	2.47	0.50
2:CB:186:ALA:HB3	2:CB:197:VAL:HG11	1.93	0.50
1:CA:406:G:N2	4:CD:119:GLN:HE22	2.09	0.50
4:CD:61:LYS:NZ	4:CD:72:GLU:OE2	2.42	0.50
6:CF:69:GLU:O	6:CF:72:VAL:HG12	2.12	0.50
7:CG:76:ARG:HB3	7:CG:156:TRP:CH2	2.47	0.50
12:CL:117:ARG:CZ	12:CL:117:ARG:HB2	2.41	0.50
26:DA:1300:U:O2'	26:DA:1635:G:OP1	2.27	0.50
26:DA:1996:C:H4'	26:DA:1997:G:OP1	2.11	0.50
26:DA:2302:G:C2'	26:DA:2303:G:H5'	2.41	0.50
26:DA:2657:A:O3'	32:DH:160:LYS:NZ	2.45	0.50
34:DN:73:THR:OG1	34:DN:82:LEU:HD11	2.11	0.50
1:AA:1030(C):G:H2'	1:AA:1030(D):A:C8	2.47	0.49
1:AA:1391:U:H2'	1:AA:1392:G:C8	2.47	0.49
1:AA:991:U:O2'	1:AA:992:U:OP2	2.23	0.49
4:AD:196:LEU:O	4:AD:198:VAL:N	2.41	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:AI:49:PRO:HG2	9:AI:81:ILE:HG23	1.93	0.49
10:AJ:61:GLU:OE1	14:AN:58:LYS:NZ	2.41	0.49
1:AA:376:G:H5'	16:AP:5:ARG:HB3	1.92	0.49
48:B1:85:LEU:HB3	48:B1:89:GLU:HG2	1.94	0.49
51:B4:61:ARG:HG3	51:B4:62:ARG:N	2.26	0.49
26:BA:1779:U:H2'	61:BA:5061:HOH:O	2.11	0.49
26:BA:2128:C:O2'	26:BA:2129:C:H5'	2.12	0.49
26:BA:2278:A:OP2	47:B0:12:ASN:ND2	2.45	0.49
26:BA:282:A:H2'	26:BA:282:A:N3	2.27	0.49
26:BA:646:A:H2'	26:BA:647:G:O4'	2.12	0.49
26:BA:747:U:O2	26:BA:2014:A:H1'	2.12	0.49
28:BD:9:TYR:CZ	28:BD:13:ARG:HG2	2.47	0.49
26:BA:1009:A:P	34:BN:37:LYS:HZ1	2.32	0.49
38:BR:28:LEU:HD12	38:BR:48:VAL:HG21	1.94	0.49
41:BU:74:LEU:H	41:BU:74:LEU:HD12	1.77	0.49
44:BX:35:THR:HG22	44:BX:38:GLU:H	1.77	0.49
1:CA:1039:C:H2'	1:CA:1040:U:O4'	2.11	0.49
1:CA:1387:G:H2'	1:CA:1388:C:C6	2.47	0.49
10:CJ:67:THR:O	10:CJ:67:THR:OG1	2.30	0.49
20:CT:50:GLU:HG3	20:CT:100:ILE:HD13	1.94	0.49
47:D0:37:LEU:HD13	47:D0:79:VAL:HG11	1.94	0.49
26:DA:1037:G:H2'	26:DA:1038:C:O4'	2.12	0.49
26:DA:1359:A:N6	26:DA:1372:U:H3	2.08	0.49
26:DA:2128:C:H5'	26:DA:2173:A:C2	2.47	0.49
35:DO:1:MET:HG3	35:DO:67:LYS:HG2	1.93	0.49
36:DP:99:LEU:HD23	36:DP:99:LEU:H	1.77	0.49
26:DA:1278:A:OP1	38:DR:36:THR:HG23	2.12	0.49
46:DZ:117:LEU:HD11	46:DZ:144:LEU:HD13	1.93	0.49
1:AA:1053:G:O2'	61:AA:4100:HOH:O	2.19	0.49
1:AA:1095:U:P	1:AA:1108:G:H1	2.35	0.49
1:AA:1125:U:O2'	1:AA:1127:G:N7	2.24	0.49
1:AA:1399:C:C2	1:AA:1502:A:N6	2.80	0.49
2:AB:103:THR:HA	2:AB:180:LEU:HD11	1.93	0.49
26:BA:1774:C:H6	26:BA:1774:C:O5'	1.95	0.49
26:BA:2259:G:C8	26:BA:2427:C:C4	3.00	0.49
39:BS:14:VAL:O	39:BS:18:ILE:HG12	2.11	0.49
45:BY:92:ASN:HB3	45:BY:94:LYS:N	2.25	0.49
46:BZ:7:ALA:HB3	46:BZ:61:LEU:HD12	1.93	0.49
1:CA:137:C:H2'	1:CA:138:G:H8	1.76	0.49
1:CA:155:C:H2'	1:CA:156:G:O4'	2.11	0.49
2:CB:163:PHE:HA	2:CB:185:ILE:HG12	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:CN:48:ALA:HB2	14:CN:53:LEU:HD12	1.94	0.49
26:DA:1359:A:H2'	26:DA:1360:A:H5'	1.94	0.49
26:DA:1721:G:H8	26:DA:1741:A:H62	1.60	0.49
26:DA:2294:C:H5''	39:DS:10:ARG:HD2	1.94	0.49
26:DA:2483:C:H2'	26:DA:2484:G:O4'	2.11	0.49
26:DA:996:A:C2	26:DA:997:G:C8	3.00	0.49
34:DN:30:ILE:HG23	34:DN:52:VAL:HG11	1.94	0.49
26:DA:2849:U:P	40:DT:95:ARG:HH12	2.35	0.49
1:AA:1008:C:H2'	1:AA:1009:G:O4'	2.12	0.49
2:AB:20:GLU:HA	2:AB:21:ARG:HH21	1.78	0.49
26:BA:2345:G:H4'	26:BA:2346:A:H5''	1.94	0.49
26:BA:271(K):U:H1'	33:BI:50:ARG:CZ	2.43	0.49
26:BA:196:A:O2'	26:BA:805:G:O6	2.26	0.49
28:BD:70:TRP:HB3	28:BD:190:TYR:CE1	2.46	0.49
38:BR:21:TYR:OH	38:BR:43:GLU:HG2	2.12	0.49
26:BA:1155:A:OP1	41:BU:55:ARG:HD3	2.12	0.49
46:BZ:117:LEU:CD1	46:BZ:144:LEU:HD22	2.39	0.49
1:CA:110:C:H2'	1:CA:111:G:O4'	2.12	0.49
1:CA:984:C:O5'	1:CA:984:C:H6	1.94	0.49
4:CD:57:ARG:NE	4:CD:205:GLU:OE2	2.44	0.49
15:CO:3:ILE:O	15:CO:3:ILE:HG12	2.13	0.49
20:CT:18:GLN:O	20:CT:22:ARG:HG3	2.12	0.49
26:DA:2805:G:H2'	26:DA:2807:G:H8	1.75	0.49
26:DA:286:C:H2'	26:DA:287:C:C6	2.47	0.49
26:DA:335:C:H4'	45:DY:73:ARG:CZ	2.42	0.49
30:DF:129:PHE:CD2	30:DF:163:VAL:HG21	2.48	0.49
32:DH:89:ILE:O	32:DH:129:THR:HG23	2.13	0.49
34:DN:38:HIS:CE1	34:DN:39:ARG:HG3	2.46	0.49
39:DS:68:GLN:O	39:DS:71:ARG:HG3	2.13	0.49
42:DV:62:LEU:HD11	42:DV:95:LEU:HB2	1.93	0.49
44:DX:31:HIS:CD2	44:DX:33:LYS:HB2	2.47	0.49
46:DZ:104:PHE:HA	46:DZ:139:VAL:HB	1.95	0.49
1:AA:1003:G:H2'	1:AA:1004:A:H4'	1.92	0.49
1:AA:110:C:H2'	1:AA:111:G:O4'	2.12	0.49
1:AA:1346:A:OP1	9:AI:120:ARG:NH1	2.45	0.49
1:AA:920:U:H2'	1:AA:921:U:C6	2.48	0.49
23:AW:63:G:H2'	23:AW:64:A:O4'	2.13	0.49
26:BA:83:G:N2	26:BA:103:A:OP2	2.44	0.49
26:BA:2815:C:H5'	52:B5:29:THR:HG21	1.94	0.49
26:BA:831:G:O2'	36:BP:38:GLN:NE2	2.44	0.49
37:BQ:16:ARG:HG2	37:BQ:18:LYS:HE2	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:875:C:H1'	8:CH:15:ASN:HD21	1.77	0.49
10:CJ:62:HIS:HB3	14:CN:59:ALA:HB3	1.93	0.49
26:DA:10:G:H2'	26:DA:11:G:C8	2.47	0.49
26:DA:1264:G:H2'	26:DA:2014:A:N6	2.27	0.49
26:DA:528:A:C2	26:DA:2042:A:H2'	2.47	0.49
30:DF:11:VAL:HG22	30:DF:125:LEU:HB2	1.94	0.49
30:DF:13:SER:OG	30:DF:16:GLY:O	2.26	0.49
34:DN:67:LEU:HD13	34:DN:87:LEU:HD13	1.94	0.49
35:DO:73:ASP:HB2	40:DT:82:LEU:HD13	1.93	0.49
1:AA:1523:G:OP1	11:AK:123:LYS:NZ	2.30	0.49
2:AB:88:ALA:HB2	2:AB:219:VAL:HG13	1.94	0.49
4:AD:166:LYS:HB2	4:AD:168:ARG:NH1	2.26	0.49
12:AL:33:ARG:HH11	12:AL:62:SER:HB3	1.77	0.49
25:AY:50:U:N3	25:AY:64:A:H2	2.05	0.49
36:BP:50:ARG:HG2	55:B8:61:LEU:HD11	1.95	0.49
26:BA:2029:G:H2'	26:BA:2031:A:OP1	2.12	0.49
26:BA:8:A:H2'	26:BA:9:U:C6	2.47	0.49
26:BA:956:G:P	37:BQ:14:ARG:HH22	2.36	0.49
1:CA:444:C:H2'	1:CA:445:G:H8	1.78	0.49
1:CA:528:C:H5'	1:CA:529:G:OP2	2.13	0.49
1:CA:91:C:H2'	1:CA:92:C:C6	2.48	0.49
4:CD:173:TRP:CD1	4:CD:189:PRO:HG3	2.47	0.49
1:CA:923:A:OP1	5:CE:21:ALA:HB2	2.11	0.49
20:CT:53:LEU:HA	20:CT:56:MET:HG2	1.94	0.49
26:DA:1778:U:H2'	26:DA:1784:A:N6	2.28	0.49
26:DA:2408:U:H2'	26:DA:2409:G:C8	2.46	0.49
26:DA:2471:C:N4	26:DA:2476:A:O2'	2.43	0.49
26:DA:2558:C:H2'	26:DA:2559:C:O4'	2.13	0.49
27:DB:41:U:H5	31:DG:70:VAL:N	2.09	0.49
31:DG:43:LEU:HD11	31:DG:153:ARG:HG2	1.93	0.49
42:DV:100:ARG:NH1	42:DV:100:ARG:HG3	2.10	0.49
1:AA:1492:A:H2'	1:AA:1493:A:C8	2.48	0.49
1:AA:630:G:O2'	1:AA:631:G:H5'	2.13	0.49
1:AA:674:G:OP1	6:AF:87:ARG:NH2	2.43	0.49
4:AD:166:LYS:HB2	4:AD:168:ARG:CZ	2.42	0.49
10:AJ:16:LEU:HD21	10:AJ:70:ARG:HG2	1.93	0.49
1:AA:1244:C:OP1	21:AU:9:ARG:HB2	2.13	0.49
26:BA:55:G:O2'	26:BA:127:A:N1	2.39	0.49
26:BA:1292:U:H2'	26:BA:1293:C:C6	2.47	0.49
26:BA:1356:G:OP1	61:BA:5239:HOH:O	2.20	0.49
26:BA:1794:U:H2'	26:BA:1795:C:H6	1.78	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:BA:2319:G:N1	39:BS:3:ARG:HA	2.28	0.49
1:CA:1287:A:N3	1:CA:1353:G:O2'	2.42	0.49
1:CA:45:U:H2'	1:CA:46:G:C8	2.47	0.49
2:CB:77:ALA:HB2	2:CB:211:ILE:HD13	1.94	0.49
12:CL:33:ARG:HG2	12:CL:60:LEU:HD12	1.94	0.49
23:CW:76:31M:O	24:CX:76:A:O2'	2.19	0.49
26:DA:1153:C:OP1	41:DU:92:ARG:NH1	2.42	0.49
26:DA:2058:A:N7	61:DA:3876:HOH:O	2.34	0.49
26:DA:2123:G:H2'	26:DA:2124:G:C8	2.47	0.49
26:DA:639:U:H2'	26:DA:640:C:C6	2.48	0.49
28:DD:275:LYS:HG3	28:DD:276:LYS:HA	1.94	0.49
31:DG:103:LEU:HD22	31:DG:178:PHE:HZ	1.77	0.49
31:DG:16:ARG:HB2	31:DG:17:PRO:HD3	1.94	0.49
26:DA:300:A:H3'	45:DY:84:ARG:HH22	1.77	0.49
1:AA:130:A:H5'	17:AQ:63:ARG:HE	1.78	0.49
24:AX:66:C:H2'	24:AX:67:C:O4'	2.13	0.49
25:AY:51:U:H2'	25:AY:52:G:C8	2.48	0.49
26:BA:2291:U:H2'	26:BA:2292:C:C6	2.48	0.49
26:BA:548:A:O2'	26:BA:549:G:OP1	2.27	0.49
26:BA:1278:A:OP1	38:BR:36:THR:HG23	2.12	0.49
1:CA:1002:G:N3	1:CA:1003:G:H8	2.10	0.49
1:CA:838:G:N2	1:CA:848:C:N3	2.58	0.49
1:CA:8:A:H5'	5:CE:101:ILE:HG22	1.95	0.49
6:CF:11:ASN:HB3	6:CF:14:LEU:HG	1.95	0.49
1:CA:539:A:OP2	12:CL:115:LYS:NZ	2.45	0.49
49:D2:32:LEU:HD23	49:D2:53:LEU:HB3	1.94	0.49
26:DA:588:U:H2'	26:DA:589:C:C6	2.46	0.49
26:DA:764:A:H5'	28:DD:210:GLY:HA2	1.94	0.49
26:DA:989:G:H4'	26:DA:990:A:OP1	2.12	0.49
44:DX:12:VAL:HG22	44:DX:29:TRP:CE2	2.47	0.49
1:AA:1030(D):A:N6	1:AA:1031:G:H21	2.10	0.49
1:AA:865:A:C2	1:AA:918:A:H4'	2.45	0.49
3:AC:114:PRO:HA	3:AC:185:GLY:HA3	1.94	0.49
1:AA:625:G:H4'	16:AP:16:HIS:CD2	2.48	0.49
23:AW:58:A:H2	23:AW:60:U:HO2'	1.59	0.49
24:AX:21:A:N6	24:AX:46:G:H2'	2.27	0.49
25:AY:22:G:H2'	25:AY:23:A:H8	1.75	0.49
51:B4:26:SER:OG	51:B4:27:THR:N	2.45	0.49
31:BG:28:VAL:O	31:BG:31:VAL:HG12	2.13	0.49
61:BA:4985:HOH:O	36:BP:39:LYS:HE3	2.12	0.49
1:CA:1479:C:H2'	1:CA:1480:G:H8	1.77	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:539:A:H2'	1:CA:540:G:H8	1.76	0.49
1:CA:815:A:N7	1:CA:1509:C:O2'	2.41	0.49
10:CJ:38:ILE:HD11	10:CJ:71:LEU:HD22	1.94	0.49
26:DA:25:U:C4	26:DA:26:G:C6	3.00	0.49
41:DU:86:ALA:O	42:DV:49:THR:HG23	2.13	0.49
7:AG:152:ALA:O	7:AG:155:ARG:HB3	2.13	0.49
19:AS:41:VAL:O	19:AS:43:GLU:N	2.45	0.49
19:AS:63:THR:OG1	19:AS:65:ASN:ND2	2.46	0.49
26:BA:1899:G:H2'	26:BA:1899:G:N3	2.28	0.49
26:BA:2140:C:H1'	26:BA:2152:G:H22	1.77	0.49
26:BA:885:C:H3'	26:BA:886:C:C5'	2.40	0.49
36:BP:50:ARG:HH21	55:B8:7:HIS:HD2	1.59	0.49
44:BX:31:HIS:HD2	44:BX:33:LYS:H	1.59	0.49
1:CA:1029:C:N4	1:CA:1033:G:O6	2.46	0.49
1:CA:1217:C:H2'	1:CA:1218:C:O4'	2.13	0.49
3:CC:48:TYR:HE1	3:CC:118:GLN:HG3	1.78	0.49
5:CE:34:VAL:HG11	5:CE:63:ARG:HG3	1.94	0.49
7:CG:126:ASP:O	7:CG:130:GLY:N	2.46	0.49
9:CI:23:ASN:ND2	9:CI:25:LYS:HG2	2.27	0.49
1:CA:376:G:H5''	16:CP:5:ARG:HB2	1.94	0.49
1:CA:1494:G:H4'	26:DA:1913:A:N7	2.28	0.49
26:DA:2154:G:C2	26:DA:2155:G:C8	3.01	0.49
26:DA:812:C:H2'	26:DA:813:U:H6	1.77	0.49
46:DZ:5:LEU:HD21	46:DZ:43:GLU:HB3	1.94	0.49
1:AA:1216:G:OP1	14:AN:2:ALA:HA	2.13	0.49
1:AA:72:C:H2'	1:AA:73:G:O4'	2.13	0.49
4:AD:119:GLN:HG2	4:AD:123:HIS:CD2	2.47	0.49
12:AL:117:ARG:HB3	12:AL:122:THR:HB	1.95	0.49
26:BA:2347:C:O2'	53:B6:21:TYR:OH	2.30	0.49
26:BA:1165:U:H2'	26:BA:1166:C:C6	2.48	0.49
26:BA:2042:A:OP1	61:BA:5120:HOH:O	2.20	0.49
26:BA:183:C:N4	26:BA:213:A:H61	2.10	0.49
28:BD:26:LYS:HB3	28:BD:83:GLU:HG2	1.94	0.49
30:BF:116:ASP:OD1	30:BF:119:ARG:NH2	2.46	0.49
24:AX:57:A:O4'	31:BG:78:SER:OG	2.31	0.49
26:BA:2319:G:C2	39:BS:3:ARG:HA	2.48	0.49
46:BZ:41:LEU:HD21	46:BZ:83:PRO:HG2	1.94	0.49
1:CA:1411:C:H2'	1:CA:1412:C:C6	2.47	0.49
1:CA:78:G:H2'	1:CA:79:G:H5''	1.95	0.49
8:CH:83:ILE:HB	8:CH:137:VAL:HG13	1.94	0.49
24:CX:9:G:N2	24:CX:46:G:OP2	2.46	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:CY:18:G:C2	25:CY:55:PSU:C4	3.00	0.49
26:DA:1268:A:H2'	26:DA:1269:A:O4'	2.12	0.49
26:DA:1512:U:H2'	26:DA:1513:C:C6	2.48	0.49
28:DD:132:PRO:HG2	28:DD:135:PHE:HD2	1.78	0.49
35:DO:122:LEU:HD13	40:DT:72:VAL:HG11	1.94	0.49
1:AA:236:G:OP1	17:AQ:40:LYS:NZ	2.45	0.48
11:AK:48:ILE:HD12	11:AK:63:LEU:HB2	1.95	0.48
23:AW:25:C:C2'	23:AW:26:A:H5'	2.43	0.48
24:AX:47:U:H5''	24:AX:48:C:OP1	2.13	0.48
27:BB:102:A:N7	61:BB:318:HOH:O	2.35	0.48
1:CA:1118:C:H1'	1:CA:1179:A:C4	2.48	0.48
25:CY:29:G:N2	25:CY:41:C:N3	2.61	0.48
55:D8:33:ASN:HA	55:D8:36:LYS:HD2	1.94	0.48
26:DA:131:G:OP1	61:DA:3791:HOH:O	2.19	0.48
26:DA:2037:G:H2'	26:DA:2038:G:C8	2.48	0.48
26:DA:2278:A:OP1	37:DQ:11:LYS:HD2	2.12	0.48
26:DA:2376:A:N3	39:DS:106:ARG:NH2	2.52	0.48
1:AA:1049:U:OP1	14:AN:3:ARG:HB2	2.14	0.48
26:BA:1364:G:P	48:B1:3:LYS:HG3	2.53	0.48
53:B6:8:LYS:HG2	55:B8:34:TRP:CG	2.49	0.48
30:BF:164:ARG:O	30:BF:168:ARG:HB2	2.12	0.48
1:CA:1138:G:C6	1:CA:1140:C:H1'	2.48	0.48
1:CA:189(L):G:H2'	1:CA:190:U:C6	2.48	0.48
1:CA:392:G:H2'	1:CA:393:A:H8	1.77	0.48
1:CA:50:A:H1'	1:CA:52:G:C8	2.48	0.48
1:CA:976:G:OP1	14:CN:32:SER:N	2.34	0.48
2:CB:119:GLU:OE2	2:CB:153:ARG:NH2	2.41	0.48
3:CC:78:GLY:HA3	3:CC:83:ARG:H	1.76	0.48
9:CI:86:VAL:HA	9:CI:89:ASN:O	2.13	0.48
23:CW:21:A:O2'	23:CW:22:G:OP1	2.28	0.48
56:D9:10:ILE:HD12	56:D9:32:HIS:HA	1.94	0.48
26:DA:2137:C:H42	26:DA:2154:G:H1	1.59	0.48
26:DA:2206:G:H5'	26:DA:2207:G:N7	2.28	0.48
26:DA:222:A:H5''	26:DA:421:U:OP1	2.13	0.48
26:DA:652(B):A:N1	26:DA:655:A:H1'	2.29	0.48
33:DI:40:THR:HG23	33:DI:43:ASN:HD21	1.77	0.48
39:DS:41:ASP:OD2	39:DS:44:LYS:HE2	2.13	0.48
43:DW:60:ASN:HD22	43:DW:60:ASN:N	2.11	0.48
1:AA:1284:C:OP2	1:AA:1285:A:O2'	2.29	0.48
1:AA:1302:U:OP1	13:AM:13:LYS:HE3	2.13	0.48
1:AA:621:A:H2'	1:AA:622:A:C8	2.48	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:163:PHE:CD2	2:AB:185:ILE:HG13	2.48	0.48
2:AB:76:GLN:H	2:AB:76:GLN:CD	2.16	0.48
3:AC:6:HIS:CD2	3:AC:8:ILE:HB	2.48	0.48
7:AG:80:VAL:HB	7:AG:85:TYR:HE2	1.77	0.48
8:AH:13:ILE:O	8:AH:17:THR:HG23	2.13	0.48
25:AY:32:PSU:C2	25:AY:33:U:H5	2.32	0.48
51:B4:53:GLU:C	51:B4:55:ARG:N	2.65	0.48
26:BA:2138:C:C2	26:BA:2154:G:C2	3.02	0.48
26:BA:247:G:H4'	26:BA:386:G:C5	2.48	0.48
34:BN:4:TYR:CD2	41:BU:100:VAL:HG11	2.48	0.48
34:BN:58:ASP:OD1	34:BN:58:ASP:N	2.40	0.48
37:BQ:52:VAL:HA	37:BQ:55:VAL:HG12	1.94	0.48
1:CA:73:G:C6	1:CA:97:G:C6	3.01	0.48
7:CG:20:ASP:HB3	7:CG:23:VAL:HB	1.95	0.48
8:CH:64:LYS:HG2	8:CH:79:VAL:HG21	1.94	0.48
8:CH:20:TYR:CE1	8:CH:76:PRO:HG2	2.48	0.48
25:CY:7:A:N6	25:CY:66:U:N3	2.17	0.48
26:DA:1309:G:H3'	54:D7:9:ARG:HH12	1.78	0.48
26:DA:1478:G:HO2'	26:DA:1558:A:H2	1.62	0.48
26:DA:1922:G:H2'	26:DA:1923:U:O4'	2.13	0.48
32:DH:164:TYR:HB2	32:DH:167:GLU:HB2	1.95	0.48
1:AA:1118:C:OP1	9:AI:104:ARG:NH1	2.42	0.48
1:AA:1279:A:O2'	1:AA:1281:U:OP2	2.20	0.48
1:AA:1425:U:H2'	1:AA:1426:C:C6	2.48	0.48
1:AA:627:G:H2'	1:AA:628:G:H8	1.78	0.48
23:AW:26:A:N1	23:AW:44:G:N2	2.61	0.48
55:B8:23:VAL:CG1	55:B8:47:LYS:HD3	2.43	0.48
56:B9:7:VAL:HG12	56:B9:34:GLN:HB3	1.94	0.48
26:BA:1786:A:H1'	26:BA:1938:A:N6	2.28	0.48
26:BA:2119:A:C2	26:BA:2170:A:H2'	2.48	0.48
26:BA:2640:G:OP1	34:BN:97:ARG:NH2	2.46	0.48
26:BA:2771:C:H2'	26:BA:2772:C:C6	2.48	0.48
26:BA:630:G:OP1	55:B8:47:LYS:NZ	2.41	0.48
26:BA:800:A:H8	26:BA:800:A:OP1	1.96	0.48
35:BO:98:VAL:HG22	35:BO:118:ALA:HA	1.96	0.48
36:BP:63:PRO:HD3	55:B8:27:THR:HG22	1.94	0.48
39:BS:3:ARG:HE	39:BS:4:LEU:N	2.11	0.48
1:CA:1030(A):G:N3	1:CA:1030(C):G:H8	2.11	0.48
1:CA:1035:A:H2'	1:CA:1036:G:C8	2.48	0.48
1:CA:339:C:H2'	1:CA:340:U:C6	2.49	0.48
6:CF:76:ALA:O	6:CF:80:ARG:HG3	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:CO:26:GLU:HB3	15:CO:81:LEU:HD13	1.96	0.48
25:CY:35:A:H2'	25:CY:36:A:O4'	2.13	0.48
26:DA:2126:A:H4'	26:DA:2127:G:OP1	2.13	0.48
26:DA:2602:A:H4'	26:DA:2603:G:O5'	2.14	0.48
26:DA:2853:C:H2'	26:DA:2854:G:H8	1.77	0.48
28:DD:137:PRO:O	28:DD:140:THR:HG23	2.14	0.48
7:AG:150:ALA:HB2	11:AK:50:TYR:OH	2.13	0.48
1:AA:130:A:H5'	17:AQ:63:ARG:NE	2.27	0.48
26:BA:1405:U:H2'	26:BA:1406:U:H6	1.78	0.48
26:BA:323:G:C8	30:BF:171:PRO:HG3	2.48	0.48
30:BF:192:LEU:HD13	30:BF:194:MET:HE2	1.96	0.48
33:BI:85:GLU:HB3	33:BI:86:THR:H	1.52	0.48
46:BZ:111:VAL:C	46:BZ:113:ALA:H	2.17	0.48
1:CA:1002:G:H2'	1:CA:1003:G:H8	1.78	0.48
1:CA:1006:C:H2'	1:CA:1007:C:C6	2.49	0.48
1:CA:141:A:H1'	1:CA:182:U:O2	2.13	0.48
2:CB:71:VAL:HG23	2:CB:163:PHE:O	2.14	0.48
5:CE:12:LEU:HB3	5:CE:31:LEU:HB2	1.95	0.48
19:CS:17:GLU:O	19:CS:17:GLU:HG2	2.14	0.48
25:CY:69:G:C2	25:CY:70:G:H1'	2.48	0.48
26:DA:2203:U:H4'	28:DD:151:LYS:HG2	1.95	0.48
31:DG:43:LEU:HD12	31:DG:45:GLU:HG3	1.96	0.48
34:DN:38:HIS:ND1	34:DN:39:ARG:HG3	2.28	0.48
38:DR:103:ARG:NH1	38:DR:108:GLY:O	2.42	0.48
41:DU:78:THR:O	41:DU:117:GLN:NE2	2.46	0.48
13:AM:84:ILE:HG13	13:AM:85:GLY:HA2	1.94	0.48
48:B1:72:GLU:O	48:B1:76:ARG:HG3	2.13	0.48
26:BA:1540:U:H2'	26:BA:1541:G:O4'	2.13	0.48
26:BA:1668:A:H4'	26:BA:1669:A:O5'	2.14	0.48
26:BA:184:C:H2'	26:BA:185:U:H6	1.78	0.48
26:BA:2141:G:N3	26:BA:2142:C:H1'	2.29	0.48
26:BA:893:C:H2'	26:BA:894:C:H6	1.79	0.48
29:BE:178:GLU:OE2	29:BE:178:GLU:N	2.46	0.48
33:BI:47:LEU:O	33:BI:51:ILE:HG13	2.13	0.48
33:BI:61:ARG:HD2	33:BI:61:ARG:N	2.28	0.48
1:CA:1029:C:N4	1:CA:1032:G:C6	2.77	0.48
1:CA:1190:G:OP1	3:CC:5:ILE:N	2.38	0.48
1:CA:1262:C:H2'	1:CA:1263:C:H6	1.79	0.48
1:CA:189(C):C:H2'	1:CA:189(D):C:O4'	2.14	0.48
1:CA:428:G:H4'	1:CA:429:U:O5'	2.12	0.48
2:CB:178:ARG:NH2	8:CH:68:ARG:HH12	2.10	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:CI:16:ARG:HH11	9:CI:66:ARG:HH11	1.62	0.48
26:DA:1364:G:P	48:D1:3:LYS:HG3	2.53	0.48
26:DA:184:C:H2'	26:DA:185:U:C6	2.48	0.48
26:DA:861:A:N3	27:DB:79:C:O2'	2.41	0.48
30:DF:183:VAL:O	30:DF:187:VAL:HG23	2.13	0.48
40:DT:59:THR:HG23	40:DT:78:LEU:HB3	1.96	0.48
1:AA:1429:C:H2'	1:AA:1430:C:C6	2.48	0.48
1:AA:62:U:OP1	1:AA:385:C:O2'	2.26	0.48
8:AH:51:VAL:HG12	8:AH:52:ASP:N	2.28	0.48
25:AY:63:G:C2	25:AY:64:A:H1'	2.48	0.48
26:BA:1231:G:H2'	26:BA:1232:G:C8	2.48	0.48
26:BA:1996:C:H4'	26:BA:1997:G:OP1	2.12	0.48
26:BA:2129:C:H2'	26:BA:2130:U:H6	1.77	0.48
26:BA:2140:C:C2	26:BA:2151:G:N2	2.82	0.48
26:BA:2386:C:H2'	26:BA:2387:U:C6	2.49	0.48
26:BA:288:C:H2'	26:BA:289:A:H8	1.79	0.48
1:CA:1060:C:H2'	1:CA:1061:G:H8	1.77	0.48
1:CA:1119:C:C4	1:CA:1154:G:O6	2.66	0.48
1:CA:1135:U:H2'	1:CA:1137:C:O2	2.14	0.48
1:CA:408:A:H4'	4:CD:112:VAL:HG21	1.96	0.48
1:CA:742:G:P	15:CO:35:ARG:HH22	2.36	0.48
19:CS:27:GLU:HG2	19:CS:47:HIS:NE2	2.28	0.48
26:DA:952:G:H5''	26:DA:953:A:OP2	2.14	0.48
31:DG:125:PHE:HB3	31:DG:166:ASP:OD1	2.14	0.48
35:DO:4:PRO:O	35:DO:5:GLN:HB2	2.14	0.48
44:DX:20:GLY:HA2	44:DX:23:GLU:OE2	2.14	0.48
1:AA:1158:C:H5	1:AA:1181:G:N1	2.06	0.48
6:AF:69:GLU:CD	6:AF:69:GLU:H	2.16	0.48
7:AG:111:ARG:HD2	7:AG:123:GLU:HB2	1.95	0.48
10:AJ:11:PHE:CE1	10:AJ:67:THR:HG22	2.49	0.48
19:AS:64:GLU:O	19:AS:67:VAL:HG23	2.14	0.48
24:AX:55:PSU:O2'	24:AX:57:A:N7	2.33	0.48
26:BA:1665:A:H2'	26:BA:1666:G:O4'	2.14	0.48
26:BA:196:A:H2'	26:BA:196:A:N3	2.27	0.48
26:BA:2328:A:H2'	26:BA:2329:G:H8	1.75	0.48
28:BD:70:TRP:HB3	28:BD:190:TYR:CZ	2.49	0.48
31:BG:11:TYR:CZ	31:BG:16:ARG:HD3	2.48	0.48
31:BG:66:GLN:HB3	31:BG:92:VAL:HG21	1.94	0.48
39:BS:59:LYS:HE3	39:BS:60:GLY:H	1.79	0.48
1:CA:1125:U:H3'	1:CA:1126:U:H5''	1.96	0.48
1:CA:1228:C:OP1	13:CM:115:LYS:N	2.23	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CB:81:VAL:HB	2:CB:94:ASN:HD21	1.78	0.48
7:CG:12:LEU:HD12	7:CG:12:LEU:H	1.78	0.48
14:CN:27:CYS:SG	14:CN:29:ARG:HB2	2.53	0.48
53:D6:11:LEU:HB2	53:D6:21:TYR:HB2	1.95	0.48
26:DA:1472:A:H2'	26:DA:1473:G:O4'	2.13	0.48
26:DA:171:G:H2'	26:DA:172:C:C6	2.49	0.48
26:DA:2162:G:H4'	26:DA:2172:U:O2'	2.13	0.48
26:DA:2695:C:H2'	26:DA:2696:U:C6	2.49	0.48
26:DA:851:U:O2'	50:D3:42:ALA:O	2.30	0.48
29:DE:108:SER:HB3	29:DE:165:VAL:HG21	1.96	0.48
30:DF:120:GLU:CB	30:DF:122:LYS:HG2	2.44	0.48
46:DZ:110:GLY:HA3	46:DZ:145:GLU:HA	1.96	0.48
1:AA:1149:C:H2'	1:AA:1150:U:H6	1.77	0.48
1:AA:328:C:H4'	1:AA:329:A:H5'	1.96	0.48
4:AD:3:ARG:HD3	4:AD:118:ARG:CD	2.44	0.48
5:AE:36:ASP:OD1	5:AE:38:GLN:N	2.38	0.48
47:B0:53:MET:HG3	47:B0:59:LEU:HD23	1.96	0.48
26:BA:2116:G:N2	26:BA:2162:G:OP1	2.46	0.48
26:BA:2183:C:H2'	26:BA:2184:G:H8	1.78	0.48
26:BA:2791:C:OP2	26:BA:2791:C:H6	1.96	0.48
26:BA:582:G:H2'	26:BA:583:G:C8	2.49	0.48
26:BA:848:G:H2'	26:BA:849:A:C8	2.48	0.48
39:BS:15:ARG:NE	39:BS:88:ASP:OD2	2.45	0.48
1:CA:1009:G:H22	1:CA:1021:G:H1'	1.78	0.48
1:CA:1133:G:N2	1:CA:1141:C:N3	2.58	0.48
1:CA:707:C:H2'	1:CA:708:C:C6	2.49	0.48
2:CB:46:LYS:O	2:CB:50:GLU:HB2	2.14	0.48
3:CC:32:LEU:HD12	3:CC:59:ARG:HH22	1.79	0.48
1:CA:10:A:OP2	5:CE:126:ARG:HD2	2.14	0.48
5:CE:33:VAL:HG13	5:CE:112:LEU:HD12	1.96	0.48
5:CE:84:PHE:N	5:CE:87:SER:O	2.45	0.48
20:CT:10:LEU:HD23	20:CT:12:ALA:HB2	1.95	0.48
26:DA:1434:A:H61	26:DA:1558:A:N6	2.12	0.48
26:DA:1363:C:O2'	26:DA:1809:A:N3	2.37	0.48
26:DA:2118:U:C4	26:DA:2149:G:H1'	2.48	0.48
26:DA:2293:C:H42	26:DA:2339:G:H1	1.61	0.48
26:DA:2540:C:H2'	26:DA:2541:A:O4'	2.14	0.48
26:DA:390:A:H4'	26:DA:391:G:H5'	1.94	0.48
26:DA:77:C:H42	26:DA:109:G:H1	1.61	0.48
26:DA:828:U:H2'	26:DA:829:A:C8	2.49	0.48
28:DD:108:PRO:HB3	28:DD:143:HIS:CE1	2.49	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:DG:15:VAL:HG13	31:DG:175:LEU:HD23	1.96	0.48
34:DN:34:LEU:O	34:DN:49:GLY:HA3	2.13	0.48
37:DQ:36:ALA:HB2	37:DQ:103:MET:SD	2.54	0.48
1:AA:1118:C:H1'	1:AA:1179:A:C5	2.49	0.48
1:AA:501:C:H2'	1:AA:502:G:H8	1.78	0.48
9:AI:99:LEU:HB3	9:AI:101:PHE:CD1	2.49	0.48
10:AJ:49:VAL:HG23	14:AN:41:ARG:HD2	1.96	0.48
12:AL:34:ARG:NH2	61:AL:201:HOH:O	2.25	0.48
23:AW:47:U:H5'	23:AW:47:U:C6	2.45	0.48
26:BA:2099:U:H2'	26:BA:2100:G:C8	2.49	0.48
26:BA:2286:A:H4'	26:BA:2287:A:O4'	2.14	0.48
26:BA:493:G:O6	61:BA:4550:HOH:O	2.19	0.48
26:BA:2572:A:C8	29:BE:144:ARG:HD2	2.49	0.48
32:BH:154:PRO:HB3	32:BH:163:TYR:CE2	2.49	0.48
35:BO:16:ALA:HB2	35:BO:52:VAL:HG21	1.96	0.48
1:CA:1030(A):G:N3	1:CA:1030(C):G:C8	2.81	0.48
1:CA:1063:C:H3'	1:CA:1064:G:H2'	1.96	0.48
1:CA:1179:A:H2'	1:CA:1180:A:O4'	2.13	0.48
1:CA:1058:G:H1	1:CA:1199:U:H3	1.62	0.48
1:CA:1333:A:H2'	1:CA:1334:G:O4'	2.14	0.48
1:CA:93:G:C2'	1:CA:96:U:H5'	2.44	0.48
3:CC:87:LEU:O	3:CC:91:LEU:N	2.36	0.48
6:CF:33:TYR:CD2	6:CF:75:LEU:HD23	2.49	0.48
12:CL:53:ARG:HH12	12:CL:92:ASP:HB2	1.79	0.48
53:D6:6:ARG:NH1	53:D6:26:ASN:HB2	2.28	0.48
26:DA:1889:A:H2'	26:DA:1890:A:C8	2.49	0.48
26:DA:2586:C:OP2	26:DA:2608:G:N1	2.42	0.48
26:DA:2820:A:OP1	38:DR:4:LEU:HD23	2.14	0.48
26:DA:272(E):G:C2	26:DA:364:C:C2	3.02	0.48
28:DD:73:VAL:HG13	28:DD:120:GLY:HA3	1.95	0.48
30:DF:29:ASN:O	30:DF:112:MET:HE1	2.13	0.48
46:DZ:138:GLU:H	46:DZ:156:LYS:HZ1	1.62	0.48
1:AA:1137:C:H6	1:AA:1137:C:H3'	1.77	0.47
25:AY:58:A:H4'	25:AY:59:U:OP1	2.14	0.47
25:AY:5:G:C2	25:AY:6:G:C4	3.02	0.47
26:BA:527:C:C5	26:BA:2779:U:H2'	2.49	0.47
30:BF:150:GLY:HA2	30:BF:172:TRP:CD2	2.49	0.47
31:BG:16:ARG:HE	31:BG:31:VAL:HG11	1.79	0.47
36:BP:50:ARG:HD3	55:B8:7:HIS:CD2	2.49	0.47
1:CA:1121:U:C4	1:CA:1122:U:C4	3.01	0.47
1:CA:130:A:O2'	1:CA:131:C:O5'	2.28	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:1371:G:O3'	9:CI:69:GLY:HA3	2.14	0.47
1:CA:89:C:H2'	1:CA:90:U:O4'	2.14	0.47
1:CA:933:G:O6	7:CG:3:ARG:NH2	2.47	0.47
2:CB:139:LYS:O	2:CB:143:GLU:HG3	2.14	0.47
2:CB:212:GLN:NE2	2:CB:234:PRO:O	2.46	0.47
3:CC:101:LEU:HD12	3:CC:102:ASN:N	2.29	0.47
5:CE:6:PHE:HB3	5:CE:35:GLY:C	2.34	0.47
26:DA:1365:A:OP2	48:D1:3:LYS:HG2	2.14	0.47
26:DA:2564:A:C2	26:DA:2647:U:H4'	2.49	0.47
27:DB:14:U:H5'	27:DB:70:C:O2	2.13	0.47
1:AA:950:U:H2'	1:AA:951:G:H8	1.80	0.47
5:AE:90:VAL:O	5:AE:120:THR:HA	2.14	0.47
13:AM:123:ALA:HB2	23:AW:39:PSU:H1'	1.95	0.47
13:AM:79:LYS:HA	13:AM:82:MET:HE2	1.96	0.47
19:AS:40:ILE:HD11	19:AS:74:PHE:HE1	1.78	0.47
26:BA:667:U:O2	55:B8:2:PRO:HD2	2.14	0.47
32:BH:117:PRO:HG3	32:BH:123:PHE:CD2	2.49	0.47
33:BI:130:TYR:N	33:BI:138:ILE:O	2.42	0.47
35:BO:4:PRO:O	35:BO:5:GLN:HB2	2.14	0.47
36:BP:82:GLY:HA2	36:BP:113:LYS:O	2.13	0.47
1:CA:1125:U:C2'	1:CA:1126:U:H5''	2.44	0.47
1:CA:1298:C:H4'	1:CA:1299:A:H5'	1.96	0.47
1:CA:392:G:H2'	1:CA:393:A:C8	2.48	0.47
1:CA:646:U:H2'	1:CA:647:C:H6	1.75	0.47
1:CA:657:G:H4'	15:CO:28:GLN:HG2	1.96	0.47
20:CT:24:LEU:HA	20:CT:24:LEU:HD13	1.69	0.47
23:CW:8:4SU:S4	23:CW:14:A:N7	2.88	0.47
24:CX:67:C:C2'	24:CX:68:C:H5'	2.43	0.47
26:DA:1641:A:H2'	26:DA:1642:G:O4'	2.14	0.47
26:DA:2141:G:H2'	26:DA:2142:C:O4'	2.14	0.47
26:DA:2304:G:H22	26:DA:2312:U:H3	1.61	0.47
26:DA:2776:A:H4'	26:DA:2777:G:H5''	1.96	0.47
26:DA:817:C:H2'	26:DA:818:G:O4'	2.14	0.47
26:DA:93:G:H2'	26:DA:94:C:C6	2.49	0.47
1:AA:165:C:H2'	1:AA:166:G:H8	1.79	0.47
1:AA:371:G:O2'	1:AA:373:A:N7	2.47	0.47
1:AA:596:C:OP2	61:AA:4083:HOH:O	2.20	0.47
1:AA:950:U:H2'	1:AA:951:G:C8	2.49	0.47
3:AC:118:GLN:HG2	3:AC:118:GLN:H	1.45	0.47
55:B8:42:ARG:HD2	61:B8:205:HOH:O	2.15	0.47
26:BA:1709:U:H2'	26:BA:1710:C:C6	2.48	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:BA:446:G:OP1	41:BU:3:ARG:NH1	2.42	0.47
26:BA:900:A:H2'	26:BA:901:A:O4'	2.14	0.47
33:BI:114:LEU:HD13	33:BI:130:TYR:HD1	1.78	0.47
37:BQ:34:LEU:HD11	37:BQ:129:THR:HB	1.95	0.47
1:CA:1128:C:H1'	1:CA:1147:C:N4	2.25	0.47
1:CA:934:C:OP1	61:CA:4164:HOH:O	2.20	0.47
2:CB:80:ILE:HD11	2:CB:212:GLN:HA	1.96	0.47
10:CJ:8:LEU:HB3	10:CJ:16:LEU:HD22	1.95	0.47
1:CA:1320:C:O4'	19:CS:73:GLU:HG3	2.13	0.47
21:CU:12:LYS:HD3	21:CU:22:ARG:HB3	1.96	0.47
26:DA:322:A:OP1	30:DF:168:ARG:HD2	2.14	0.47
26:DA:39:C:H2'	26:DA:40:C:C6	2.49	0.47
26:DA:615:G:OP1	30:DF:40:GLN:HG2	2.14	0.47
28:DD:71:ASP:HB3	28:DD:103:ARG:NH2	2.28	0.47
29:DE:144:ARG:HB3	29:DE:145:LYS:H	1.48	0.47
29:DE:178:GLU:N	29:DE:178:GLU:OE2	2.42	0.47
32:DH:7:LEU:O	32:DH:69:ARG:NH1	2.40	0.47
37:DQ:37:LEU:HD21	37:DQ:130:LYS:HE2	1.96	0.47
42:DV:5:VAL:HG11	42:DV:57:VAL:HG21	1.96	0.47
44:DX:4:ALA:HB1	44:DX:42:ALA:HA	1.95	0.47
1:AA:461:A:O2'	1:AA:470:C:H5'	2.13	0.47
3:AC:134:ILE:HG22	3:AC:168:ALA:HB3	1.96	0.47
7:AG:111:ARG:HB3	7:AG:113:GLU:OE2	2.14	0.47
10:AJ:47:PHE:HB2	10:AJ:63:PHE:HB2	1.96	0.47
26:BA:1701:A:OP2	61:BA:5017:HOH:O	2.20	0.47
1:AA:1495:U:O2'	26:BA:1919:A:N1	2.40	0.47
26:BA:2712:U:OP1	26:BA:2714:G:H4'	2.14	0.47
26:BA:899:A:HO2'	26:BA:900:A:H8	1.60	0.47
27:BB:66:A:N6	27:BB:108:U:H2'	2.28	0.47
26:BA:616:G:H5'	30:BF:205:ARG:HD2	1.96	0.47
41:BU:86:ALA:O	42:BV:49:THR:HG23	2.14	0.47
1:CA:1030(A):G:N2	1:CA:1030(C):G:H3'	2.30	0.47
1:CA:1181:G:O2'	1:CA:1182:G:N7	2.47	0.47
1:CA:736:C:H2'	1:CA:737:A:C8	2.49	0.47
1:CA:1057:G:H5'	3:CC:155:GLY:HA2	1.95	0.47
19:CS:32:LYS:HE3	19:CS:57:HIS:CD2	2.49	0.47
26:DA:816:C:OP1	26:DA:1185:C:O2'	2.22	0.47
35:DO:7:TYR:CZ	35:DO:44:LYS:HG3	2.50	0.47
42:DV:21:ARG:HG2	42:DV:91:TYR:CD2	2.49	0.47
1:AA:1027:C:H2'	1:AA:1028:C:C6	2.49	0.47
12:AL:97:ARG:HB2	12:AL:98:TYR:CE2	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:AW:76:31M:HNH1	26:BA:2061:G:H22	1.62	0.47
25:AY:32:PSU:C2	25:AY:33:U:C5	3.02	0.47
25:AY:50:U:H2'	25:AY:51:U:C6	2.48	0.47
26:BA:1031:G:H21	56:B9:36:GLN:HE22	1.62	0.47
32:BH:20:ALA:HB1	32:BH:21:PRO:HD2	1.97	0.47
35:BO:120:GLU:HG2	35:BO:122:LEU:HG	1.97	0.47
26:BA:302:C:OP2	45:BY:73:ARG:NH2	2.46	0.47
1:CA:727:G:P	1:CA:742:G:H21	2.38	0.47
2:CB:120:ALA:O	2:CB:122:PHE:N	2.43	0.47
3:CC:69:HIS:CD2	3:CC:104:GLN:HB3	2.49	0.47
4:CD:173:TRP:NE1	4:CD:189:PRO:HG3	2.29	0.47
8:CH:33:GLU:HG2	8:CH:48:TYR:CE1	2.49	0.47
1:CA:1328:C:O2'	13:CM:29:ARG:NH2	2.45	0.47
21:CU:15:ARG:HB2	21:CU:15:ARG:HH11	1.79	0.47
26:DA:709:U:H2'	26:DA:710:G:C8	2.50	0.47
28:DD:4:LYS:HB3	28:DD:18:VAL:CG2	2.44	0.47
29:DE:1:MET:HE1	29:DE:199:ARG:HD2	1.95	0.47
33:DI:31:LEU:HD21	33:DI:38:LEU:HG	1.96	0.47
1:AA:1179:A:H4'	9:AI:103:THR:HA	1.97	0.47
1:AA:1210:C:N4	1:AA:1211:U:O4	2.47	0.47
2:AB:166:ASP:O	2:AB:170:GLU:N	2.39	0.47
1:AA:1191:A:H5''	3:AC:4:LYS:HZ2	1.79	0.47
4:AD:175:SER:OG	4:AD:184:LYS:HB2	2.14	0.47
25:AY:18:G:H1	25:AY:55:PSU:H1'	1.80	0.47
25:AY:36:A:N6	25:AY:37:MIA:C6	2.78	0.47
26:BA:1178:C:O5'	26:BA:1178:C:H6	1.96	0.47
26:BA:143:G:H1'	44:BX:37:THR:HG21	1.97	0.47
1:CA:952:U:H4'	1:CA:964:A:N1	2.30	0.47
3:CC:42:LEU:HA	3:CC:45:LYS:HZ2	1.80	0.47
4:CD:57:ARG:NH2	5:CE:107:ARG:HD3	2.28	0.47
7:CG:89:MET:SD	7:CG:155:ARG:HB2	2.55	0.47
14:CN:26:ARG:HB3	14:CN:43:CYS:SG	2.54	0.47
24:CX:23:C:H2'	24:CX:24:U:C6	2.49	0.47
26:DA:2528:U:H5''	56:D9:31:LYS:HE2	1.97	0.47
26:DA:1410:G:H2'	26:DA:1411:C:C6	2.49	0.47
26:DA:1528(A):A:H2'	26:DA:1529:G:O4'	2.15	0.47
26:DA:310:A:H1'	26:DA:311:A:H2'	1.95	0.47
61:DA:3829:HOH:O	30:DF:68:LYS:HE2	2.14	0.47
32:DH:86:GLU:OE2	32:DH:132:ARG:NH2	2.47	0.47
1:AA:46:G:O2'	1:AA:365:U:O2	2.31	0.47
2:AB:188:ALA:HB1	2:AB:192:SER:OG	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:B6:16:CYS:SG	53:B6:18:ARG:HD3	2.54	0.47
26:BA:1045:A:OP1	26:BA:1046:A:H3'	2.15	0.47
26:BA:2117:A:O2'	26:BA:2118:U:H5''	2.15	0.47
26:BA:2701:C:H2'	26:BA:2702:U:H2'	1.96	0.47
31:BG:28:VAL:HG23	31:BG:29:TRP:CD1	2.50	0.47
32:BH:69:ARG:HG3	32:BH:70:THR:N	2.30	0.47
33:BI:93:THR:OG1	33:BI:96:ASP:OD1	2.24	0.47
41:BU:85:LYS:HE2	41:BU:117:GLN:HA	1.97	0.47
45:BY:30:VAL:HG13	45:BY:37:VAL:HG12	1.97	0.47
1:CA:1133:G:H2'	1:CA:1134:G:C8	2.49	0.47
1:CA:1186:G:O3'	9:CI:113:LYS:NZ	2.46	0.47
1:CA:988:G:C4'	1:CA:1014:A:H61	2.28	0.47
2:CB:211:ILE:O	2:CB:215:LEU:HB2	2.14	0.47
2:CB:54:THR:HG23	2:CB:199:TYR:HB3	1.96	0.47
9:CI:88:TYR:CD1	9:CI:89:ASN:HB2	2.49	0.47
10:CJ:37:PRO:HA	10:CJ:72:VAL:HG12	1.97	0.47
22:CV:14:A:OP1	22:CV:14:A:H8	1.97	0.47
48:D1:3:LYS:HB2	48:D1:61:ARG:NH1	2.30	0.47
26:DA:1514:U:H2'	26:DA:1515:G:H8	1.80	0.47
26:DA:1877:A:H5'	26:DA:1878:G:OP2	2.15	0.47
26:DA:2751:G:C8	32:DH:2:SER:HA	2.49	0.47
26:DA:2788:C:H2'	26:DA:2789:C:C6	2.50	0.47
26:DA:897:C:H3'	26:DA:898:C:C6	2.50	0.47
28:DD:5:LYS:HE3	28:DD:5:LYS:HB3	1.52	0.47
29:DE:5:LEU:HD11	29:DE:79:ARG:HB2	1.96	0.47
31:DG:121:ASN:HB3	31:DG:124:SER:HB2	1.97	0.47
1:AA:1360:A:H2'	1:AA:1361:G:O4'	2.15	0.47
1:AA:1346:A:N1	1:AA:1374:A:H5''	2.30	0.47
2:AB:102:LEU:HB3	2:AB:180:LEU:HD12	1.96	0.47
2:AB:63:MET:HB3	2:AB:225:ALA:HB1	1.97	0.47
3:AC:32:LEU:HD13	3:AC:59:ARG:HD3	1.97	0.47
25:AY:27:G:N2	25:AY:44:G:N3	2.63	0.47
26:BA:1173:G:N2	26:BA:1177:A:OP2	2.31	0.47
26:BA:2110:G:H4'	26:BA:2111:C:OP2	2.15	0.47
40:BT:53:ARG:NH1	40:BT:53:ARG:HB3	2.30	0.47
1:CA:109:A:C6	1:CA:326:G:C6	3.03	0.47
1:CA:627:G:H2'	1:CA:628:G:H8	1.78	0.47
2:CB:115:LEU:HD11	2:CB:153:ARG:CZ	2.44	0.47
10:CJ:46:ARG:HG2	10:CJ:64:GLU:HB3	1.97	0.47
13:CM:10:PRO:HD2	13:CM:18:ALA:HB1	1.95	0.47
13:CM:92:HIS:CE1	13:CM:98:VAL:HG11	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:DA:855:G:O2'	47:D0:27:GLU:OE2	2.31	0.47
48:D1:3:LYS:HB2	48:D1:61:ARG:HH12	1.80	0.47
26:DA:1196:C:H2'	26:DA:1197:G:H8	1.79	0.47
26:DA:118:A:N3	26:DA:178:G:H1'	2.30	0.47
26:DA:2086:U:H2'	26:DA:2087:G:C8	2.49	0.47
26:DA:2364:C:H2'	26:DA:2365:G:O4'	2.14	0.47
32:DH:144:VAL:O	32:DH:148:ILE:HG12	2.15	0.47
46:DZ:108:PRO:HB2	46:DZ:111:VAL:HG23	1.96	0.47
1:AA:1293:G:H2'	1:AA:1294:G:C8	2.49	0.47
1:AA:407:G:OP1	4:AD:115:ARG:NH2	2.48	0.47
26:BA:1311:G:O2'	54:B7:47:ARG:NH2	2.47	0.47
26:BA:41:C:H2'	26:BA:42:G:O4'	2.15	0.47
46:BZ:107:THR:HA	46:BZ:108:PRO:HD3	1.77	0.47
1:CA:1027:C:OP1	1:CA:1027:C:H4'	2.14	0.47
1:CA:1179:A:C6	1:CA:1180:A:C4	3.03	0.47
1:CA:1343:G:H2'	1:CA:1344:C:C6	2.50	0.47
1:CA:337:C:H2'	1:CA:338:A:H8	1.79	0.47
3:CC:6:HIS:HB3	14:CN:49:HIS:ND1	2.30	0.47
8:CH:73:ASP:OD1	8:CH:75:ARG:HD3	2.15	0.47
24:CX:44:A:C6	24:CX:45:G:C6	3.02	0.47
51:D4:53:GLU:HG2	51:D4:55:ARG:N	2.29	0.47
26:DA:1025:G:C4	26:DA:1135:C:H1'	2.49	0.47
26:DA:1270:C:H5''	26:DA:1271:G:O5'	2.15	0.47
26:DA:121:G:H4'	26:DA:149:A:H5'	1.97	0.47
26:DA:2306:C:H3'	26:DA:2307:G:H2'	1.97	0.47
26:DA:2506:U:OP1	29:DE:144:ARG:NH2	2.48	0.47
26:DA:2722:G:H2'	26:DA:2723:C:C6	2.50	0.47
26:DA:797:C:H2'	26:DA:798:G:O4'	2.14	0.47
43:DW:14:PRO:HG2	43:DW:78:GLU:HG2	1.97	0.47
1:AA:1028:C:H2'	1:AA:1029:C:H4'	1.96	0.47
1:AA:1132:C:H2'	1:AA:1133:G:C8	2.50	0.47
1:AA:1443:G:N2	1:AA:1459:C:O2	2.37	0.47
1:AA:299:G:O6	61:AA:4081:HOH:O	2.14	0.47
2:AB:17:PHE:CD2	2:AB:44:LEU:HD21	2.48	0.47
1:AA:1227:A:P	13:AM:111:LYS:HZ2	2.37	0.47
26:BA:1243:G:O2'	36:BP:7:ARG:NH2	2.47	0.47
28:BD:72:LYS:HB3	28:BD:75:ILE:HD12	1.97	0.47
1:CA:1118:C:H1'	1:CA:1179:A:C5	2.50	0.47
1:CA:1139:G:H4'	1:CA:1140:C:OP1	2.14	0.47
1:CA:1305:G:H5'	21:CU:4:GLY:C	2.36	0.47
9:CI:16:ARG:HH11	9:CI:64:THR:HG21	1.80	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:CS:32:LYS:HA	19:CS:50:ALA:HB3	1.96	0.47
24:CX:19:G:H4'	24:CX:20:U:OP2	2.15	0.47
26:DA:77:C:OP1	49:D2:59:ARG:HD3	2.14	0.47
26:DA:2166:G:H3'	26:DA:2167:U:C5'	2.40	0.47
26:DA:2563:U:H4'	35:DO:28:SER:HA	1.97	0.47
26:DA:315:G:H2'	26:DA:316:C:C6	2.50	0.47
40:DT:29:ARG:HB3	40:DT:87:ASP:HB2	1.97	0.47
1:AA:1030(B):C:H2'	1:AA:1030(B):C:O2	2.15	0.47
1:AA:156:G:N1	1:AA:165:C:N3	2.55	0.47
2:AB:19:HIS:O	2:AB:39:ILE:HG23	2.15	0.47
15:AO:74:ASP:CG	15:AO:77:ARG:HG3	2.35	0.47
36:BP:59:LEU:HD11	55:B8:10:ALA:HB2	1.97	0.47
2:CB:185:ILE:HG22	2:CB:199:TYR:HD2	1.79	0.47
4:CD:140:VAL:HG11	4:CD:146:ILE:HD11	1.95	0.47
7:CG:44:TYR:O	7:CG:47:CYS:HB2	2.15	0.47
8:CH:124:ALA:O	8:CH:128:GLY:N	2.48	0.47
13:CM:54:VAL:HA	13:CM:57:ARG:HB3	1.97	0.47
1:CA:136:C:O2'	16:CP:63:GLY:O	2.24	0.47
23:CW:29:G:N2	23:CW:41:C:N3	2.56	0.47
26:DA:511:U:H4'	26:DA:1235:G:H4'	1.96	0.47
26:DA:1514:U:H2'	26:DA:1515:G:C8	2.50	0.47
26:DA:2298:A:C8	26:DA:2299:G:C8	3.03	0.47
26:DA:2319:G:N2	39:DS:3:ARG:HA	2.30	0.47
26:DA:2477:C:N4	56:D9:10:ILE:HG23	2.30	0.47
26:DA:571:A:N6	26:DA:2499:C:O3'	2.47	0.47
27:DB:115:G:H2'	27:DB:116:G:O4'	2.15	0.47
31:DG:143:GLU:H	31:DG:143:GLU:HG2	1.41	0.47
46:DZ:57:ILE:HD12	46:DZ:71:VAL:HG23	1.97	0.47
1:AA:1028:C:N4	1:AA:1033:G:H1	2.10	0.46
1:AA:1183:A:HO2'	1:AA:1184:G:P	2.35	0.46
1:AA:1530:G:H4'	1:AA:1530:G:OP1	2.14	0.46
1:AA:161:A:H2'	1:AA:162:A:C8	2.50	0.46
1:AA:163:C:H2'	1:AA:164:U:C6	2.49	0.46
1:AA:346:G:C3'	1:AA:347:G:H4'	2.45	0.46
1:AA:625:G:H2'	1:AA:626:U:H6	1.79	0.46
1:AA:953:G:N7	13:AM:104:ARG:NH2	2.63	0.46
2:AB:30:ARG:HG3	2:AB:31:TYR:CD1	2.50	0.46
23:AW:52:G:H4'	37:BQ:56:ARG:HH12	1.80	0.46
26:BA:1587:A:H2'	26:BA:1588:C:C6	2.50	0.46
26:BA:1641:A:H2'	26:BA:1642:G:O4'	2.14	0.46
26:BA:303:U:H2'	26:BA:304:G:H8	1.80	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:BA:620:G:N3	26:BA:620:G:H5'	2.30	0.46
38:BR:104:ARG:HG3	38:BR:111:LEU:HD21	1.97	0.46
1:CA:309:G:O2'	1:CA:607:A:N1	2.48	0.46
4:CD:25:ARG:NH1	4:CD:30:LYS:O	2.48	0.46
17:CQ:26:GLN:HG2	17:CQ:37:LYS:HG2	1.96	0.46
1:CA:1456:G:N1	20:CT:51:GLU:OE1	2.45	0.46
26:DA:1116:C:H2'	26:DA:1117:G:H8	1.79	0.46
26:DA:1169:G:O5'	26:DA:1169:G:H8	1.98	0.46
26:DA:1430:C:H2'	26:DA:1431:U:C6	2.49	0.46
26:DA:2059:A:O2'	30:DF:69:HIS:HD2	1.98	0.46
26:DA:2516:G:O6	26:DA:2517:C:N4	2.48	0.46
26:DA:2846:G:H2'	26:DA:2847:U:O4'	2.14	0.46
26:DA:854:G:H2'	26:DA:855:G:C8	2.50	0.46
26:DA:1797:C:H4'	28:DD:257:LEU:O	2.15	0.46
42:DV:40:LEU:HB2	42:DV:46:VAL:HG13	1.96	0.46
1:AA:1002:G:H3'	1:AA:1003:G:H8	1.81	0.46
1:AA:1182:G:C4'	1:AA:1183:A:H5'	2.44	0.46
1:AA:382:A:H2'	1:AA:383:A:C8	2.49	0.46
2:AB:102:LEU:HD23	2:AB:182:ILE:HD12	1.98	0.46
2:AB:17:PHE:HB2	2:AB:44:LEU:HD11	1.96	0.46
2:AB:21:ARG:H	2:AB:21:ARG:HD2	1.80	0.46
5:AE:43:LEU:HD21	5:AE:132:ALA:HB1	1.97	0.46
23:AW:6:G:N1	23:AW:67:C:N4	2.39	0.46
26:BA:1028:A:N6	26:BA:1125:G:H2'	2.30	0.46
26:BA:1179:C:H2'	26:BA:1180:C:H6	1.80	0.46
26:BA:2010:G:H5''	43:BW:42:ARG:HB2	1.98	0.46
26:BA:2887:U:H2'	26:BA:2888:C:C6	2.49	0.46
26:BA:744:G:OP1	29:BE:132:HIS:ND1	2.43	0.46
30:BF:93:LYS:HD3	30:BF:93:LYS:HA	1.68	0.46
31:BG:146:TYR:O	31:BG:146:TYR:HD1	1.98	0.46
1:CA:772:U:H2'	1:CA:773:G:O4'	2.15	0.46
2:CB:76:GLN:HG3	2:CB:206:ASP:O	2.15	0.46
7:CG:76:ARG:HB3	7:CG:156:TRP:HH2	1.80	0.46
8:CH:82:HIS:NE2	8:CH:84:ARG:HG2	2.30	0.46
10:CJ:23:ILE:HA	10:CJ:23:ILE:HD13	1.77	0.46
16:CP:40:ASP:O	16:CP:48:TRP:HB2	2.16	0.46
23:CW:76:31M:N	24:CX:76:A:O3'	2.49	0.46
25:CY:74:C:H4'	48:D1:23:LYS:HE3	1.97	0.46
26:DA:1630:G:H2'	26:DA:1631:C:C6	2.51	0.46
26:DA:1786:A:H1'	26:DA:1938:A:N6	2.31	0.46
26:DA:1932:A:H2'	26:DA:1933:G:O4'	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:DA:2141:G:C8	26:DA:2151:G:N2	2.83	0.46
26:DA:229:A:H5''	26:DA:230:U:H5'	1.96	0.46
26:DA:2318:G:H4'	26:DA:2319:G:OP1	2.14	0.46
26:DA:2516:G:C6	26:DA:2517:C:C4	3.03	0.46
26:DA:2647:U:H2'	26:DA:2648:C:C6	2.51	0.46
26:DA:2836:U:H2'	26:DA:2837:G:C8	2.50	0.46
26:DA:528:A:OP2	34:DN:114:ARG:NH1	2.48	0.46
37:DQ:133:ARG:HG2	37:DQ:134:ARG:N	2.30	0.46
40:DT:16:ARG:HH11	40:DT:16:ARG:HB3	1.80	0.46
42:DV:60:GLU:HB3	42:DV:95:LEU:HB3	1.97	0.46
1:AA:406:G:H4'	4:AD:3:ARG:HH22	1.80	0.46
1:AA:743:U:H2'	1:AA:744:C:C6	2.51	0.46
2:AB:59:GLU:HG3	2:AB:225:ALA:HB2	1.96	0.46
4:AD:163:GLU:O	4:AD:165:MET:N	2.48	0.46
15:AO:18:PHE:CZ	15:AO:21:ASP:HB3	2.50	0.46
18:AR:58:LEU:HB3	18:AR:62:GLU:HG3	1.98	0.46
25:AY:12:U:C2	25:AY:24:G:C2	3.03	0.46
25:AY:69:G:C5	25:AY:70:G:C8	3.03	0.46
26:BA:1107:G:H2'	26:BA:1107:G:N3	2.29	0.46
26:BA:278:A:O2'	26:BA:279:C:OP1	2.23	0.46
26:BA:527:C:C4	26:BA:2779:U:H2'	2.50	0.46
26:BA:615:G:OP1	30:BF:40:GLN:HG2	2.15	0.46
26:BA:1653:G:H3'	38:BR:2:ARG:HD3	1.96	0.46
45:BY:55:TYR:CD2	45:BY:55:TYR:N	2.84	0.46
46:BZ:137:ILE:HA	46:BZ:156:LYS:HZ1	1.80	0.46
46:BZ:5:LEU:O	46:BZ:59:LEU:HA	2.15	0.46
1:CA:1492:A:H2'	1:CA:1493:A:C8	2.51	0.46
8:CH:44:PHE:CE2	8:CH:109:ILE:HG12	2.51	0.46
22:CV:16:A:N6	24:CX:36:U:H3	2.12	0.46
25:CY:69:G:C6	25:CY:70:G:C8	3.04	0.46
26:DA:2263:C:N4	47:D0:15:ASP:OD1	2.47	0.46
56:D9:13:LYS:HD3	56:D9:28:GLU:OE2	2.15	0.46
24:CX:13:C:O2'	26:DA:1924:C:H4'	2.15	0.46
26:DA:2510:C:C4	26:DA:2511:U:C4	3.03	0.46
26:DA:724:U:H2'	26:DA:725:G:O4'	2.15	0.46
26:DA:8:A:H2'	26:DA:9:U:H6	1.81	0.46
29:DE:50:GLY:HA2	29:DE:77:ILE:O	2.14	0.46
2:AB:109:SER:O	2:AB:112:VAL:HG22	2.15	0.46
2:AB:210:SER:O	2:AB:214:ILE:HG12	2.16	0.46
7:AG:113:GLU:HG3	7:AG:118:VAL:HG12	1.96	0.46
7:AG:138:LYS:NZ	7:AG:142:GLU:OE2	2.49	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:AW:19:G:H4'	23:AW:20:U:OP1	2.16	0.46
23:AW:8:4SU:O2'	23:AW:46:7MG:N2	2.49	0.46
24:AX:17:C:H5'	24:AX:61:C:OP1	2.16	0.46
26:BA:2792:G:N2	26:BA:2805:G:H1'	2.31	0.46
29:BE:149:ARG:N	61:BE:406:HOH:O	2.38	0.46
37:BQ:37:LEU:HD21	37:BQ:130:LYS:HB2	1.98	0.46
43:BW:9:TYR:HA	43:BW:100:THR:HG23	1.98	0.46
1:CA:1318:A:H5''	19:CS:3:ARG:HH22	1.80	0.46
1:CA:1499:A:H1'	1:CA:1520:G:H5'	1.96	0.46
24:CX:37:A:H2'	24:CX:38:A:O4'	2.16	0.46
25:CY:15:G:C2	25:CY:48:C:N3	2.82	0.46
26:DA:1359:A:N1	26:DA:1372:U:O4	2.47	0.46
26:DA:2745:C:C4	26:DA:2746:U:C4	3.03	0.46
26:DA:2870:C:H5''	38:DR:65:LEU:HD21	1.97	0.46
26:DA:28:A:C2	26:DA:513:A:C8	3.03	0.46
26:DA:647:G:H8	26:DA:647:G:O5'	1.98	0.46
26:DA:995:C:N3	34:DN:2:LYS:HA	2.31	0.46
1:AA:1003:G:C2	1:AA:1004:A:N3	2.84	0.46
1:AA:224:C:H2'	1:AA:225:C:H6	1.81	0.46
9:AI:8:GLY:HA3	9:AI:76:ALA:O	2.15	0.46
10:AJ:70:ARG:HA	10:AJ:70:ARG:HD3	1.83	0.46
11:AK:82:VAL:N	11:AK:107:SER:O	2.45	0.46
25:AY:36:A:H2'	25:AY:37:MIA:O4'	2.15	0.46
49:B2:32:LEU:HD13	49:B2:36:ARG:NH1	2.30	0.46
26:BA:2130:U:H2'	26:BA:2131:G:N2	2.31	0.46
26:BA:236:C:H2'	26:BA:237:C:C6	2.50	0.46
26:BA:2748:A:H5'	32:BH:4:ILE:HD12	1.97	0.46
30:BF:28:ILE:O	30:BF:30:PRO:HD3	2.15	0.46
1:CA:69:G:H2'	1:CA:70:G:C8	2.51	0.46
1:CA:90:U:O2'	1:CA:91:C:H5'	2.15	0.46
1:CA:992:U:H6	1:CA:992:U:H5''	1.80	0.46
2:CB:149:LEU:HD22	2:CB:152:PHE:HD2	1.80	0.46
19:CS:27:GLU:HB2	19:CS:28:LYS:NZ	2.31	0.46
19:CS:27:GLU:HG2	19:CS:47:HIS:HE2	1.80	0.46
48:D1:83:GLU:HA	48:D1:84:GLY:HA2	1.62	0.46
26:DA:195:A:H2'	26:DA:198:C:N4	2.31	0.46
26:DA:2502:G:H5''	26:DA:2503:A:H5''	1.98	0.46
26:DA:383:U:H2'	26:DA:385:C:H5	1.81	0.46
26:DA:783:A:O2'	26:DA:785:G:OP1	2.24	0.46
26:DA:811:U:H2'	36:DP:21:ARG:HA	1.96	0.46
29:DE:1:MET:O	29:DE:84:PHE:HB2	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:DB:55:U:O3'	31:DG:27:ASN:ND2	2.49	0.46
32:DH:86:GLU:HB3	32:DH:165:ALA:HB2	1.97	0.46
1:AA:1025:U:O2	1:AA:1036:G:C6	2.66	0.46
1:AA:1136:U:H5'	1:AA:1137:C:N3	2.30	0.46
2:AB:61:LEU:HD23	2:AB:68:ILE:HD11	1.96	0.46
4:AD:110:PHE:HE1	4:AD:176:LEU:HD13	1.80	0.46
1:AA:1351:U:O4	9:AI:118:LYS:NZ	2.49	0.46
18:AR:65:ILE:O	18:AR:69:THR:HG23	2.16	0.46
26:BA:1021:A:H3'	26:BA:1021:A:C8	2.50	0.46
26:BA:1176:G:H1'	26:BA:1177:A:C5'	2.38	0.46
26:BA:1495:A:H2'	26:BA:1496:A:C8	2.51	0.46
26:BA:1697:G:OP2	26:BA:1698:A:O2'	2.14	0.46
26:BA:1859:A:N6	26:BA:1883:G:O2'	2.48	0.46
26:BA:191:A:H2'	26:BA:192:C:C6	2.51	0.46
26:BA:2128:C:H2'	26:BA:2129:C:C6	2.50	0.46
26:BA:484:C:H2'	26:BA:485:C:C6	2.51	0.46
40:BT:51:ARG:HG3	40:BT:98:LYS:HD2	1.96	0.46
43:BW:13:SER:HA	43:BW:14:PRO:HD3	1.84	0.46
1:CA:1002:G:N3	1:CA:1003:G:C8	2.84	0.46
1:CA:1095:U:C4	1:CA:1096:C:C4	3.03	0.46
1:CA:1134:G:H2'	1:CA:1135:U:H5'	1.98	0.46
1:CA:1291:G:C6	1:CA:1292:U:C4	3.04	0.46
1:CA:630:G:H2'	1:CA:631:G:H8	1.81	0.46
14:CN:6:LEU:HB3	14:CN:23:ARG:NH2	2.30	0.46
18:CR:26:LEU:CD2	18:CR:42:ARG:HD2	2.46	0.46
25:CY:35:A:N6	25:CY:36:A:N1	2.63	0.46
52:D5:16:ARG:HD2	52:D5:20:ARG:NH1	2.31	0.46
26:DA:1310:G:OP2	54:D7:9:ARG:NH1	2.49	0.46
26:DA:1611:C:H2'	26:DA:1612:C:H5'	1.98	0.46
26:DA:191:A:H2'	26:DA:192:C:C6	2.50	0.46
26:DA:740:U:H2'	26:DA:741:G:C8	2.51	0.46
2:AB:189:ASP:OD1	2:AB:189:ASP:N	2.39	0.46
3:AC:134:ILE:HG23	3:AC:151:VAL:HB	1.98	0.46
4:AD:3:ARG:HD3	4:AD:118:ARG:HD2	1.97	0.46
26:BA:1204:A:N6	26:BA:1240:U:H2'	2.30	0.46
26:BA:1300:U:H4'	26:BA:1301:A:H5'	1.97	0.46
26:BA:2086:U:H2'	26:BA:2087:G:C8	2.51	0.46
26:BA:2141:G:N7	26:BA:2151:G:C2	2.84	0.46
26:BA:2199:A:OP2	26:BA:2200:C:H5	1.99	0.46
26:BA:2630:G:H2'	26:BA:2631:G:H8	1.80	0.46
26:BA:882:G:H2'	26:BA:883:G:O4'	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:BG:47:LYS:O	31:BG:51:ARG:HG2	2.16	0.46
37:BQ:14:ARG:HG2	37:BQ:41:TRP:HH2	1.79	0.46
1:CA:937:A:H1'	1:CA:1379:G:N2	2.30	0.46
8:CH:6:ILE:O	8:CH:10:LEU:HG	2.16	0.46
10:CJ:30:SER:O	10:CJ:81:THR:HG23	2.16	0.46
25:CY:50:U:C2	25:CY:64:A:N1	2.84	0.46
26:DA:2347:C:O2'	53:D6:21:TYR:OH	2.34	0.46
26:DA:1913:A:H4'	26:DA:1914:C:O5'	2.15	0.46
26:DA:195:A:H2'	26:DA:198:C:H41	1.80	0.46
26:DA:2291:U:O2'	26:DA:2374:C:H1'	2.16	0.46
26:DA:2821:A:H2'	26:DA:2822:G:C8	2.51	0.46
26:DA:999:U:O2'	26:DA:1000:A:H5'	2.16	0.46
31:DG:10:LYS:HG3	31:DG:14:GLU:OE1	2.16	0.46
33:DI:77:LEU:HD11	33:DI:101:LEU:HB2	1.98	0.46
39:DS:27:SER:HA	39:DS:88:ASP:HB3	1.96	0.46
1:AA:1429:C:H2'	1:AA:1430:C:H6	1.80	0.46
1:AA:93:G:O2'	1:AA:96:U:H5'	2.16	0.46
3:AC:20:SER:OG	3:AC:40:ARG:NH1	2.48	0.46
11:AK:73:MET:HG2	11:AK:103:LEU:HD21	1.98	0.46
61:BA:5273:HOH:O	47:B0:41:ARG:HA	2.15	0.46
50:B3:26:LEU:O	50:B3:35:ARG:NE	2.49	0.46
51:B4:68:ARG:HD2	51:B4:69:LYS:H	1.81	0.46
26:BA:2533:A:H2'	26:BA:2534:A:O4'	2.16	0.46
26:BA:271(V):G:O6	61:BA:4948:HOH:O	2.20	0.46
26:BA:536:A:H2'	26:BA:537:C:C6	2.50	0.46
33:BI:85:GLU:OE1	33:BI:85:GLU:HA	2.16	0.46
1:CA:1220:G:H5'	19:CS:34:TRP:O	2.15	0.46
1:CA:1457:G:OP1	20:CT:39:LYS:NZ	2.37	0.46
1:CA:450:G:H4'	16:CP:41:PRO:HB2	1.98	0.46
2:CB:28:PHE:HD1	2:CB:194:PRO:HG3	1.81	0.46
2:CB:30:ARG:HG3	2:CB:31:TYR:CD1	2.50	0.46
7:CG:79:ARG:HB3	7:CG:80:VAL:H	1.37	0.46
26:DA:774:A:N3	26:DA:774:A:H2'	2.30	0.46
31:DG:25:TYR:HB3	31:DG:30:GLU:HB3	1.98	0.46
1:AA:1237:C:O2'	1:AA:1300:G:N2	2.43	0.46
1:AA:1302:U:OP2	13:AM:21:TYR:OH	2.24	0.46
1:AA:262:A:C6	1:AA:263:A:C6	3.03	0.46
1:AA:6:G:O2'	1:AA:7:G:H5'	2.16	0.46
7:AG:111:ARG:NH2	7:AG:126:ASP:OD2	2.48	0.46
52:B5:42:PRO:HB2	52:B5:43:HIS:ND1	2.31	0.46
26:BA:2141:G:C4	26:BA:2142:C:H1'	2.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:BA:857:C:N4	26:BA:858:U:O4	2.49	0.46
30:BF:29:ASN:H	30:BF:112:MET:CE	2.28	0.46
38:BR:36:THR:HG22	38:BR:37:THR:H	1.81	0.46
1:CA:1004:A:N7	1:CA:1037:C:H2'	2.31	0.46
1:CA:1006:C:H2'	1:CA:1007:C:O4'	2.16	0.46
1:CA:1317:C:H5	14:CN:18:VAL:HG21	1.80	0.46
1:CA:1516:G:N2	1:CA:1519:A:OP2	2.49	0.46
1:CA:202:U:O2'	1:CA:203:U:O5'	2.31	0.46
2:CB:100:GLY:HA2	2:CB:103:THR:OG1	2.15	0.46
2:CB:150:SER:OG	2:CB:151:GLY:N	2.48	0.46
2:CB:218:ALA:O	2:CB:222:ILE:HG23	2.15	0.46
4:CD:92:VAL:O	4:CD:96:LEU:HD22	2.16	0.46
8:CH:121:ASP:OD1	8:CH:121:ASP:N	2.49	0.46
26:DA:1032:A:H2	26:DA:1122:G:H22	1.61	0.46
26:DA:1484:G:C6	26:DA:1485:G:N7	2.84	0.46
25:CY:76:A:O2'	26:DA:2394:C:N3	2.44	0.46
26:DA:2687:U:H2'	26:DA:2688:U:O4'	2.16	0.46
26:DA:307:G:H22	26:DA:310:A:P	2.38	0.46
31:DG:44:GLY:O	31:DG:47:LYS:HB2	2.15	0.46
44:DX:92:LEU:HA	44:DX:92:LEU:HD12	1.83	0.46
46:DZ:150:LEU:HD12	46:DZ:150:LEU:HA	1.78	0.46
1:AA:1273:G:H3'	1:AA:1274:G:C8	2.51	0.46
1:AA:1457:G:H2'	1:AA:1458:G:C8	2.51	0.46
1:AA:93:G:C2'	1:AA:96:U:H5'	2.46	0.46
5:AE:12:LEU:HB3	5:AE:31:LEU:HB2	1.98	0.46
13:AM:4:ILE:HD12	13:AM:57:ARG:HA	1.97	0.46
26:BA:2011:U:OP1	43:BW:42:ARG:HD3	2.16	0.46
26:BA:2359:C:H2'	26:BA:2360:A:O4'	2.16	0.46
26:BA:2675:A:H5'	35:BO:29:ASN:O	2.15	0.46
26:BA:2803:C:H2'	26:BA:2804:C:C6	2.51	0.46
1:CA:994:A:C5	1:CA:1216:G:H4'	2.51	0.46
2:CB:96:ARG:HD2	2:CB:98:LEU:HD22	1.97	0.46
3:CC:121:ALA:HB2	3:CC:198:VAL:HG21	1.98	0.46
3:CC:36:ASP:O	3:CC:40:ARG:HG3	2.16	0.46
1:CA:664:G:H5''	18:CR:64:ARG:NH2	2.31	0.46
47:D0:82:ARG:HA	47:D0:83:PRO:HD3	1.78	0.46
26:DA:1477:A:H2'	26:DA:1478:G:O4'	2.14	0.46
26:DA:1539:G:H2'	26:DA:1540:U:O4'	2.16	0.46
26:DA:1857:G:C6	26:DA:1858:G:N1	2.84	0.46
26:DA:1913:A:H4'	26:DA:1914:C:C5'	2.46	0.46
26:DA:2119:A:H2	26:DA:2171:A:H5'	1.81	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:DA:330:A:HO2'	26:DA:331:A:H8	1.61	0.46
26:DA:517:C:O2'	43:DW:18:ARG:NH2	2.49	0.46
27:DB:5:C:N4	27:DB:116:G:H1	2.13	0.46
27:DB:80:U:H2'	27:DB:81:G:C8	2.51	0.46
33:DI:90:GLY:O	33:DI:121:LYS:HE3	2.16	0.46
38:DR:98:LEU:HB2	38:DR:113:LEU:HD11	1.98	0.46
1:AA:1075:C:H2'	1:AA:1076:C:H5''	1.98	0.45
1:AA:691:G:OP2	11:AK:26:ASN:ND2	2.38	0.45
2:AB:45:GLN:O	2:AB:49:GLU:HB2	2.16	0.45
50:B3:43:ILE:O	50:B3:47:VAL:HG23	2.16	0.45
26:BA:1178:C:H2'	26:BA:1179:C:C6	2.51	0.45
26:BA:271(O):C:H2'	26:BA:271(P):C:C6	2.51	0.45
33:BI:77:LEU:HB2	33:BI:142:VAL:HG12	1.97	0.45
42:BV:21:ARG:HG2	42:BV:91:TYR:CD1	2.51	0.45
1:CA:1084:G:C5	1:CA:1085:U:C4	3.04	0.45
1:CA:976:G:C8	1:CA:1362:C:N4	2.84	0.45
1:CA:1423:G:H2'	1:CA:1424:C:H6	1.80	0.45
1:CA:59:A:H3'	1:CA:331:G:H22	1.81	0.45
1:CA:920:U:H2'	1:CA:921:U:H6	1.77	0.45
7:CG:111:ARG:HB3	7:CG:113:GLU:OE2	2.16	0.45
1:CA:689:C:P	11:CK:46:GLY:HA3	2.56	0.45
12:CL:8:ASN:O	12:CL:12:ARG:HG3	2.16	0.45
15:CO:74:ASP:OD1	15:CO:76:GLU:HB2	2.16	0.45
19:CS:27:GLU:HB3	19:CS:28:LYS:HA	1.96	0.45
26:DA:1300:U:H4'	26:DA:1301:A:O5'	2.16	0.45
26:DA:601:C:O2'	30:DF:104:LYS:NZ	2.44	0.45
26:DA:754:C:H2'	26:DA:755:C:C6	2.50	0.45
28:DD:72:LYS:HB3	28:DD:75:ILE:HD12	1.98	0.45
33:DI:102:SER:O	33:DI:106:GLY:N	2.37	0.45
26:DA:385:C:O2	36:DP:71:VAL:HG21	2.16	0.45
1:AA:1034:G:H3'	1:AA:1035:A:C8	2.51	0.45
1:AA:59:A:H3'	1:AA:331:G:H22	1.81	0.45
2:AB:16:HIS:CB	2:AB:204:ASN:HB3	2.31	0.45
3:AC:155:GLY:HA3	3:AC:196:LEU:HD22	1.97	0.45
4:AD:162:LEU:CD1	4:AD:181:MET:HG2	2.46	0.45
5:AE:27:ARG:HB2	5:AE:27:ARG:HE	1.48	0.45
15:AO:61:GLY:O	15:AO:65:ARG:HG3	2.16	0.45
53:B6:11:LEU:HB3	53:B6:49:HIS:HB3	1.98	0.45
26:BA:2567:G:H2'	26:BA:2568:C:C6	2.51	0.45
26:BA:2846:G:H2'	26:BA:2847:U:O4'	2.16	0.45
26:BA:911:A:H2'	37:BQ:9:TYR:OH	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:BA:1842:G:O2'	28:BD:253:GLN:NE2	2.49	0.45
26:BA:1803:A:H4'	28:BD:259:THR:HG23	1.98	0.45
31:BG:16:ARG:NE	31:BG:31:VAL:HG11	2.30	0.45
1:CA:1323:G:H2'	1:CA:1324:A:C8	2.51	0.45
1:CA:775:G:N2	1:CA:804:U:O4	2.48	0.45
3:CC:164:ARG:HG2	3:CC:165:THR:H	1.81	0.45
2:CB:178:ARG:NH2	8:CH:68:ARG:HH22	2.12	0.45
9:CI:99:LEU:HB3	9:CI:101:PHE:CE2	2.51	0.45
13:CM:37:THR:HG21	13:CM:56:LEU:HA	1.97	0.45
17:CQ:66:SER:OG	17:CQ:69:LYS:HB2	2.16	0.45
47:D0:53:MET:HG2	47:D0:57:PHE:HA	1.98	0.45
26:DA:1027:A:C6	26:DA:1126:A:C4	3.04	0.45
26:DA:1991:U:H2'	26:DA:1992:G:H5''	1.97	0.45
26:DA:2379:G:O2'	39:DS:17:ARG:NH2	2.36	0.45
26:DA:698:C:O2'	26:DA:734:A:N6	2.49	0.45
26:DA:752:A:P	54:D7:3:ARG:HH22	2.39	0.45
28:DD:96:HIS:CD2	28:DD:102:LYS:HG2	2.52	0.45
33:DI:93:THR:HG22	33:DI:119:PRO:HB3	1.97	0.45
38:DR:29:LEU:HA	38:DR:29:LEU:HD12	1.78	0.45
1:AA:1243:C:H2'	1:AA:1244:C:C6	2.50	0.45
2:AB:16:HIS:CE1	2:AB:214:ILE:HD11	2.46	0.45
10:AJ:31:GLY:HA2	10:AJ:32:ALA:HA	1.44	0.45
26:BA:1301:A:C8	26:BA:1303:G:C8	3.04	0.45
26:BA:2141:G:C6	26:BA:2142:C:C2	3.04	0.45
26:BA:90:U:H4'	26:BA:92:A:H5'	1.99	0.45
28:BD:52:ARG:NH2	61:BD:411:HOH:O	2.22	0.45
31:BG:45:GLU:HG2	31:BG:45:GLU:H	1.36	0.45
34:BN:38:HIS:NE2	34:BN:50:ASP:OD2	2.50	0.45
1:CA:1053:G:C3'	1:CA:1054:C:H5'	2.45	0.45
1:CA:21:G:H2'	1:CA:22:G:C8	2.51	0.45
1:CA:580:U:H2'	1:CA:581:G:O4'	2.16	0.45
2:CB:97:TRP:CZ3	2:CB:101:MET:HB2	2.52	0.45
11:CK:81:ASP:OD1	11:CK:106:LYS:HB2	2.17	0.45
16:CP:19:ILE:N	16:CP:37:GLY:O	2.49	0.45
19:CS:41:VAL:HG12	19:CS:43:GLU:H	1.80	0.45
26:DA:2127:G:N1	26:DA:2161:C:O2	2.34	0.45
26:DA:2468:G:C2	26:DA:2481:G:N3	2.85	0.45
26:DA:2653:U:O2'	32:DH:110:SER:HB3	2.15	0.45
39:DS:3:ARG:HE	39:DS:4:LEU:N	2.15	0.45
1:AA:1251:A:H2'	1:AA:1252:A:C8	2.52	0.45
1:AA:1273:G:H3'	1:AA:1274:G:H8	1.81	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:356:A:N7	61:AA:4035:HOH:O	2.36	0.45
4:AD:138:TYR:HE1	4:AD:140:VAL:HA	1.81	0.45
5:AE:18:ARG:HE	5:AE:27:ARG:HH21	1.64	0.45
7:AG:91:VAL:HB	7:AG:96:GLN:HG2	1.99	0.45
13:AM:15:VAL:HG22	13:AM:43:THR:O	2.17	0.45
31:BG:31:VAL:HA	31:BG:32:PRO:HD2	1.79	0.45
36:BP:121:LYS:O	36:BP:123:LEU:N	2.45	0.45
1:CA:56:U:H2'	1:CA:57:G:C8	2.52	0.45
1:CA:991:U:H3'	1:CA:1212:U:N3	2.32	0.45
3:CC:79:ARG:H	3:CC:82:GLU:HB3	1.82	0.45
5:CE:90:VAL:O	5:CE:120:THR:HA	2.17	0.45
6:CF:28:ARG:HH11	6:CF:28:ARG:HB2	1.82	0.45
11:CK:45:GLY:O	11:CK:50:TYR:HB2	2.17	0.45
50:D3:4:LEU:O	50:D3:36:VAL:HA	2.17	0.45
26:DA:241:A:H8	26:DA:241:A:OP1	2.00	0.45
26:DA:583:G:OP2	41:DU:10:ARG:NH1	2.49	0.45
26:DA:94(A):G:H2'	26:DA:95:G:O4'	2.16	0.45
29:DE:9:VAL:HG13	29:DE:25:VAL:O	2.16	0.45
26:DA:2019:A:C4'	41:DU:34:LYS:HD2	2.47	0.45
45:DY:86:ARG:HD2	45:DY:100:ALA:HA	1.98	0.45
2:AB:150:SER:OG	2:AB:151:GLY:N	2.49	0.45
2:AB:22:LYS:H	2:AB:40:HIS:CE1	2.35	0.45
4:AD:170:VAL:HG12	4:AD:171:GLY:N	2.32	0.45
5:AE:12:LEU:HD22	5:AE:13:ILE:N	2.32	0.45
6:AF:44:GLY:HA2	6:AF:59:TYR:CE2	2.52	0.45
18:AR:31:LEU:HD11	18:AR:62:GLU:HB2	1.98	0.45
1:AA:1305:G:H5''	21:AU:4:GLY:HA3	1.98	0.45
32:BH:11:VAL:HG13	32:BH:15:VAL:HG22	1.98	0.45
35:BO:7:TYR:CZ	35:BO:44:LYS:HG3	2.52	0.45
46:BZ:105:VAL:N	46:BZ:139:VAL:O	2.41	0.45
1:CA:1097:C:O2'	1:CA:1169:A:N3	2.41	0.45
1:CA:189(F):U:O2	17:CQ:63:ARG:NH2	2.50	0.45
1:CA:22:G:H4'	1:CA:885:G:C8	2.52	0.45
6:CF:46:ARG:HH21	18:CR:37:VAL:HG11	1.81	0.45
12:CL:69:TYR:CE2	12:CL:71:PRO:HA	2.52	0.45
1:CA:1218:C:OP2	14:CN:9:LYS:NZ	2.49	0.45
15:CO:17:ARG:HG3	15:CO:17:ARG:HH11	1.82	0.45
20:CT:43:LEU:HD13	20:CT:51:GLU:HB3	1.98	0.45
20:CT:53:LEU:O	20:CT:57:ARG:HG3	2.16	0.45
36:DP:63:PRO:HG2	55:D8:25:MET:HB2	1.99	0.45
26:DA:2287:A:N1	26:DA:2346:A:N7	2.65	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:DA:2447:G:N2	26:DA:2450:A:OP2	2.46	0.45
26:DA:468:G:N7	54:D7:39:ARG:NH2	2.63	0.45
42:DV:5:VAL:CG1	42:DV:57:VAL:HG21	2.47	0.45
26:DA:25:U:H5'	43:DW:78:GLU:O	2.16	0.45
1:AA:1030(C):G:H2'	1:AA:1030(D):A:H8	1.81	0.45
1:AA:300:A:O2'	1:AA:564:C:N3	2.39	0.45
1:AA:8:A:N7	4:AD:208:SER:OG	2.48	0.45
3:AC:181:ASN:C	3:AC:181:ASN:HD22	2.20	0.45
10:AJ:55:LYS:O	10:AJ:57:LYS:N	2.50	0.45
11:AK:41:THR:OG1	11:AK:42:TRP:N	2.50	0.45
1:AA:836:G:OP1	18:AR:61:LYS:NZ	2.49	0.45
26:BA:1300:U:H4'	26:BA:1301:A:H5''	1.99	0.45
26:BA:2544:G:H1'	26:BA:2646:C:H4'	1.99	0.45
26:BA:528:A:N1	26:BA:2042:A:H2'	2.31	0.45
29:BE:7:VAL:HG12	29:BE:27:LEU:HB3	1.98	0.45
33:BI:102:SER:OG	33:BI:103:ARG:N	2.50	0.45
46:BZ:138:GLU:N	46:BZ:156:LYS:HD3	2.30	0.45
1:CA:1009:G:C2	1:CA:1010:G:C4	3.04	0.45
1:CA:1054:C:O2'	1:CA:1055:A:C5'	2.64	0.45
1:CA:93:G:C6	1:CA:96:U:C4	3.05	0.45
1:CA:97:G:O2'	1:CA:98:G:H5''	2.17	0.45
25:CY:21:A:N6	25:CY:46:7MG:H81	2.32	0.45
55:D8:62:LEU:HB3	55:D8:65:GLU:HG3	1.97	0.45
26:DA:1463:C:H2'	26:DA:1464:C:H6	1.81	0.45
26:DA:2450:A:OP1	26:DA:2497:A:O2'	2.35	0.45
26:DA:251:A:H5''	36:DP:50:ARG:HH11	1.81	0.45
26:DA:1782:C:H1'	26:DA:2609:U:H5''	1.98	0.45
26:DA:686:G:H21	26:DA:788:A:H61	1.65	0.45
26:DA:93:G:H2'	26:DA:94:C:H6	1.82	0.45
28:DD:17:THR:O	28:DD:211:ARG:NH2	2.45	0.45
41:DU:27:LEU:HD23	41:DU:30:LYS:HB2	1.98	0.45
42:DV:100:ARG:HH11	42:DV:100:ARG:CG	2.17	0.45
45:DY:13:VAL:HG12	45:DY:74:PRO:HA	1.99	0.45
46:DZ:113:ALA:HB3	46:DZ:146:ILE:HD11	1.97	0.45
1:AA:692:U:O2'	1:AA:694:A:N7	2.42	0.45
1:AA:78:G:C6	1:AA:91:C:N4	2.83	0.45
2:AB:158:LEU:HA	2:AB:159:PRO:HD3	1.83	0.45
4:AD:61:LYS:HA	4:AD:203:VAL:HG22	1.98	0.45
16:AP:5:ARG:NH1	16:AP:24:ALA:HA	2.31	0.45
25:AY:50:U:C4	25:AY:64:A:N1	2.84	0.45
53:B6:13:CYS:SG	53:B6:47:THR:HG21	2.56	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:BA:141:A:H8	26:BA:1408:C:O2'	2.00	0.45
26:BA:1794:U:H2'	26:BA:1795:C:C6	2.50	0.45
28:BD:5:LYS:HE3	28:BD:5:LYS:HB3	1.56	0.45
33:BI:136:VAL:N	33:BI:137:PRO:HD3	2.32	0.45
36:BP:135:LEU:HD23	36:BP:135:LEU:HA	1.77	0.45
37:BQ:18:LYS:HB2	37:BQ:18:LYS:HE3	1.72	0.45
1:CA:1000:U:C2	1:CA:1041:A:N1	2.83	0.45
1:CA:297:G:N2	1:CA:300:A:OP2	2.49	0.45
1:CA:335:C:H2'	1:CA:336:C:C6	2.51	0.45
2:CB:55:PHE:O	2:CB:59:GLU:N	2.33	0.45
3:CC:156:ARG:NH2	3:CC:159:GLY:O	2.27	0.45
15:CO:54:ARG:HD3	15:CO:58:MET:CE	2.47	0.45
23:CW:47:U:H3'	23:CW:48:C:C5'	2.47	0.45
25:CY:70:G:H2'	25:CY:71:G:H5'	1.99	0.45
26:DA:2348:U:O4	26:DA:2382:G:N1	2.50	0.45
26:DA:30:G:H2'	26:DA:31:C:C6	2.52	0.45
26:DA:864:G:C6	26:DA:865:C:N4	2.85	0.45
31:DG:74:LYS:O	31:DG:84:LYS:HD2	2.16	0.45
35:DO:107:ARG:CZ	40:DT:36:GLU:HG2	2.46	0.45
44:DX:92:LEU:C	44:DX:94:GLY:H	2.18	0.45
1:AA:1003:G:C2'	1:AA:1004:A:H4'	2.47	0.45
1:AA:300:A:H2'	1:AA:301:G:O4'	2.17	0.45
4:AD:121:VAL:O	4:AD:134:ASP:HA	2.15	0.45
4:AD:98:GLU:OE1	4:AD:103:ASN:ND2	2.33	0.45
1:AA:279:A:C4	17:AQ:98:LEU:HD23	2.51	0.45
26:BA:1783:A:H5'	26:BA:2608:G:H4'	1.98	0.45
1:CA:1048:G:OP1	14:CN:3:ARG:HD2	2.17	0.45
1:CA:58:C:O2'	1:CA:388:G:N7	2.40	0.45
11:CK:34:ASP:OD2	11:CK:38:ASN:HB2	2.17	0.45
24:CX:9:G:O2'	24:CX:10:G:N7	2.37	0.45
26:DA:1740:G:H2'	26:DA:1741:A:C8	2.51	0.45
26:DA:1027:A:C2	26:DA:2488:A:H5'	2.52	0.45
26:DA:270:A:N1	26:DA:366:C:H4'	2.32	0.45
26:DA:2637:U:H1'	26:DA:2782:G:N2	2.32	0.45
26:DA:443:A:OP2	26:DA:614(B):G:N2	2.38	0.45
26:DA:848:G:C4	26:DA:933:A:H8	2.35	0.45
26:DA:94(A):G:C6	26:DA:95:G:C5	3.05	0.45
30:DF:64:ILE:HG21	30:DF:78:ILE:HG23	1.99	0.45
37:DQ:118:LEU:HB3	37:DQ:131:ILE:HD12	1.97	0.45
40:DT:65:LYS:HE2	40:DT:67:SER:HB2	1.98	0.45
1:AA:189(A):C:N4	1:AA:189(J):G:H1	2.15	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:662:G:H2'	1:AA:663:A:H8	1.79	0.45
8:AH:51:VAL:HG21	8:AH:60:ARG:HB2	1.98	0.45
11:AK:38:ASN:HA	11:AK:39:PRO:HD3	1.86	0.45
23:AW:18:G:O2'	23:AW:57:G:N2	2.39	0.45
25:AY:7:A:O2'	25:AY:49:C:OP2	2.21	0.45
26:BA:1957:C:H2'	26:BA:1958:C:C6	2.52	0.45
26:BA:2080:G:OP1	48:B1:35:THR:HG21	2.17	0.45
26:BA:729:G:C6	28:BD:208:LYS:HB2	2.52	0.45
26:BA:897:C:C4	26:BA:898:C:N4	2.85	0.45
31:BG:11:TYR:O	31:BG:16:ARG:HG2	2.17	0.45
34:BN:14:VAL:HG11	34:BN:138:LEU:HD12	1.99	0.45
45:BY:34:LYS:O	45:BY:34:LYS:HG3	2.15	0.45
1:CA:1010:G:H22	1:CA:1020:U:H1'	1.82	0.45
1:CA:1374:A:O2'	7:CG:28:ASN:HB3	2.16	0.45
2:CB:19:HIS:CG	2:CB:20:GLU:H	2.34	0.45
2:CB:15:VAL:HG21	2:CB:213:LEU:HD12	1.98	0.45
9:CI:4:TYR:HB2	9:CI:19:LEU:HB2	1.99	0.45
13:CM:33:ALA:HA	13:CM:59:TYR:CE2	2.51	0.45
23:CW:18:G:O6	23:CW:55:PSU:H1'	2.17	0.45
23:CW:76:31M:HD1	23:CW:76:31M:HA	1.41	0.45
26:DA:1116:C:H2'	26:DA:1117:G:C8	2.52	0.45
26:DA:1395:A:OP1	61:DA:4546:HOH:O	2.21	0.45
26:DA:2052:G:H4'	29:DE:143:ASN:O	2.16	0.45
26:DA:2305:A:H2'	26:DA:2306:C:O4'	2.17	0.45
26:DA:263:C:H2'	26:DA:264:C:O4'	2.17	0.45
27:DB:66:A:N6	27:DB:108:U:H3'	2.32	0.45
27:DB:11:C:H3'	27:DB:12:C:C6	2.52	0.45
28:DD:96:HIS:HD2	28:DD:102:LYS:HG2	1.81	0.45
28:DD:10:THR:OG1	28:DD:13:ARG:HG2	2.16	0.45
40:DT:117:ASP:OD2	40:DT:120:ARG:NE	2.41	0.45
42:DV:40:LEU:HB2	42:DV:46:VAL:HG22	1.99	0.45
1:AA:1442(B):A:N3	40:BT:118:ARG:NH2	2.65	0.45
25:AY:54:5MU:H73	25:AY:55:PSU:O2	2.17	0.45
53:B6:40:CYS:HA	53:B6:41:PRO:HD3	1.78	0.45
26:BA:250:G:P	55:B8:13:ARG:HH22	2.39	0.45
26:BA:2168:G:O6	26:BA:2171:A:H8	1.99	0.45
26:BA:2576:G:H1'	61:BA:4454:HOH:O	2.17	0.45
26:BA:2893:G:HO2'	26:BA:2894:G:P	2.38	0.45
26:BA:899:A:O2'	26:BA:900:A:H8	2.00	0.45
26:BA:973:A:OP2	61:BA:4141:HOH:O	2.20	0.45
30:BF:184:TYR:O	30:BF:188:ARG:HG3	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:BA:4103:HOH:O	30:BF:68:LYS:HE2	2.17	0.45
32:BH:98:LEU:HD12	32:BH:102:ALA:O	2.16	0.45
42:BV:55:ALA:HB2	42:BV:101:GLY:HA2	1.99	0.45
1:CA:1028:C:N3	1:CA:1033:G:C6	2.84	0.45
1:CA:1133:G:C4	1:CA:1134:G:C8	3.04	0.45
1:CA:1338:G:C6	1:CA:1339:A:C6	3.05	0.45
1:CA:200:G:H1	1:CA:217:C:N4	2.09	0.45
1:CA:582:U:OP2	1:CA:758:G:N1	2.45	0.45
1:CA:986:A:H2'	1:CA:987:G:O4'	2.17	0.45
1:CA:1191:A:OP2	3:CC:3:ASN:ND2	2.49	0.45
5:CE:79:GLU:OE1	8:CH:104:ARG:HA	2.17	0.45
26:DA:1427:A:H4'	26:DA:1428:C:O5'	2.15	0.45
26:DA:2303:G:O2'	31:DG:132:ASN:ND2	2.44	0.45
26:DA:2607:G:O6	61:DA:4661:HOH:O	2.20	0.45
26:DA:492:A:H2'	26:DA:493:G:O4'	2.17	0.45
30:DF:36:VAL:HG11	30:DF:183:VAL:HG11	1.99	0.45
34:DN:37:LYS:NZ	61:DN:5101:HOH:O	2.49	0.45
39:DS:106:ARG:HG3	39:DS:112:PHE:CZ	2.51	0.45
45:DY:5:MET:HG2	45:DY:30:VAL:HG11	1.99	0.45
1:AA:6:G:H4'	1:AA:298:A:H4'	1.99	0.44
1:AA:636:U:H2'	1:AA:637:G:C8	2.52	0.44
6:AF:18:GLN:HA	6:AF:21:LEU:HD12	1.99	0.44
36:BP:50:ARG:NH2	55:B8:7:HIS:HD2	2.15	0.44
26:BA:1371:G:H2'	26:BA:1372:U:C5	2.50	0.44
26:BA:2615:U:H2'	26:BA:2616:C:H6	1.82	0.44
26:BA:271(P):C:O3'	33:BI:42:SER:OG	2.27	0.44
1:CA:1070:U:H2'	1:CA:1071:C:C6	2.52	0.44
1:CA:1249:C:O4'	9:CI:70:LYS:HE2	2.17	0.44
1:CA:1386:G:C2	1:CA:1387:G:C8	3.04	0.44
1:CA:353:A:H8	1:CA:353:A:H5'	1.82	0.44
1:CA:501:C:H2'	1:CA:502:G:C8	2.52	0.44
1:CA:866:C:C4	1:CA:867:G:H1'	2.52	0.44
2:CB:187:LEU:HA	2:CB:201:ILE:HB	1.98	0.44
17:CQ:6:LEU:O	17:CQ:58:GLU:HA	2.16	0.44
20:CT:46:GLU:O	20:CT:46:GLU:HG2	2.16	0.44
1:CA:1326:C:H5''	21:CU:18:TYR:O	2.17	0.44
25:CY:66:U:H2'	25:CY:67:C:O4'	2.17	0.44
26:DA:1794:U:H2'	26:DA:1795:C:C6	2.53	0.44
26:DA:2203:U:H2'	26:DA:2205:C:H6	1.81	0.44
26:DA:2298:A:H2'	26:DA:2299:G:O4'	2.16	0.44
26:DA:307:G:H21	26:DA:330:A:N6	2.10	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:DA:182:A:H2	26:DA:433:C:O2	2.00	0.44
27:DB:66:A:H61	27:DB:109:C:H5'	1.82	0.44
37:DQ:58:PHE:CE2	37:DQ:109:VAL:HG21	2.52	0.44
46:DZ:157:LEU:C	46:DZ:161:VAL:HG11	2.37	0.44
1:AA:1149:C:P	9:AI:9:ARG:HH21	2.40	0.44
1:AA:767:A:N7	61:AA:4048:HOH:O	2.36	0.44
1:AA:923:A:OP1	5:AE:21:ALA:HB2	2.17	0.44
16:AP:20:VAL:HG21	16:AP:32:TYR:CD2	2.52	0.44
25:AY:41:C:H2'	25:AY:42:C:C6	2.53	0.44
26:BA:1019:U:H3	26:BA:1142(A):A:N6	2.10	0.44
26:BA:1630:G:H2'	26:BA:1631:C:C6	2.53	0.44
26:BA:2649:U:H2'	26:BA:2650:U:C6	2.51	0.44
26:BA:305:U:H2'	26:BA:306:U:C6	2.52	0.44
26:BA:470:A:OP1	30:BF:59:TYR:HE1	1.99	0.44
1:CA:153:C:H2'	1:CA:154:C:C6	2.52	0.44
2:CB:213:LEU:O	2:CB:217:ARG:HB2	2.17	0.44
8:CH:44:PHE:HE2	8:CH:109:ILE:HG12	1.82	0.44
9:CI:99:LEU:HB3	9:CI:101:PHE:CD2	2.52	0.44
15:CO:54:ARG:HD3	15:CO:58:MET:HE2	1.99	0.44
56:D9:3:VAL:HA	56:D9:35:ARG:O	2.18	0.44
26:DA:686:G:N2	26:DA:788:A:H61	2.14	0.44
27:DB:72:G:H1'	27:DB:105:A:H61	1.82	0.44
31:DG:138:GLN:OE1	31:DG:138:GLN:N	2.43	0.44
33:DI:133:HIS:HD2	33:DI:136:VAL:HG23	1.82	0.44
39:DS:34:HIS:O	39:DS:97:ARG:NH2	2.50	0.44
45:DY:52:SER:HB2	45:DY:53:PRO:HD2	1.99	0.44
1:AA:620:C:H2'	1:AA:621:A:O4'	2.16	0.44
3:AC:52:LEU:HA	3:AC:70:VAL:HG23	1.99	0.44
9:AI:99:LEU:HB3	9:AI:101:PHE:HE1	1.80	0.44
26:BA:1378:A:OP1	54:B7:10:ARG:NH2	2.51	0.44
26:BA:2661:G:H2'	26:BA:2662:A:C8	2.51	0.44
26:BA:2849:U:H4'	26:BA:2868:A:C2	2.52	0.44
26:BA:675:A:C8	26:BA:804:A:C6	3.05	0.44
29:BE:79:ARG:HA	29:BE:79:ARG:HD3	1.82	0.44
32:BH:54:ARG:HD3	32:BH:65:HIS:ND1	2.32	0.44
46:BZ:108:PRO:CG	46:BZ:117:LEU:HD22	2.47	0.44
1:CA:1273:G:H3'	1:CA:1274:G:C8	2.51	0.44
3:CC:131:ARG:NH1	5:CE:50:GLU:HG3	2.32	0.44
4:CD:173:TRP:CE2	4:CD:189:PRO:HG3	2.53	0.44
4:CD:47:ARG:HH11	4:CD:49:ARG:HH21	1.65	0.44
12:CL:33:ARG:HD3	12:CL:62:SER:HB3	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:CS:30:LEU:CD1	19:CS:50:ALA:HB2	2.48	0.44
1:CA:1318:A:H5''	19:CS:3:ARG:NH2	2.32	0.44
51:D4:57:GLU:HA	51:D4:58:ARG:HA	1.71	0.44
26:DA:2153:G:N2	26:DA:2154:G:N3	2.65	0.44
31:DG:173:LEU:HB3	31:DG:178:PHE:CG	2.53	0.44
31:DG:28:VAL:O	31:DG:31:VAL:HG12	2.18	0.44
36:DP:88:LEU:HD11	36:DP:114:ILE:HD12	1.99	0.44
46:DZ:128:VAL:HG23	46:DZ:160:GLY:O	2.17	0.44
1:AA:769:G:H4'	1:AA:1513:A:H4'	1.99	0.44
3:AC:27:LYS:NZ	3:AC:27:LYS:HA	2.32	0.44
10:AJ:38:ILE:HD11	10:AJ:71:LEU:HD23	1.98	0.44
23:AW:51:U:H2'	23:AW:52:G:H8	1.83	0.44
24:AX:31:G:N7	24:AX:32:5MC:HM52	2.32	0.44
25:AY:40:C:H2'	25:AY:41:C:C6	2.52	0.44
26:BA:2384:G:OP2	47:B0:55:ARG:NH1	2.51	0.44
26:BA:1184:G:H5'	50:B3:29:ARG:NH1	2.32	0.44
26:BA:141:A:C8	26:BA:1408:C:O2'	2.69	0.44
26:BA:1268:A:C2	26:BA:2013:A:C4	3.05	0.44
26:BA:311:A:C6	26:BA:328:U:C4	3.06	0.44
27:BB:4:C:H2'	27:BB:5:C:C6	2.52	0.44
33:BI:101:LEU:HD13	33:BI:107:VAL:O	2.16	0.44
40:BT:37:GLY:HA2	40:BT:38:ASN:HA	1.69	0.44
1:CA:1054:C:HO2'	1:CA:1055:A:P	2.36	0.44
1:CA:1084:G:OP1	1:CA:1086:U:C2	2.70	0.44
1:CA:1324:A:O4'	1:CA:1362:C:H4'	2.17	0.44
1:CA:142:G:H2'	1:CA:143:A:O4'	2.16	0.44
1:CA:551:U:H2'	1:CA:552:U:H6	1.81	0.44
2:CB:80:ILE:HD11	2:CB:212:GLN:CA	2.48	0.44
4:CD:163:GLU:O	4:CD:166:LYS:N	2.44	0.44
10:CJ:5:ARG:HA	10:CJ:73:ASP:HA	2.00	0.44
17:CQ:66:SER:H	17:CQ:69:LYS:HB3	1.82	0.44
1:CA:1305:G:H5'	21:CU:4:GLY:HA3	1.99	0.44
25:CY:7:A:N1	25:CY:66:U:O2	2.50	0.44
49:D2:16:LEU:O	49:D2:67:LYS:NZ	2.47	0.44
26:DA:1035:U:H2'	26:DA:1036:G:C8	2.52	0.44
26:DA:1219:G:H1	26:DA:1230:C:H42	1.64	0.44
26:DA:2370:G:C6	26:DA:2371:G:C6	3.06	0.44
29:DE:181:LEU:HD12	29:DE:181:LEU:HA	1.84	0.44
35:DO:71:ARG:NE	35:DO:105:GLU:OE2	2.40	0.44
44:DX:59:VAL:HB	44:DX:76:ARG:HB2	1.99	0.44
1:AA:1028:C:H2'	1:AA:1029:C:C4'	2.47	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1241:G:H2'	1:AA:1242:C:C6	2.53	0.44
1:AA:162:A:O5'	1:AA:162:A:H8	2.01	0.44
2:AB:51:LEU:HD23	2:AB:201:ILE:HD12	2.00	0.44
2:AB:21:ARG:CD	2:AB:21:ARG:H	2.30	0.44
4:AD:105:VAL:HG13	4:AD:110:PHE:HB2	1.99	0.44
4:AD:177:ASP:HB3	4:AD:182:LYS:HG2	2.00	0.44
8:AH:6:ILE:HD11	8:AH:31:PHE:HD2	1.82	0.44
8:AH:86:ILE:HG13	8:AH:133:LEU:HD22	2.00	0.44
3:AC:12:LEU:O	14:AN:57:ARG:NH2	2.50	0.44
50:B3:31:LEU:HD23	50:B3:31:LEU:HA	1.69	0.44
26:BA:1001:A:H2'	26:BA:1002:G:O4'	2.18	0.44
26:BA:848:G:O6	26:BA:928:G:H2'	2.17	0.44
28:BD:232:PRO:HB3	28:BD:244:ARG:CZ	2.48	0.44
26:BA:2052:G:H4'	29:BE:143:ASN:O	2.17	0.44
33:BI:27:ARG:HD2	48:B1:71:TYR:CZ	2.51	0.44
26:BA:2849:U:OP2	40:BT:95:ARG:NH1	2.50	0.44
1:CA:1226:C:H4'	19:CS:80:TYR:OH	2.17	0.44
1:CA:1441:G:O5'	1:CA:1441:G:H8	2.00	0.44
1:CA:537:G:H2'	1:CA:538:G:C8	2.53	0.44
1:CA:938:A:C6	1:CA:939:G:C5	3.06	0.44
2:CB:74:LYS:HB3	2:CB:169:LYS:HE2	1.98	0.44
3:CC:33:LEU:HD12	3:CC:36:ASP:HB3	1.99	0.44
7:CG:51:GLN:O	7:CG:55:GLY:HA2	2.16	0.44
26:DA:1153:C:H5''	41:DU:62:ILE:HD13	2.00	0.44
26:DA:1463:C:H2'	26:DA:1464:C:C6	2.53	0.44
26:DA:1472:A:N6	26:DA:1519:G:H1'	2.32	0.44
26:DA:1894:C:H2'	26:DA:1895:C:C6	2.53	0.44
26:DA:2156:G:H8	26:DA:2156:G:O5'	1.99	0.44
26:DA:250:G:C6	26:DA:251:A:C6	3.05	0.44
26:DA:2892:A:N6	26:DA:2893:G:O6	2.51	0.44
26:DA:900:A:HO2'	26:DA:901:A:P	2.40	0.44
28:DD:79:VAL:HG21	28:DD:111:LEU:HD11	1.99	0.44
35:DO:103:ALA:HB1	35:DO:105:GLU:OE1	2.16	0.44
37:DQ:35:VAL:HG12	37:DQ:130:LYS:O	2.18	0.44
1:AA:1513:A:H2'	1:AA:1514:C:C6	2.53	0.44
1:AA:636:U:H2'	1:AA:637:G:H8	1.83	0.44
1:AA:92:C:H2'	1:AA:93:G:H8	1.80	0.44
6:AF:33:TYR:CD2	6:AF:75:LEU:HD23	2.53	0.44
9:AI:4:TYR:CE1	9:AI:88:TYR:HD1	2.36	0.44
26:BA:1178:C:H2'	26:BA:1179:C:H6	1.82	0.44
26:BA:2115:G:C2	26:BA:2117:A:N7	2.86	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:BA:2093:G:C6	26:BA:2225:A:C8	3.06	0.44
26:BA:2303:G:O2'	31:BG:132:ASN:ND2	2.44	0.44
23:AW:56:C:OP1	26:BA:897:C:H5'	2.18	0.44
26:BA:910:A:N1	26:BA:2277:G:H1'	2.32	0.44
26:BA:1153:C:OP1	41:BU:92:ARG:NH1	2.50	0.44
45:BY:102:CYS:SG	45:BY:103:GLY:N	2.91	0.44
1:CA:1493:A:H5''	1:CA:1494:G:OP2	2.18	0.44
1:CA:1508:G:H2'	1:CA:1509:C:C6	2.52	0.44
1:CA:37:U:O2'	1:CA:500:G:H4'	2.17	0.44
1:CA:826:C:H2'	1:CA:827:U:C6	2.53	0.44
4:CD:161:ASN:HD22	4:CD:161:ASN:N	2.16	0.44
8:CH:51:VAL:HG11	8:CH:60:ARG:NH1	2.33	0.44
12:CL:24:VAL:O	12:CL:24:VAL:HG12	2.17	0.44
16:CP:9:PHE:CE1	16:CP:18:ARG:HD2	2.52	0.44
23:CW:39:PSU:H2'	23:CW:40:C:H6	1.83	0.44
26:DA:2336:A:H61	47:D0:43:THR:CG2	2.29	0.44
26:DA:2880:C:O3'	38:DR:90:ARG:NH1	2.51	0.44
26:DA:556:G:H2'	26:DA:557:U:C6	2.52	0.44
27:DB:3:C:H2'	27:DB:4:C:H6	1.83	0.44
27:DB:46:A:H2'	27:DB:47:C:C6	2.52	0.44
29:DE:77:ILE:CD1	29:DE:195:LEU:HD13	2.46	0.44
31:DG:128:ARG:HE	31:DG:128:ARG:HB2	1.67	0.44
35:DO:77:ILE:HB	40:DT:74:ARG:HD3	2.00	0.44
1:AA:346:G:N3	1:AA:347:G:H1'	2.33	0.44
1:AA:434:U:H2'	1:AA:435:C:C6	2.52	0.44
1:AA:630:G:H2'	1:AA:631:G:H8	1.83	0.44
1:AA:674:G:H2'	1:AA:675:A:H8	1.83	0.44
1:AA:952:U:H2'	1:AA:953:G:H8	1.80	0.44
3:AC:140:ARG:HB2	3:AC:140:ARG:HE	1.51	0.44
7:AG:46:ALA:O	7:AG:50:ILE:HG23	2.18	0.44
10:AJ:38:ILE:HD11	10:AJ:71:LEU:HB3	1.99	0.44
15:AO:53:HIS:O	15:AO:56:LEU:HB3	2.18	0.44
1:AA:1326:C:OP1	21:AU:12:LYS:NZ	2.50	0.44
23:AW:22:G:H2'	23:AW:23:A:C8	2.53	0.44
49:B2:30:ARG:O	49:B2:34:GLU:HG3	2.17	0.44
54:B7:11:LYS:HE3	54:B7:15:THR:OG1	2.18	0.44
26:BA:2319:G:N2	39:BS:3:ARG:HA	2.33	0.44
26:BA:251:A:C5	26:BA:252:G:H1'	2.52	0.44
26:BA:530:G:N3	26:BA:530:G:O4'	2.50	0.44
32:BH:125:VAL:HG12	32:BH:127:GLU:O	2.18	0.44
32:BH:164:TYR:HB2	32:BH:167:GLU:HB2	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:BH:24:VAL:HG22	32:BH:35:VAL:HB	1.99	0.44
33:BI:79:ILE:HB	33:BI:144:VAL:HG12	2.00	0.44
39:BS:58:LEU:HD23	39:BS:58:LEU:HA	1.70	0.44
46:BZ:155:LEU:HD12	46:BZ:156:LYS:H	1.81	0.44
1:CA:1134:G:C2'	1:CA:1135:U:H5'	2.48	0.44
1:CA:1170:A:H2'	1:CA:1171:G:O4'	2.17	0.44
1:CA:576:G:O6	1:CA:880:C:O2'	2.30	0.44
1:CA:696:A:H8	1:CA:696:A:O5'	2.01	0.44
1:CA:79:G:N2	1:CA:80:G:C4	2.86	0.44
2:CB:224:GLN:HA	2:CB:228:GLY:O	2.18	0.44
2:CB:74:LYS:HG3	2:CB:77:ALA:HB3	1.99	0.44
6:CF:69:GLU:H	6:CF:69:GLU:CD	2.17	0.44
8:CH:68:ARG:NH1	8:CH:74:PRO:HB3	2.32	0.44
1:CA:684:A:O2'	11:CK:39:PRO:O	2.34	0.44
13:CM:40:ASN:ND2	13:CM:41:PRO:HD2	2.33	0.44
23:CW:14:A:N6	23:CW:21:A:H2	2.15	0.44
23:CW:38:A:H2'	23:CW:39:PSU:O4'	2.18	0.44
23:CW:76:31M:H4'	26:DA:2506:U:O2'	2.17	0.44
50:D3:18:ASP:N	50:D3:18:ASP:OD1	2.44	0.44
26:DA:1016:G:H2'	26:DA:1017:G:O4'	2.18	0.44
26:DA:2144:U:O3'	26:DA:2145:C:H2'	2.17	0.44
26:DA:2242:G:H2'	26:DA:2243:U:O4'	2.18	0.44
26:DA:582:G:H2'	26:DA:583:G:C8	2.53	0.44
26:DA:656:G:H2'	26:DA:657:U:O4'	2.18	0.44
26:DA:828:U:H4'	26:DA:831:G:N1	2.32	0.44
28:DD:108:PRO:HG2	28:DD:111:LEU:HB2	1.99	0.44
28:DD:164:GLN:NE2	28:DD:166:GLN:OE1	2.46	0.44
30:DF:39:TRP:HB3	30:DF:101:LEU:HD22	2.00	0.44
1:AA:1118:C:H2'	1:AA:1119:C:H6	1.83	0.44
1:AA:1118:C:H1'	1:AA:1179:A:C4	2.53	0.44
1:AA:184:G:H2'	1:AA:185:A:H8	1.81	0.44
1:AA:299:G:H2'	1:AA:300:A:C8	2.53	0.44
1:AA:406:G:N3	4:AD:119:GLN:NE2	2.60	0.44
1:AA:68:G:C2	1:AA:69:G:H1'	2.53	0.44
1:AA:731:G:H5'	1:AA:766:A:H4'	2.00	0.44
1:AA:1250:A:H4'	9:AI:68:GLY:N	2.33	0.44
15:AO:54:ARG:O	15:AO:58:MET:HG3	2.18	0.44
16:AP:53:VAL:HG13	16:AP:79:VAL:HG22	1.99	0.44
20:AT:72:LEU:HD23	20:AT:72:LEU:HA	1.84	0.44
21:AU:15:ARG:HH11	21:AU:15:ARG:HB2	1.82	0.44
23:AW:51:U:H2'	23:AW:52:G:C8	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:BA:2030:A:H4'	26:BA:2031:A:C8	2.53	0.44
26:BA:2059:A:OP2	61:BA:4337:HOH:O	2.21	0.44
26:BA:875:G:H2'	26:BA:876:C:O4'	2.17	0.44
29:BE:73:GLU:HG3	29:BE:73:GLU:H	1.63	0.44
1:CA:1040:U:C4	1:CA:1041:A:C8	3.05	0.44
1:CA:1245:A:H2'	1:CA:1246:C:O4'	2.17	0.44
4:CD:47:ARG:NH1	4:CD:49:ARG:HH21	2.16	0.44
9:CI:4:TYR:CZ	9:CI:88:TYR:HD2	2.36	0.44
14:CN:26:ARG:HD2	14:CN:43:CYS:HB3	2.00	0.44
19:CS:19:VAL:O	19:CS:23:ASN:ND2	2.50	0.44
25:CY:65:G:H2'	25:CY:66:U:C6	2.53	0.44
50:D3:23:LEU:O	50:D3:27:GLY:N	2.50	0.44
51:D4:40:HIS:ND1	51:D4:43:TYR:HD2	2.15	0.44
26:DA:330:A:H2	26:DA:1210:A:H2'	1.83	0.44
26:DA:1288:U:C2	26:DA:1327:C:O2	2.71	0.44
26:DA:2680:C:OP2	29:DE:111:ARG:NH2	2.50	0.44
26:DA:888:C:H5''	26:DA:889:C:OP2	2.18	0.44
28:DD:13:ARG:HD2	28:DD:13:ARG:HA	1.71	0.44
28:DD:237:GLU:OE2	61:DD:401:HOH:O	2.21	0.44
30:DF:11:VAL:HB	30:DF:18:ARG:HB3	1.99	0.44
34:DN:15:LEU:HD12	34:DN:137:LYS:HG2	1.99	0.44
1:AA:958:A:C6	1:AA:959:A:N1	2.86	0.44
8:AH:96:GLY:N	8:AH:99:GLU:OE2	2.28	0.44
11:AK:33:THR:HA	11:AK:39:PRO:HA	2.00	0.44
16:AP:20:VAL:HG23	16:AP:35:LYS:HA	2.00	0.44
26:BA:1636:C:H2'	26:BA:1637:A:C8	2.53	0.44
26:BA:2364:C:H2'	26:BA:2365:G:O4'	2.18	0.44
26:BA:574:C:N3	29:BE:145:LYS:NZ	2.63	0.44
26:BA:876:C:H2'	26:BA:877:U:O4'	2.18	0.44
28:BD:83:GLU:OE1	28:BD:104:TYR:OH	2.28	0.44
29:BE:143:ASN:HD22	29:BE:147:PRO:CD	2.31	0.44
32:BH:3:ARG:HH12	32:BH:65:HIS:HB3	1.83	0.44
34:BN:67:LEU:O	34:BN:88:GLU:HG3	2.17	0.44
35:BO:2:ILE:HD12	35:BO:6:THR:HG21	1.99	0.44
44:BX:88:LYS:NZ	44:BX:90:GLU:OE1	2.33	0.44
1:CA:292:G:N7	1:CA:293:G:H1'	2.33	0.44
1:CA:35:G:H2'	1:CA:36:C:C6	2.53	0.44
2:CB:192:SER:O	2:CB:194:PRO:HD3	2.17	0.44
6:CF:3:ARG:HB3	6:CF:93:SER:HB2	2.00	0.44
8:CH:39:LEU:HA	8:CH:39:LEU:HD13	1.74	0.44
12:CL:69:TYR:HE2	12:CL:71:PRO:HA	1.83	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:CY:30:G:C2	25:CY:31:A:C8	3.06	0.44
26:DA:1032:A:H4'	56:D9:16:VAL:HG11	2.00	0.44
26:DA:1301:A:H2	26:DA:1626:G:N3	2.14	0.44
26:DA:2070:G:H2'	26:DA:2071:A:H8	1.83	0.44
26:DA:2615:U:OP1	61:DA:4004:HOH:O	2.21	0.44
26:DA:265:A:C8	26:DA:266:G:H1'	2.53	0.44
26:DA:26:G:C6	26:DA:27:G:N1	2.86	0.44
26:DA:328:U:H4'	45:DY:68:HIS:CG	2.52	0.44
26:DA:911:A:H2'	37:DQ:9:TYR:OH	2.18	0.44
26:DA:927:G:H2'	26:DA:928:G:O4'	2.17	0.44
31:DG:111:LEU:HB3	31:DG:117:PHE:CE2	2.53	0.44
39:DS:35:ILE:HD11	39:DS:101:LEU:HD12	1.99	0.44
1:AA:1001(A):G:C6	1:AA:1002:G:C5	3.06	0.43
1:AA:1118:C:H2'	1:AA:1119:C:C6	2.53	0.43
1:AA:401:C:H2'	1:AA:402:G:C8	2.53	0.43
1:AA:858:G:O6	1:AA:869:G:H3'	2.18	0.43
2:AB:16:HIS:HD2	2:AB:17:PHE:H	1.56	0.43
4:AD:11:LEU:HD23	4:AD:66:ARG:HB3	1.99	0.43
9:AI:22:GLY:N	9:AI:58:HIS:O	2.39	0.43
1:AA:276:G:O3'	17:AQ:68:ARG:NH1	2.51	0.43
26:BA:1440:G:H2'	26:BA:1441:G:O4'	2.18	0.43
26:BA:1826:G:H2'	26:BA:1827:C:O4'	2.17	0.43
26:BA:2685:G:H5'	35:BO:68:GLU:OE1	2.18	0.43
26:BA:970:C:H2'	26:BA:971:C:C6	2.53	0.43
30:BF:140:LEU:HD21	30:BF:170:LEU:HD11	2.00	0.43
39:BS:3:ARG:HE	39:BS:4:LEU:H	1.66	0.43
46:BZ:111:VAL:CG2	46:BZ:117:LEU:HB2	2.48	0.43
46:BZ:7:ALA:O	46:BZ:62:PRO:HD3	2.18	0.43
1:CA:1095:U:H2'	1:CA:1096:C:O4'	2.18	0.43
1:CA:1118:C:N1	1:CA:1119:C:H5	2.16	0.43
1:CA:1136:U:H5''	1:CA:1137:C:C5	2.53	0.43
1:CA:1423:G:H2'	1:CA:1424:C:C6	2.53	0.43
2:CB:7:VAL:HG12	2:CB:8:LYS:HG2	2.00	0.43
3:CC:6:HIS:HA	3:CC:7:PRO:HD3	1.71	0.43
7:CG:18:TYR:HB3	7:CG:59:LEU:HD13	2.00	0.43
9:CI:26:VAL:HG13	9:CI:61:ALA:HB3	1.99	0.43
13:CM:72:ALA:O	13:CM:76:ALA:N	2.42	0.43
25:CY:37:MIA:H3'	25:CY:38:A:H8	1.82	0.43
26:DA:2742:C:OP1	56:D9:35:ARG:HD3	2.18	0.43
26:DA:2164:C:H5	26:DA:2165:G:N3	2.16	0.43
26:DA:2347:C:H2'	26:DA:2348:U:C6	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:DA:2732:G:OP1	29:DE:203:LYS:NZ	2.43	0.43
26:DA:668:G:H5'	26:DA:669:G:OP2	2.18	0.43
33:DI:88:ILE:HD11	33:DI:144:VAL:HG11	2.00	0.43
33:DI:57:ARG:O	33:DI:61:ARG:HG2	2.18	0.43
34:DN:4:TYR:CD2	41:DU:100:VAL:HG11	2.52	0.43
37:DQ:27:VAL:O	37:DQ:29:PHE:N	2.51	0.43
41:DU:76:TYR:HH	41:DU:92:ARG:HH11	1.63	0.43
45:DY:10:GLY:O	45:DY:26:LYS:HD3	2.18	0.43
37:DQ:139:GLU:HG2	46:DZ:122:ARG:HG3	2.00	0.43
37:DQ:29:PHE:O	46:DZ:122:ARG:NH2	2.51	0.43
1:AA:1305:G:H22	1:AA:1331:G:H1'	1.82	0.43
1:AA:339:C:H2'	1:AA:340:U:C6	2.54	0.43
1:AA:646:U:H2'	1:AA:647:C:C6	2.53	0.43
4:AD:112:VAL:HG23	4:AD:116:GLN:OE1	2.18	0.43
4:AD:188:LEU:HA	4:AD:189:PRO:HD3	1.80	0.43
4:AD:65:ARG:HG2	4:AD:75:PHE:CD2	2.53	0.43
9:AI:23:ASN:ND2	9:AI:25:LYS:HG2	2.33	0.43
25:AY:57:G:C2	25:AY:58:A:H5'	2.53	0.43
26:BA:127:A:H5''	26:BA:128:C:C6	2.53	0.43
26:BA:1358:G:N2	26:BA:1372:U:C5	2.86	0.43
26:BA:2320:A:H2'	26:BA:2320:A:N3	2.34	0.43
26:BA:2447:G:N2	26:BA:2450:A:OP2	2.51	0.43
26:BA:363(A):A:H2'	26:BA:363(B):G:C8	2.53	0.43
26:BA:94:C:H2'	26:BA:94(A):G:O4'	2.19	0.43
35:BO:78:ARG:NH2	40:BT:73:GLU:OE2	2.49	0.43
41:BU:117:GLN:H	41:BU:117:GLN:HG2	1.42	0.43
46:BZ:150:LEU:HA	46:BZ:150:LEU:HD12	1.78	0.43
1:CA:1115:C:H2'	1:CA:1116:C:C6	2.53	0.43
1:CA:1152:A:C6	1:CA:1153:C:C4	3.06	0.43
1:CA:766:A:OP2	61:CA:4021:HOH:O	2.21	0.43
2:CB:20:GLU:HG3	2:CB:191:ASP:HB3	1.99	0.43
3:CC:18:TRP:CE3	3:CC:18:TRP:N	2.85	0.43
3:CC:47:LEU:HD12	3:CC:68:VAL:HG11	2.00	0.43
7:CG:26:PHE:CD2	7:CG:62:PHE:HE1	2.36	0.43
9:CI:108:VAL:HG12	9:CI:109:VAL:H	1.84	0.43
10:CJ:16:LEU:HD23	10:CJ:94:VAL:HG22	1.99	0.43
13:CM:50:GLU:O	13:CM:54:VAL:HG22	2.18	0.43
19:CS:80:TYR:CZ	19:CS:82:GLY:HA2	2.53	0.43
51:D4:26:SER:OG	51:D4:27:THR:N	2.51	0.43
26:DA:2006:C:O5'	26:DA:2006:C:H6	2.00	0.43
26:DA:2172:U:O2'	26:DA:2173:A:OP1	2.30	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:DA:2626:C:H2'	26:DA:2627:G:O4'	2.18	0.43
26:DA:288:C:H2'	26:DA:289:A:H8	1.82	0.43
26:DA:601:C:O2	26:DA:605:C:H4'	2.18	0.43
26:DA:817:C:OP2	61:DA:4676:HOH:O	2.21	0.43
26:DA:903:C:H2'	26:DA:904:C:H6	1.81	0.43
26:DA:910:A:N1	26:DA:2277:G:H1'	2.32	0.43
37:DQ:68:ILE:HD13	37:DQ:103:MET:HG2	2.00	0.43
38:DR:21:TYR:CZ	38:DR:43:GLU:HG2	2.52	0.43
46:DZ:154:ASP:N	46:DZ:154:ASP:OD1	2.39	0.43
1:AA:1240:U:OP2	7:AG:116:ALA:N	2.44	0.43
1:AA:335:C:H2'	1:AA:336:C:C6	2.54	0.43
3:AC:52:LEU:HD11	3:AC:55:VAL:CG2	2.48	0.43
5:AE:41:VAL:HG23	5:AE:67:VAL:HG12	2.00	0.43
9:AI:61:ALA:HB1	9:AI:63:ILE:HD11	2.01	0.43
14:AN:24:CYS:HB2	14:AN:33:VAL:HG12	2.01	0.43
20:AT:92:LEU:HA	20:AT:92:LEU:HD23	1.84	0.43
26:BA:1594:G:H2'	26:BA:1595:G:O4'	2.18	0.43
26:BA:1970:A:H4'	26:BA:1971:A:OP1	2.18	0.43
26:BA:2406:U:H2'	26:BA:2406:U:OP2	2.19	0.43
30:BF:33:LEU:HD13	30:BF:112:MET:HE2	2.00	0.43
43:BW:14:PRO:HG2	43:BW:78:GLU:CG	2.45	0.43
1:CA:1016:A:H2'	1:CA:1017:G:O4'	2.18	0.43
1:CA:1002:G:N2	1:CA:1039:C:C4	2.86	0.43
1:CA:1080:A:H5''	1:CA:1081:G:OP2	2.19	0.43
1:CA:757:U:O2'	1:CA:879:C:O2	2.31	0.43
4:CD:111:ALA:HB1	4:CD:116:GLN:HB3	2.00	0.43
7:CG:27:ILE:HD12	7:CG:40:ALA:HA	2.00	0.43
16:CP:3:LYS:O	16:CP:21:VAL:HA	2.18	0.43
16:CP:60:LEU:HD13	16:CP:60:LEU:HA	1.84	0.43
6:CF:94:GLN:NE2	18:CR:72:ARG:HH12	2.16	0.43
20:CT:90:GLN:O	20:CT:93:GLU:HB3	2.18	0.43
51:D4:56:VAL:HG13	51:D4:57:GLU:H	1.83	0.43
26:DA:2674:G:H2'	26:DA:2675:A:C8	2.53	0.43
26:DA:324:A:H2'	26:DA:325:G:O4'	2.19	0.43
26:DA:623:G:H2'	26:DA:624:C:C6	2.54	0.43
35:DO:25:LEU:HD12	35:DO:38:VAL:HG12	1.99	0.43
1:AA:374:A:C6	1:AA:375:U:C4	3.05	0.43
1:AA:814:A:H2'	1:AA:816:A:H5''	1.99	0.43
2:AB:213:LEU:HD22	2:AB:214:ILE:HD13	2.00	0.43
3:AC:6:HIS:HA	3:AC:7:PRO:HD3	1.83	0.43
7:AG:65:ALA:O	7:AG:69:VAL:HG23	2.17	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1302:U:H5	13:AM:17:VAL:HG21	1.83	0.43
13:AM:70:LEU:O	13:AM:74:VAL:HG23	2.19	0.43
21:AU:5:ASP:O	21:AU:11:GLY:HA3	2.18	0.43
26:BA:2168:G:H5'	26:BA:2169:A:H5''	2.00	0.43
26:BA:2377:A:H2'	26:BA:2378:A:C8	2.53	0.43
23:AW:76:31M:HE1	26:BA:2451:A:C6	2.53	0.43
26:BA:2543:G:H2'	26:BA:2544:G:C8	2.53	0.43
26:BA:590:A:H2'	26:BA:591:C:O4'	2.18	0.43
26:BA:886:C:H4'	26:BA:886:C:OP1	2.17	0.43
30:BF:64:ILE:HD12	30:BF:65:TRP:CZ3	2.54	0.43
44:BX:50:LYS:N	44:BX:87:GLN:OE1	2.48	0.43
1:CA:1366:C:H2'	1:CA:1367:C:C6	2.53	0.43
1:CA:1399:C:C2	1:CA:1502:A:N6	2.87	0.43
3:CC:34:LEU:HG	3:CC:38:ARG:NH1	2.31	0.43
14:CN:37:PHE:HZ	14:CN:56:VAL:HG21	1.83	0.43
51:D4:68:ARG:O	51:D4:69:LYS:HB3	2.18	0.43
26:DA:813:U:HO2'	26:DA:1225:G:HO2'	1.67	0.43
26:DA:1881:C:H2'	26:DA:1882:C:O4'	2.19	0.43
26:DA:2410:G:H2'	26:DA:2411:A:O4'	2.19	0.43
26:DA:2820:A:C5	38:DR:4:LEU:HD11	2.53	0.43
26:DA:540:C:H2'	26:DA:541:C:C6	2.53	0.43
26:DA:627:A:H4'	26:DA:628:G:H5'	2.00	0.43
34:DN:57:ALA:HB1	34:DN:96:GLU:HA	2.01	0.43
30:DF:33:LEU:HB3	36:DP:6:LEU:HD21	2.01	0.43
45:DY:89:PHE:CE2	45:DY:95:LYS:HB2	2.53	0.43
1:AA:262:A:H4'	20:AT:75:ASN:HB2	2.00	0.43
5:AE:105:VAL:O	5:AE:109:ILE:HD12	2.19	0.43
6:AF:10:LEU:HB2	6:AF:59:TYR:HB3	2.01	0.43
10:AJ:45:ARG:HG2	10:AJ:47:PHE:CZ	2.53	0.43
1:AA:1456:G:O3'	20:AT:39:LYS:NZ	2.52	0.43
23:AW:56:C:H5'	26:BA:896:A:H1'	2.00	0.43
26:BA:1171:G:H3'	26:BA:1173:G:H5'	2.01	0.43
26:BA:1177:A:H2'	26:BA:1177:A:N3	2.33	0.43
26:BA:1431:U:H2'	26:BA:1432:C:C6	2.54	0.43
26:BA:1918:A:O2'	26:BA:1920:C:N4	2.51	0.43
31:BG:122:PRO:HD3	31:BG:181:ARG:HG2	2.00	0.43
32:BH:33:LEU:HD21	32:BH:136:ILE:HG13	2.00	0.43
33:BI:81:VAL:O	33:BI:146:ALA:HA	2.19	0.43
1:CA:1279:A:O2'	1:CA:1282:C:N4	2.51	0.43
1:CA:722:A:N6	1:CA:724:G:C2	2.87	0.43
2:CB:35:GLU:HB2	2:CB:40:HIS:HD2	1.82	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:CL:83:VAL:HG23	12:CL:107:ALA:HB2	2.01	0.43
16:CP:55:ARG:HD2	16:CP:55:ARG:HA	1.88	0.43
25:CY:4:C:H2'	25:CY:5:G:H5'	2.00	0.43
26:DA:1817:G:OP1	28:DD:88:ARG:NH2	2.48	0.43
26:DA:2134:A:C2	26:DA:2159:G:H4'	2.53	0.43
26:DA:2134:A:H3'	26:DA:2135:A:C8	2.53	0.43
26:DA:2516:G:C6	26:DA:2517:C:N4	2.86	0.43
27:DB:28:C:OP2	39:DS:33:LYS:NZ	2.32	0.43
28:DD:182:LEU:HB2	28:DD:272:ALA:HB3	2.01	0.43
31:DG:45:GLU:HG2	31:DG:45:GLU:H	1.43	0.43
32:DH:98:LEU:HD12	32:DH:102:ALA:O	2.18	0.43
41:DU:79:PHE:CZ	41:DU:83:LEU:HD21	2.54	0.43
45:DY:43:ASN:OD1	45:DY:65:ALA:HB3	2.19	0.43
1:AA:1061:G:H1'	10:AJ:56:HIS:CE1	2.53	0.43
13:AM:120:LYS:HE3	23:AW:40:C:O2'	2.19	0.43
19:AS:52:TYR:HA	19:AS:56:GLN:O	2.18	0.43
25:AY:33:U:H2'	25:AY:34:G:H5''	2.00	0.43
51:B4:59:PHE:C	51:B4:61:ARG:H	2.21	0.43
26:BA:1258:C:H2'	26:BA:1259:G:O4'	2.19	0.43
26:BA:1720:U:H2'	26:BA:1721:G:O4'	2.18	0.43
25:AY:71:G:H4'	26:BA:1851:U:H4'	2.00	0.43
26:BA:2183:C:O2'	26:BA:2184:G:OP1	2.35	0.43
26:BA:2591:C:H2'	26:BA:2592:G:C8	2.54	0.43
26:BA:2791:C:H5'	26:BA:2893:G:N2	2.34	0.43
28:BD:137:PRO:O	28:BD:140:THR:HG23	2.18	0.43
31:BG:43:LEU:HB3	31:BG:44:GLY:H	1.55	0.43
34:BN:67:LEU:HA	34:BN:67:LEU:HD12	1.80	0.43
40:BT:118:ARG:HD2	40:BT:118:ARG:HA	1.61	0.43
1:CA:1009:G:N2	1:CA:1010:G:H1'	2.33	0.43
1:CA:1030(A):G:C2	1:CA:1030(C):G:H8	2.36	0.43
1:CA:693:G:H2'	1:CA:694:A:C8	2.53	0.43
9:CI:43:ALA:HB2	9:CI:74:ILE:CD1	2.49	0.43
14:CN:47:LEU:O	14:CN:51:GLY:N	2.51	0.43
1:CA:750:G:N2	15:CO:23:GLY:O	2.48	0.43
24:CX:15:G:H2'	24:CX:59:A:N1	2.34	0.43
23:CW:76:31M:HAM	24:CX:76:A:O3'	2.19	0.43
26:DA:2695:C:H2'	26:DA:2696:U:H6	1.84	0.43
26:DA:69:C:N4	61:DA:4335:HOH:O	2.52	0.43
26:DA:782:A:H5'	26:DA:783:A:N7	2.34	0.43
28:DD:142:VAL:HG13	28:DD:191:ALA:HB1	2.00	0.43
46:DZ:153:SER:HB3	46:DZ:167:PRO:HA	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1198:G:H2'	1:AA:1199:U:C6	2.54	0.43
1:AA:90:U:O2'	1:AA:91:C:H5'	2.19	0.43
2:AB:200:ILE:HD13	2:AB:200:ILE:H	1.84	0.43
2:AB:36:ARG:C	2:AB:38:GLY:H	2.21	0.43
7:AG:46:ALA:HA	7:AG:49:ILE:HD12	2.01	0.43
8:AH:41:ARG:NH2	8:AH:123:GLU:OE2	2.51	0.43
19:AS:27:GLU:HB3	19:AS:28:LYS:HB3	2.01	0.43
48:B1:50:ARG:HG2	48:B1:59:THR:HB	2.00	0.43
53:B6:10:LEU:HG	53:B6:54:ILE:HG13	2.00	0.43
26:BA:1045:A:H1'	26:BA:1047:G:C2	2.53	0.43
26:BA:2292:C:H2'	26:BA:2293:C:H6	1.83	0.43
26:BA:2706:G:N7	61:BA:4733:HOH:O	2.37	0.43
33:BI:50:ARG:HA	33:BI:53:ALA:HB3	2.01	0.43
42:BV:34:GLU:HB3	42:BV:56:SER:HB2	2.00	0.43
43:BW:19:LEU:HB3	52:B5:25:LEU:HD11	2.01	0.43
1:CA:1011:G:C2	1:CA:1012:U:H1'	2.54	0.43
1:CA:1014:A:H2'	1:CA:1015:A:C8	2.54	0.43
1:CA:1110:A:OP2	61:CA:4091:HOH:O	2.21	0.43
1:CA:1442(A):G:O2'	40:DT:118:ARG:HG2	2.18	0.43
1:CA:503:C:OP2	12:CL:116:SER:HB3	2.19	0.43
13:CM:50:GLU:HA	13:CM:53:VAL:HB	2.01	0.43
19:CS:28:LYS:HB2	19:CS:29:ARG:CB	2.48	0.43
25:CY:8:4SU:C2	25:CY:14:A:H62	2.30	0.43
26:DA:1503:U:H2'	26:DA:1504:C:C6	2.54	0.43
26:DA:2805:G:C6	26:DA:2807:G:C6	3.07	0.43
26:DA:2870:C:H2'	26:DA:2871:C:O4'	2.19	0.43
26:DA:991:C:OP2	26:DA:1186:G:H5'	2.18	0.43
30:DF:18:ARG:HG2	30:DF:19:GLU:H	1.84	0.43
32:DH:59:ARG:O	32:DH:63:SER:OG	2.36	0.43
33:DI:73:GLU:HG3	33:DI:139:GLN:O	2.18	0.43
1:AA:1151:A:O4'	10:AJ:39:PRO:HB2	2.19	0.43
1:AA:452:A:HO2'	1:AA:453:A:H8	1.65	0.43
2:AB:54:THR:HG21	2:AB:201:ILE:HD11	1.99	0.43
4:AD:64:LEU:HB2	4:AD:198:VAL:HG21	2.00	0.43
5:AE:148:VAL:O	5:AE:152:ARG:HG3	2.18	0.43
12:AL:24:VAL:O	12:AL:24:VAL:HG12	2.18	0.43
17:AQ:53:LEU:HD23	17:AQ:82:MET:HE1	2.01	0.43
49:B2:16:LEU:HB3	49:B2:20:GLU:HB2	1.99	0.43
26:BA:11:G:C2'	26:BA:12:U:H5''	2.45	0.43
26:BA:2233:U:H2'	26:BA:2234:G:C8	2.54	0.43
26:BA:197:A:N6	26:BA:2430:A:O2'	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:BA:2790:A:N3	26:BA:2790:A:H2'	2.34	0.43
15:AO:56:LEU:HD21	26:BA:715:G:C2	2.54	0.43
26:BA:848:G:N9	26:BA:933:A:H8	2.17	0.43
27:BB:48:A:H4'	39:BS:95:HIS:HD2	1.83	0.43
38:BR:53:HIS:O	38:BR:56:LYS:HB2	2.18	0.43
1:CA:1320:C:C1'	19:CS:73:GLU:HG3	2.49	0.43
1:CA:165:C:H2'	1:CA:166:G:C8	2.54	0.43
1:CA:302:G:N3	1:CA:556:C:H4'	2.33	0.43
1:CA:664:G:N2	1:CA:741:G:H1	2.04	0.43
2:CB:84:GLU:OE1	2:CB:216:SER:HA	2.18	0.43
4:CD:38:TYR:CZ	4:CD:45:GLN:HG2	2.54	0.43
7:CG:78:ARG:CZ	7:CG:79:ARG:HH12	2.32	0.43
20:CT:86:ARG:O	20:CT:90:GLN:HB2	2.19	0.43
23:CW:61:C:O2'	23:CW:62:C:H6	2.02	0.43
49:D2:53:LEU:HA	49:D2:53:LEU:HD23	1.89	0.43
26:DA:1487:G:H2'	26:DA:1488:G:O4'	2.18	0.43
26:DA:1656:C:H2'	26:DA:1657:C:H6	1.84	0.43
26:DA:2494:G:C4	26:DA:2495:G:C8	3.07	0.43
26:DA:2602:A:H4'	26:DA:2603:G:C5'	2.48	0.43
26:DA:265:A:H1'	26:DA:266:G:O4'	2.19	0.43
26:DA:644:A:H5''	26:DA:645:C:OP1	2.19	0.43
26:DA:974:G:C4	26:DA:989:G:C2	3.07	0.43
31:DG:164:GLU:OE2	31:DG:164:GLU:N	2.51	0.43
31:DG:37:VAL:O	31:DG:94:LEU:N	2.50	0.43
36:DP:101:VAL:HA	36:DP:106:LEU:O	2.18	0.43
45:DY:13:VAL:HB	45:DY:72:VAL:HG13	2.00	0.43
1:AA:1529:G:H4'	1:AA:1530:G:OP2	2.19	0.43
1:AA:402:G:C6	1:AA:403:C:C4	3.07	0.43
2:AB:88:ALA:O	2:AB:226:ARG:NH1	2.51	0.43
3:AC:6:HIS:HD2	3:AC:8:ILE:N	2.11	0.43
25:AY:49:C:N4	25:AY:65:G:N1	2.28	0.43
26:BA:1175:U:O3'	26:BA:1176:G:H4'	2.17	0.43
26:BA:1372:U:H2'	26:BA:1373:A:O4'	2.18	0.43
26:BA:2176:A:H2'	26:BA:2177:C:C6	2.54	0.43
26:BA:2181:G:O2'	26:BA:2182:G:OP1	2.34	0.43
26:BA:2296:U:OP2	39:BS:9:ARG:NH2	2.52	0.43
26:BA:2653:U:H2'	26:BA:2654:A:C8	2.53	0.43
26:BA:288:C:H2'	26:BA:289:A:C8	2.53	0.43
28:BD:71:ASP:HB3	28:BD:103:ARG:HH22	1.83	0.43
32:BH:121:ILE:HG13	32:BH:144:VAL:HG21	2.01	0.43
35:BO:104:ARG:NH1	40:BT:34:VAL:HG21	2.34	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:BZ:144:LEU:HD21	46:BZ:148:ASP:O	2.19	0.43
1:CA:1133:G:H2'	1:CA:1134:G:H8	1.84	0.43
1:CA:1289:A:H2	1:CA:1372:U:O4'	2.01	0.43
1:CA:397:A:N3	1:CA:397:A:H3'	2.34	0.43
1:CA:607:A:C2	16:CP:31:LYS:HG3	2.54	0.43
15:CO:87:ILE:HG22	15:CO:88:ARG:N	2.33	0.43
24:CX:54:5MU:O5'	24:CX:54:5MU:H6	2.02	0.43
26:DA:1262:A:H2	52:D5:10:LYS:HD2	1.83	0.43
52:D5:48:GLU:O	52:D5:60:VAL:HG11	2.18	0.43
26:DA:208:C:H2'	26:DA:209:C:C6	2.54	0.43
26:DA:2228:G:C5	26:DA:2229:C:C4	3.07	0.43
26:DA:224:G:N7	26:DA:420:C:H4'	2.33	0.43
26:DA:2400:G:H2'	26:DA:2401:U:C6	2.50	0.43
26:DA:380:U:H2'	26:DA:381:G:H8	1.83	0.43
28:DD:68:LYS:O	28:DD:69:ARG:HB2	2.19	0.43
31:DG:43:LEU:C	31:DG:45:GLU:H	2.22	0.43
33:DI:14:ASP:OD1	33:DI:15:VAL:HG12	2.19	0.43
36:DP:39:LYS:CB	36:DP:45:LEU:HG	2.47	0.43
46:DZ:156:LYS:HE3	46:DZ:158:PRO:HD3	2.01	0.43
1:AA:1015:A:H2'	1:AA:1016:A:C8	2.54	0.43
1:AA:130:A:N3	1:AA:263:A:O2'	2.38	0.43
1:AA:1342:C:H4'	9:AI:125:TYR:HB3	2.01	0.43
1:AA:584:G:H2'	1:AA:585:G:C8	2.54	0.43
1:AA:943:U:H2'	1:AA:944:G:H5'	2.00	0.43
4:AD:63:LYS:HG3	4:AD:64:LEU:N	2.33	0.43
9:AI:4:TYR:CE2	9:AI:88:TYR:HA	2.54	0.43
15:AO:25:THR:HG21	15:AO:70:LEU:HB2	2.01	0.43
20:AT:90:GLN:O	20:AT:93:GLU:HB3	2.19	0.43
25:AY:6:G:H2'	25:AY:7:A:H5'	2.01	0.43
52:B5:59:GLU:HG2	52:B5:60:VAL:H	1.83	0.43
26:BA:1380:G:OP2	61:BA:5152:HOH:O	2.22	0.43
26:BA:1826:G:H4'	28:BD:242:ARG:CZ	2.49	0.43
26:BA:224:G:H2'	26:BA:225:A:O4'	2.18	0.43
26:BA:2646:C:H2'	26:BA:2647:U:O4'	2.18	0.43
26:BA:1664:A:H1'	26:BA:2685:G:O2'	2.19	0.43
26:BA:340:A:H2'	26:BA:341:G:O4'	2.19	0.43
26:BA:657:U:H2'	26:BA:658:C:C6	2.53	0.43
26:BA:881:G:N3	26:BA:881:G:H2'	2.34	0.43
26:BA:892:G:C5	26:BA:893:C:C4	3.07	0.43
26:BA:882:G:N2	26:BA:895:U:O2	2.52	0.43
27:BB:110:G:H2'	27:BB:111:G:H8	1.84	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:BD:206:LEU:HD22	28:BD:211:ARG:HG2	2.00	0.43
31:BG:77:ILE:HD12	31:BG:82:LEU:HD12	2.00	0.43
36:BP:96:THR:OG1	36:BP:99:LEU:HG	2.18	0.43
26:BA:2292:C:P	39:BS:17:ARG:HH12	2.41	0.43
41:BU:66:ASN:O	41:BU:70:ARG:HG3	2.19	0.43
44:BX:66:LEU:HD23	44:BX:66:LEU:HA	1.73	0.43
1:CA:1144:G:C6	1:CA:1145:C:N4	2.87	0.43
1:CA:337:C:H2'	1:CA:338:A:C8	2.53	0.43
1:CA:92:C:H2'	1:CA:93:G:O4'	2.19	0.43
7:CG:33:ASP:OD1	7:CG:33:ASP:N	2.51	0.43
10:CJ:90:LEU:HA	10:CJ:91:PRO:HD3	1.83	0.43
25:CY:34:G:C6	25:CY:35:A:C6	3.07	0.43
48:D1:50:ARG:HD2	48:D1:57:GLU:OE1	2.19	0.43
54:D7:26:GLY:O	54:D7:30:VAL:HG23	2.19	0.43
26:DA:2529:G:O6	56:D9:31:LYS:NZ	2.52	0.43
26:DA:140:G:H22	26:DA:1596:A:H4'	1.83	0.43
26:DA:1668:A:O2'	26:DA:1674:G:N7	2.43	0.43
26:DA:2028:U:H2'	26:DA:2029:G:O4'	2.19	0.43
26:DA:855:G:C6	26:DA:856:C:N4	2.86	0.43
26:DA:816:C:O2'	26:DA:932:G:O6	2.37	0.43
31:DG:44:GLY:N	31:DG:88:ILE:O	2.52	0.43
35:DO:104:ARG:NH2	35:DO:121:VAL:O	2.52	0.43
27:DB:114:C:H4'	39:DS:46:VAL:HG22	2.01	0.43
42:DV:55:ALA:HA	42:DV:100:ARG:O	2.19	0.43
1:AA:1353:G:H2'	1:AA:1354:C:H6	1.84	0.42
1:AA:1504:G:OP1	1:AA:1507:A:H4'	2.19	0.42
1:AA:839:U:H3'	1:AA:840:C:C5	2.53	0.42
1:AA:96:U:OP2	1:AA:96:U:H6	2.02	0.42
2:AB:28:PHE:CD1	2:AB:190:THR:HG22	2.54	0.42
2:AB:21:ARG:HB3	2:AB:39:ILE:HA	2.00	0.42
3:AC:104:GLN:HE21	3:AC:105:GLU:H	1.66	0.42
6:AF:45:LEU:HD12	6:AF:59:TYR:HD2	1.84	0.42
13:AM:19:LEU:HB3	13:AM:25:ILE:HG21	2.01	0.42
17:AQ:62:SER:OG	17:AQ:72:ARG:HD2	2.19	0.42
20:AT:13:LEU:HD12	20:AT:14:LYS:N	2.33	0.42
24:AX:19:G:H3'	24:AX:20:U:H6	1.84	0.42
26:BA:1796:U:H2'	26:BA:1797:C:H6	1.84	0.42
26:BA:2173:A:H2'	26:BA:2174:C:O4'	2.18	0.42
26:BA:2561:A:H2'	26:BA:2562:U:O4'	2.18	0.42
26:BA:614(C):A:C4	30:BF:180:GLY:HA2	2.54	0.42
28:BD:145:VAL:HG12	28:BD:146:GLU:O	2.18	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:BT:95:ARG:HH11	40:BT:95:ARG:CG	2.26	0.42
1:CA:1286:A:H3'	1:CA:1286:A:C8	2.54	0.42
1:CA:130:A:N3	1:CA:263:A:O2'	2.49	0.42
1:CA:532:A:N6	3:CC:156:ARG:HH22	2.16	0.42
1:CA:580:U:H5''	15:CO:58:MET:HG2	2.00	0.42
1:CA:608:A:H2'	1:CA:609:A:O4'	2.18	0.42
24:CX:21:A:N6	24:CX:46:G:H2'	2.34	0.42
24:CX:8:4SU:H5''	24:CX:49:G:H5'	2.01	0.42
26:DA:1161:C:H2'	26:DA:1162:G:C8	2.53	0.42
26:DA:140:G:H1'	26:DA:141:A:H2	1.84	0.42
26:DA:2137:C:O2'	26:DA:2138:C:H5'	2.19	0.42
26:DA:2865:U:C4	26:DA:2866:U:C4	3.07	0.42
26:DA:325:G:H2'	26:DA:326:G:O4'	2.20	0.42
26:DA:414:C:O2'	26:DA:415:A:H5'	2.19	0.42
26:DA:827:U:H4'	26:DA:828:U:C6	2.53	0.42
28:DD:121:PRO:HB3	28:DD:135:PHE:CE2	2.53	0.42
28:DD:36:PRO:HA	28:DD:61:LEU:HD13	2.01	0.42
30:DF:53:THR:HG23	30:DF:55:GLY:N	2.22	0.42
31:DG:125:PHE:CZ	31:DG:170:ARG:HA	2.54	0.42
33:DI:94:ALA:O	33:DI:98:ALA:N	2.44	0.42
37:DQ:31:ASP:HA	37:DQ:134:ARG:HH11	1.83	0.42
46:DZ:55:HIS:CE1	46:DZ:135:GLU:HG3	2.51	0.42
1:AA:126:G:H4'	1:AA:634:C:O2	2.19	0.42
1:AA:1457:G:OP1	20:AT:39:LYS:NZ	2.41	0.42
1:AA:346:G:H2'	1:AA:347:G:H4'	2.01	0.42
1:AA:711:G:OP1	6:AF:54:LYS:NZ	2.35	0.42
17:AQ:76:LEU:HD12	17:AQ:77:VAL:H	1.83	0.42
24:AX:7:G:O2'	24:AX:49:G:H5'	2.19	0.42
48:B1:8:SER:HB3	48:B1:66:HIS:CD2	2.55	0.42
51:B4:39:CYS:HA	51:B4:44:THR:HG21	2.01	0.42
26:BA:1713:U:H2'	26:BA:1714:G:H8	1.84	0.42
26:BA:1991:U:H2'	26:BA:1992:G:H5''	2.00	0.42
26:BA:38:A:H2'	26:BA:39:C:C6	2.54	0.42
26:BA:528:A:C2	26:BA:2043:C:H4'	2.53	0.42
29:BE:12:THR:HG22	29:BE:13:ARG:N	2.33	0.42
40:BT:118:ARG:HH11	40:BT:118:ARG:CG	2.30	0.42
35:BO:122:LEU:HD13	40:BT:72:VAL:HG11	2.01	0.42
45:BY:35:TYR:CE2	45:BY:69:ALA:HB3	2.53	0.42
1:CA:1051:C:N4	61:CA:4001:HOH:O	2.51	0.42
1:CA:1142:G:H2'	1:CA:1143:G:O4'	2.19	0.42
1:CA:49:U:O4	1:CA:365:U:H5	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:684:A:H1'	11:CK:39:PRO:HD2	2.01	0.42
3:CC:6:HIS:HD2	3:CC:8:ILE:N	2.14	0.42
4:CD:155:LEU:HD23	4:CD:156:GLU:H	1.84	0.42
7:CG:103:TRP:CH2	7:CG:141:VAL:HG21	2.54	0.42
51:D4:62:ARG:HB2	51:D4:63:TYR:CD1	2.54	0.42
53:D6:40:CYS:HA	53:D6:41:PRO:HD3	1.90	0.42
26:DA:1235:G:C6	26:DA:1236:G:N1	2.87	0.42
26:DA:1292:U:H2'	26:DA:1293:C:C6	2.54	0.42
26:DA:1471:A:OP2	26:DA:1519:G:N1	2.42	0.42
26:DA:1587:A:H2'	26:DA:1588:C:C6	2.54	0.42
26:DA:212:G:H2'	26:DA:213:A:O4'	2.18	0.42
26:DA:2345:G:OP2	53:D6:38:LYS:NZ	2.42	0.42
26:DA:746:A:H2'	26:DA:2612:C:H5''	2.00	0.42
26:DA:760:G:H2'	26:DA:761:A:O4'	2.18	0.42
29:DE:170:LEU:HB3	29:DE:184:VAL:CG2	2.49	0.42
35:DO:23:ARG:HG3	35:DO:24:VAL:N	2.33	0.42
1:AA:1299:A:H5''	1:AA:1299:A:N3	2.35	0.42
1:AA:1236:A:O2'	1:AA:1304:G:H4'	2.19	0.42
1:AA:1317:C:N3	19:AS:37:ARG:NH2	2.63	0.42
1:AA:1410:G:H2'	1:AA:1411:C:C6	2.53	0.42
1:AA:540:G:H2'	1:AA:541:G:O4'	2.19	0.42
2:AB:166:ASP:HA	2:AB:167:PRO:HD3	1.81	0.42
4:AD:107:ARG:HD2	4:AD:107:ARG:HA	1.79	0.42
1:AA:8:A:H5'	5:AE:101:ILE:HG22	2.00	0.42
1:AA:16:A:O2'	5:AE:16:THR:HB	2.19	0.42
8:AH:86:ILE:HG22	8:AH:93:VAL:HG21	2.01	0.42
13:AM:39:ILE:HD12	13:AM:52:GLU:HG2	2.00	0.42
6:AF:89:MET:HE1	18:AR:72:ARG:HB3	2.00	0.42
20:AT:16:HIS:O	20:AT:19:SER:OG	2.25	0.42
25:AY:55:PSU:N3	25:AY:57:G:H5'	2.33	0.42
51:B4:59:PHE:N	51:B4:59:PHE:CD1	2.77	0.42
26:BA:1188:U:H4'	42:BV:79:VAL:HG22	2.01	0.42
24:AX:13:C:O2'	26:BA:1924:C:H4'	2.20	0.42
26:BA:192:C:OP1	61:BA:4017:HOH:O	2.21	0.42
26:BA:226:G:N2	26:BA:228:A:H62	2.15	0.42
26:BA:644:A:H4'	26:BA:645:C:H5	1.83	0.42
26:BA:1797:C:H4'	28:BD:257:LEU:O	2.18	0.42
30:BF:9:ILE:HA	30:BF:10:PRO:HD2	1.82	0.42
30:BF:24:LEU:HB3	30:BF:115:ALA:HB2	2.02	0.42
30:BF:89:VAL:HG12	30:BF:90:PHE:CD2	2.55	0.42
31:BG:48:GLU:HA	31:BG:51:ARG:HG3	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:BZ:136:PHE:O	46:BZ:137:ILE:HG13	2.20	0.42
1:CA:935:A:O2'	1:CA:1383:C:N3	2.44	0.42
1:CA:922:G:C6	1:CA:923:A:C6	3.07	0.42
4:CD:13:ARG:HB2	4:CD:40:PRO:HD3	2.01	0.42
12:CL:71:PRO:O	12:CL:102:ARG:HD2	2.18	0.42
19:CS:51:VAL:HB	19:CS:75:ALA:HB2	2.00	0.42
23:CW:74:C:C4	23:CW:75:C:C2	3.07	0.42
24:CX:53:G:H3'	24:CX:54:5MU:H71	2.01	0.42
25:CY:9:A:C8	25:CY:11:C:N4	2.87	0.42
53:D6:10:LEU:HD23	53:D6:22:ALA:HB2	2.01	0.42
26:DA:1545:A:H2'	26:DA:1546:C:O4'	2.20	0.42
26:DA:1575:C:H2'	26:DA:1576:U:O4'	2.19	0.42
26:DA:1656:C:H2'	26:DA:1657:C:C6	2.54	0.42
26:DA:1970:A:H4'	26:DA:1971:A:OP1	2.19	0.42
26:DA:2168:G:O3'	26:DA:2169:A:H8	2.02	0.42
26:DA:2272:U:H5''	26:DA:2273:A:OP1	2.18	0.42
26:DA:2745:C:H2'	26:DA:2746:U:O4'	2.19	0.42
26:DA:39:C:H2'	26:DA:40:C:H6	1.83	0.42
26:DA:699:A:H2'	26:DA:700:G:O4'	2.19	0.42
30:DF:33:LEU:HA	30:DF:33:LEU:HD12	1.75	0.42
32:DH:137:ASP:HB3	32:DH:140:LYS:HB3	1.99	0.42
35:DO:68:GLU:HB3	35:DO:78:ARG:HB2	2.01	0.42
37:DQ:43:THR:OG1	37:DQ:45:GLN:HG2	2.19	0.42
39:DS:67:ARG:HG3	39:DS:104:GLY:CA	2.49	0.42
41:DU:17:ILE:HG13	41:DU:32:PHE:HE1	1.83	0.42
46:DZ:138:GLU:H	46:DZ:156:LYS:NZ	2.16	0.42
1:AA:1479:C:H2'	1:AA:1480:G:H8	1.84	0.42
1:AA:741:G:H2'	1:AA:742:G:O4'	2.19	0.42
2:AB:207:ALA:O	2:AB:210:SER:HB3	2.19	0.42
20:AT:67:ALA:HA	20:AT:72:LEU:O	2.18	0.42
22:AV:15:A:O5'	22:AV:15:A:H8	2.02	0.42
24:AX:9:G:O2'	24:AX:10:G:N7	2.47	0.42
25:AY:50:U:H2'	25:AY:51:U:O4'	2.20	0.42
38:BR:98:LEU:HD12	52:B5:57:VAL:HG11	2.01	0.42
26:BA:1142(A):A:C4	26:BA:1144:G:C8	3.06	0.42
26:BA:1530:C:H1'	26:BA:1531:C:OP1	2.19	0.42
26:BA:2116:G:H2'	26:BA:2117:A:C5	2.54	0.42
26:BA:466:A:N3	26:BA:683:C:H1'	2.34	0.42
33:BI:93:THR:H	33:BI:96:ASP:HB2	1.84	0.42
34:BN:130:HIS:O	34:BN:133:GLN:HG2	2.19	0.42
46:BZ:19:ARG:HD3	46:BZ:25:PRO:CD	2.49	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:1122:U:N3	1:CA:1123:A:N7	2.67	0.42
1:CA:1410:G:H2'	1:CA:1411:C:H6	1.84	0.42
1:CA:583:A:N6	1:CA:758:G:O2'	2.52	0.42
1:CA:898:G:N2	1:CA:901:A:OP2	2.50	0.42
1:CA:924:C:O2'	1:CA:1502:A:N6	2.49	0.42
2:CB:160:ASP:N	2:CB:160:ASP:OD1	2.52	0.42
4:CD:112:VAL:HG22	4:CD:116:GLN:OE1	2.20	0.42
4:CD:121:VAL:O	4:CD:134:ASP:HA	2.20	0.42
23:CW:11:C:N4	23:CW:24:G:H1	2.14	0.42
25:CY:50:U:H2'	25:CY:51:U:C6	2.53	0.42
51:D4:33:VAL:HG12	51:D4:34:GLU:N	2.34	0.42
26:DA:1847:A:H3'	26:DA:1848:A:H5'	2.00	0.42
26:DA:2114:A:H2'	26:DA:2114:A:N3	2.34	0.42
26:DA:2110:G:C2	26:DA:2120:G:H1'	2.55	0.42
26:DA:2251:G:OP1	37:DQ:82:ARG:NH1	2.52	0.42
26:DA:2376:A:H3'	26:DA:2377:A:H8	1.85	0.42
26:DA:729:G:O2'	26:DA:763:G:H4'	2.19	0.42
26:DA:996:A:C6	26:DA:1160:G:N1	2.87	0.42
27:DB:33:G:N3	27:DB:50:G:N2	2.67	0.42
36:DP:6:LEU:HA	36:DP:6:LEU:HD23	1.78	0.42
26:DA:910:A:C5	37:DQ:13:GLN:HG3	2.55	0.42
42:DV:48:GLY:HA2	42:DV:52:VAL:HG12	2.01	0.42
1:AA:109:A:C6	1:AA:326:G:C6	3.07	0.42
1:AA:1125:U:H4'	1:AA:1126:U:OP1	2.19	0.42
1:AA:1401:G:C2	1:AA:1402:C:H1'	2.55	0.42
1:AA:1079:G:O3'	5:AE:14:ARG:NH2	2.52	0.42
5:AE:20:GLN:NE2	5:AE:21:ALA:O	2.52	0.42
8:AH:46:LYS:HG3	8:AH:64:LYS:HB2	2.02	0.42
24:AX:2:G:H2'	24:AX:2:G:N3	2.34	0.42
53:B6:11:LEU:HD23	53:B6:11:LEU:HA	1.82	0.42
26:BA:1124:C:H1'	56:B9:36:GLN:NE2	2.34	0.42
26:BA:375:C:H2'	26:BA:376:C:C6	2.54	0.42
28:BD:218:ARG:HB3	28:BD:219:PRO:HD2	2.01	0.42
31:BG:121:ASN:HA	31:BG:122:PRO:HD3	1.87	0.42
32:BH:22:GLY:HA2	32:BH:37:VAL:O	2.20	0.42
1:CA:1173:G:H2'	1:CA:1174:G:H8	1.84	0.42
1:CA:1286:A:C8	1:CA:1287:A:H4'	2.55	0.42
4:CD:158:ILE:HG22	4:CD:162:LEU:HD12	2.02	0.42
6:CF:68:PRO:HB2	6:CF:71:ARG:HG3	2.01	0.42
10:CJ:32:ALA:HB1	10:CJ:33:GLN:HA	2.00	0.42
1:CA:1297:C:P	13:CM:44:ARG:HH22	2.42	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:DA:2171:A:OP1	26:DA:2171:A:H3'	2.19	0.42
26:DA:352:G:N2	61:DA:3734:HOH:O	2.32	0.42
26:DA:744:G:OP1	29:DE:132:HIS:ND1	2.47	0.42
26:DA:864:G:N2	26:DA:913:U:C2	2.87	0.42
30:DF:139:PHE:CD2	30:DF:167:ALA:HB2	2.55	0.42
30:DF:184:TYR:CZ	30:DF:188:ARG:HD2	2.54	0.42
39:DS:57:LYS:HE3	39:DS:57:LYS:HB2	1.80	0.42
46:DZ:144:LEU:CD1	46:DZ:172:ALA:HB1	2.47	0.42
1:AA:299:G:H8	1:AA:299:G:O5'	2.02	0.42
1:AA:438:G:H4'	4:AD:123:HIS:CE1	2.55	0.42
1:AA:60:A:OP1	1:AA:111:G:N2	2.51	0.42
2:AB:24:TRP:HD1	2:AB:24:TRP:H	1.68	0.42
4:AD:166:LYS:HD3	4:AD:166:LYS:HA	1.79	0.42
25:AY:52:G:H1	25:AY:62:C:H42	1.67	0.42
26:BA:1675:C:O2	29:BE:128:SER:OG	2.37	0.42
26:BA:2181:G:HO2'	26:BA:2182:G:P	2.42	0.42
26:BA:606:U:H4'	26:BA:658:C:H4'	2.00	0.42
27:BB:110:G:H2'	27:BB:111:G:C8	2.54	0.42
28:BD:242:ARG:HD3	28:BD:242:ARG:N	2.33	0.42
31:BG:77:ILE:N	31:BG:82:LEU:O	2.48	0.42
30:BF:34:TRP:CH2	36:BP:8:PRO:HB3	2.54	0.42
40:BT:127:ALA:O	40:BT:128:GLU:HB2	2.18	0.42
1:CA:1057:G:C5	1:CA:1204:A:C2	3.07	0.42
1:CA:1092:A:C6	1:CA:1093:A:C6	3.07	0.42
1:CA:444:C:H2'	1:CA:445:G:C8	2.55	0.42
1:CA:715:A:H5''	1:CA:805:C:H1'	2.02	0.42
1:CA:792:A:H4'	1:CA:793:U:H5''	2.01	0.42
1:CA:971:G:H3'	1:CA:971:G:OP1	2.19	0.42
1:CA:979:C:H2'	1:CA:980:C:H5'	2.01	0.42
2:CB:133:LYS:O	2:CB:137:ARG:HG3	2.20	0.42
3:CC:43:LEU:HD11	3:CC:91:LEU:HD11	2.01	0.42
1:CA:1079:G:O3'	5:CE:14:ARG:NH2	2.53	0.42
23:CW:25:C:C2'	23:CW:26:A:H5'	2.49	0.42
25:CY:18:G:C2	25:CY:55:PSU:O4	2.72	0.42
26:DA:2271:G:OP1	47:D0:18:ALA:HB1	2.19	0.42
13:CM:65:LYS:CA	51:D4:50:VAL:HG11	2.49	0.42
26:DA:2365:G:O6	55:D8:39:LYS:HE3	2.19	0.42
26:DA:1151:G:C2	26:DA:1152:C:C2	3.07	0.42
26:DA:1354:A:H5''	28:DD:38:LYS:HD3	2.01	0.42
26:DA:1488:G:H5'	26:DA:1489:U:OP2	2.20	0.42
26:DA:2128:C:H2'	26:DA:2129:C:O4'	2.18	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:DA:251:A:C5	26:DA:252:G:H1'	2.55	0.42
26:DA:608:A:C6	26:DA:609:A:C6	3.08	0.42
26:DA:896:A:N6	46:DZ:146:ILE:HD13	2.34	0.42
27:DB:28:C:P	39:DS:36:TYR:HH	2.43	0.42
27:DB:33:G:C6	27:DB:34:U:C4	3.07	0.42
27:DB:73:A:C4	27:DB:105:A:C2	3.07	0.42
28:DD:264:LYS:HA	28:DD:265:PRO:HD3	1.88	0.42
29:DE:72:VAL:HA	29:DE:73:GLU:CB	2.50	0.42
31:DG:136:ARG:H	31:DG:136:ARG:HH11	1.68	0.42
33:DI:66:GLU:OE2	33:DI:69:LYS:HD3	2.18	0.42
35:DO:36:GLY:HA2	35:DO:106:LEU:HD23	2.01	0.42
26:DA:29:U:OP1	41:DU:5:LYS:NZ	2.52	0.42
1:AA:1356:G:H2'	1:AA:1357:A:C8	2.54	0.42
1:AA:971:G:N1	1:AA:1363(A):A:OP2	2.45	0.42
1:AA:877:C:OP1	8:AH:88:LYS:NZ	2.33	0.42
11:AK:111:ASP:HB2	18:AR:84:LYS:HD3	2.01	0.42
47:B0:38:VAL:HG12	47:B0:40:GLN:HG2	2.01	0.42
26:BA:118:A:H3'	26:BA:119:A:H5''	2.02	0.42
26:BA:1268:A:H2'	26:BA:1269:A:O4'	2.18	0.42
26:BA:1748:G:H5''	26:BA:1748:G:H8	1.85	0.42
26:BA:493:G:H2'	26:BA:494:G:O4'	2.19	0.42
29:BE:14:ILE:HD11	29:BE:173:VAL:HG11	2.01	0.42
40:BT:91:ARG:HD2	40:BT:120:ARG:NH1	2.35	0.42
46:BZ:110:GLY:CA	46:BZ:145:GLU:HA	2.50	0.42
46:BZ:145:GLU:H	46:BZ:148:ASP:HB2	1.84	0.42
1:CA:1053:G:C4'	1:CA:1054:C:H5'	2.50	0.42
1:CA:1325:C:O2'	1:CA:1326:C:H5'	2.18	0.42
1:CA:1446:U:H4'	1:CA:1447:A:C5	2.54	0.42
1:CA:116:A:H61	1:CA:313:A:H1'	1.84	0.42
1:CA:779:C:H2'	1:CA:780:A:O4'	2.19	0.42
2:CB:69:LEU:HB3	2:CB:162:ILE:HG22	2.01	0.42
19:CS:27:GLU:HB2	19:CS:28:LYS:HZ3	1.83	0.42
26:DA:1167:U:C2	26:DA:1168:G:C8	3.07	0.42
26:DA:2285:C:OP2	53:D6:6:ARG:NH1	2.52	0.42
26:DA:698:C:H5''	26:DA:699:A:OP1	2.20	0.42
26:DA:868:U:C4	26:DA:869:G:N7	2.88	0.42
26:DA:937:U:H2'	26:DA:938:G:O4'	2.20	0.42
28:DD:37:LEU:HD13	28:DD:87:ASN:ND2	2.34	0.42
30:DF:34:TRP:CE2	36:DP:8:PRO:HG3	2.55	0.42
44:DX:12:VAL:HG21	44:DX:27:THR:HG22	2.02	0.42
1:AA:1218:C:H2'	1:AA:1219:U:C6	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1287:A:H2	1:AA:1353:G:N3	2.18	0.42
1:AA:938:A:C6	1:AA:939:G:C5	3.07	0.42
4:AD:107:ARG:HH22	4:AD:194:LEU:CD2	2.33	0.42
6:AF:35:ALA:HA	6:AF:67:MET:HB3	2.02	0.42
12:AL:53:ARG:HG2	12:AL:69:TYR:HE1	1.84	0.42
13:AM:84:ILE:HD12	19:AS:74:PHE:CE2	2.51	0.42
24:AX:32:5MC:HM53	24:AX:33:U:O4	2.20	0.42
25:AY:52:G:H1	25:AY:62:C:N4	2.17	0.42
49:B2:32:LEU:HD13	49:B2:36:ARG:HH11	1.85	0.42
56:B9:27:CYS:SG	56:B9:28:GLU:N	2.93	0.42
26:BA:1512:U:O2'	26:BA:1513:C:H5'	2.20	0.42
26:BA:1714:G:H1	26:BA:1745(A):C:N4	2.13	0.42
26:BA:570:G:H2'	26:BA:2030:A:C5	2.55	0.42
26:BA:717:G:H2'	26:BA:718:A:O4'	2.20	0.42
31:BG:77:ILE:HG21	31:BG:80:PHE:CD2	2.55	0.42
35:BO:73:ASP:HB2	40:BT:82:LEU:HD13	2.00	0.42
1:CA:1067:A:H1'	1:CA:1068:G:O4'	2.20	0.42
1:CA:1072:G:C6	1:CA:1073:U:C4	3.08	0.42
1:CA:1233:G:H2'	1:CA:1234:C:C6	2.55	0.42
1:CA:583:A:H2'	1:CA:584:G:O4'	2.20	0.42
1:CA:685:G:C2	1:CA:686:U:C4	3.08	0.42
2:CB:137:ARG:O	2:CB:141:GLU:N	2.36	0.42
15:CO:36:ILE:HG23	15:CO:56:LEU:HD11	2.01	0.42
15:CO:5:LYS:O	15:CO:9:GLN:HG2	2.19	0.42
51:D4:9:LEU:HD23	51:D4:9:LEU:HA	1.90	0.42
56:D9:7:VAL:HG12	56:D9:34:GLN:HB3	2.01	0.42
26:DA:1198:U:H2'	26:DA:1199:U:C6	2.55	0.42
26:DA:2107:C:H2'	26:DA:2108:C:O4'	2.20	0.42
26:DA:536:A:H2'	26:DA:537:C:C6	2.55	0.42
28:DD:145:VAL:HB	28:DD:155:LEU:HB2	2.02	0.42
29:DE:9:VAL:HB	40:DT:3:ARG:HG2	2.02	0.42
34:DN:40:PRO:HB3	41:DU:68:ALA:HB2	2.01	0.42
45:DY:45:VAL:N	45:DY:63:LYS:O	2.45	0.42
46:DZ:24:LEU:HA	46:DZ:25:PRO:HD3	1.90	0.42
1:AA:1006:C:H2'	1:AA:1007:C:C6	2.55	0.42
1:AA:1029:C:N3	1:AA:1032:G:O6	2.53	0.42
1:AA:108:G:O6	20:AT:15:ARG:HD2	2.19	0.42
1:AA:1182:G:C3'	1:AA:1183:A:H5'	2.50	0.42
1:AA:130:A:O2'	1:AA:131:C:O5'	2.32	0.42
1:AA:152:A:N6	1:AA:170:U:C2	2.88	0.42
1:AA:583:A:N6	1:AA:758:G:O2'	2.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:AO:17:ARG:HH11	15:AO:17:ARG:HG3	1.84	0.42
15:AO:78:TYR:CZ	15:AO:82:ILE:HD13	2.55	0.42
17:AQ:66:SER:H	17:AQ:69:LYS:HB3	1.85	0.42
25:AY:56:C:C2	25:AY:57:G:C8	3.08	0.42
26:BA:1858:G:H21	26:BA:1883:G:H2'	1.84	0.42
26:BA:2090:G:O6	61:BA:4756:HOH:O	2.19	0.42
26:BA:2111:C:OP2	26:BA:2145:C:N4	2.51	0.42
26:BA:222:A:H3'	26:BA:421:U:H5'	2.00	0.42
26:BA:2461:C:H2'	26:BA:2462:U:C6	2.55	0.42
29:BE:14:ILE:HG12	29:BE:21:VAL:HG13	2.00	0.42
33:BI:131:LYS:HA	33:BI:137:PRO:HA	2.02	0.42
40:BT:53:ARG:CZ	40:BT:53:ARG:HB3	2.50	0.42
45:BY:54:LYS:HA	45:BY:55:TYR:HA	1.85	0.42
1:CA:1269:A:H2	1:CA:1312:G:N3	2.17	0.42
1:CA:1357:A:N6	1:CA:1363(A):A:N1	2.67	0.42
1:CA:6:G:H4'	1:CA:298:A:H4'	2.00	0.42
1:CA:344:A:H5''	1:CA:345:C:H5	1.84	0.42
3:CC:19:GLU:HB3	3:CC:55:VAL:O	2.20	0.42
3:CC:77:ILE:HG13	3:CC:78:GLY:N	2.35	0.42
11:CK:38:ASN:HA	11:CK:39:PRO:HD3	1.80	0.42
23:CW:29:G:N2	23:CW:42:C:C2	2.88	0.42
26:DA:1231:G:H2'	26:DA:1232:G:C8	2.55	0.42
26:DA:1470:G:HO2'	26:DA:1471:A:H8	1.63	0.42
26:DA:1794:U:H2'	26:DA:1795:C:H6	1.85	0.42
24:CX:3:C:H5'	26:DA:2255:G:O2'	2.20	0.42
26:DA:234:C:H2'	26:DA:235:U:C6	2.54	0.42
26:DA:839:U:H2'	26:DA:840:C:C6	2.55	0.42
28:DD:73:VAL:O	28:DD:75:ILE:HG13	2.19	0.42
31:DG:72:ARG:NH1	31:DG:87:PRO:HG3	2.35	0.42
34:DN:138:LEU:HA	34:DN:138:LEU:HD23	1.73	0.42
26:DA:863:A:P	37:DQ:22:LYS:HG3	2.60	0.42
44:DX:84:ALA:HB3	44:DX:87:GLN:NE2	2.35	0.42
46:DZ:146:ILE:H	46:DZ:146:ILE:HG13	1.62	0.42
1:AA:1314:C:H2'	1:AA:1315:U:C6	2.54	0.42
1:AA:922:G:C6	1:AA:923:A:C6	3.08	0.42
2:AB:62:ALA:HB3	2:AB:225:ALA:HB3	2.02	0.42
3:AC:112:SER:O	3:AC:116:VAL:HG23	2.20	0.42
3:AC:131:ARG:NE	3:AC:166:GLU:OE2	2.53	0.42
3:AC:56:ASP:HB2	3:AC:67:THR:HB	2.02	0.42
4:AD:170:VAL:HG11	4:AD:174:LEU:HB2	2.02	0.42
9:AI:16:ARG:HB2	9:AI:64:THR:HB	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:881:G:P	12:AL:12:ARG:HH22	2.42	0.42
13:AM:14:ARG:NH2	13:AM:41:PRO:O	2.53	0.42
18:AR:26:LEU:HD23	18:AR:29:PHE:CE2	2.55	0.42
25:AY:38:A:C5	25:AY:39:PSU:C6	3.08	0.42
25:AY:68:C:N3	25:AY:69:G:C8	2.88	0.42
50:B3:5:LYS:NZ	50:B3:34:GLU:OE2	2.40	0.42
51:B4:62:ARG:HB2	51:B4:63:TYR:CD1	2.54	0.42
26:BA:1762:A:H2'	61:BA:5184:HOH:O	2.19	0.42
26:BA:2101:G:H2'	26:BA:2102:U:C6	2.55	0.42
26:BA:2443:C:OP1	30:BF:68:LYS:HD3	2.20	0.42
27:BB:55:U:H2'	27:BB:56:G:O4'	2.20	0.42
26:BA:2619:C:H4'	29:BE:151:TYR:O	2.20	0.42
45:BY:9:LYS:HA	45:BY:10:GLY:HA2	1.71	0.42
1:CA:1154:G:C8	1:CA:1155:G:C8	3.07	0.42
1:CA:340:U:H2'	1:CA:341:C:C6	2.54	0.42
1:CA:641:U:O3'	1:CA:642:A:H8	2.03	0.42
1:CA:989:C:HO2'	1:CA:1016:A:H2	1.67	0.42
3:CC:115:LEU:HD12	3:CC:115:LEU:HA	1.80	0.42
4:CD:57:ARG:HD3	4:CD:205:GLU:HB2	2.00	0.42
10:CJ:56:HIS:CD2	10:CJ:56:HIS:H	2.38	0.42
11:CK:110:ASP:HB3	18:CR:85:LEU:HB3	2.02	0.42
13:CM:94:ARG:CZ	19:CS:80:TYR:HD2	2.33	0.42
1:CA:375:U:OP1	16:CP:69:THR:HG21	2.20	0.42
20:CT:33:ILE:HG13	20:CT:62:LEU:HD22	2.02	0.42
25:CY:15:G:H22	25:CY:48:C:N4	2.15	0.42
26:DA:1015:G:O2'	26:DA:1016:G:H5'	2.20	0.42
26:DA:1019:U:H3	26:DA:1142(A):A:N6	2.13	0.42
26:DA:526:A:N3	26:DA:2044:C:H1'	2.35	0.42
26:DA:2252:G:H2'	26:DA:2253:G:O4'	2.19	0.42
26:DA:2307:G:H8	26:DA:2307:G:OP1	2.03	0.42
26:DA:2262:U:H4'	26:DA:2328:A:H2	1.84	0.42
26:DA:2853:C:H2'	26:DA:2854:G:C8	2.54	0.42
26:DA:300:A:H3'	45:DY:84:ARG:NH2	2.35	0.42
39:DS:80:LEU:HA	39:DS:80:LEU:HD12	1.84	0.42
46:DZ:5:LEU:HA	46:DZ:5:LEU:HD22	1.82	0.42
1:AA:1003:G:N3	1:AA:1004:A:H1'	2.34	0.41
1:AA:1035:A:H8	1:AA:1035:A:O5'	2.02	0.41
1:AA:555:C:H2'	1:AA:556:C:C6	2.55	0.41
1:AA:591:U:H2'	1:AA:592:G:C8	2.54	0.41
1:AA:78:G:N2	1:AA:91:C:C2	2.88	0.41
2:AB:71:VAL:HG13	2:AB:93:VAL:CG2	2.50	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:47:LEU:CD1	3:AC:68:VAL:HG11	2.50	0.41
9:AI:93:ARG:HB2	9:AI:93:ARG:NH1	2.35	0.41
1:AA:688:G:H5'	11:AK:46:GLY:C	2.40	0.41
51:B4:63:TYR:CD1	51:B4:63:TYR:N	2.86	0.41
36:BP:63:PRO:HG2	55:B8:25:MET:HB2	2.02	0.41
33:BI:110:ASP:HA	33:BI:111:PRO:HD2	1.78	0.41
36:BP:121:LYS:HG2	36:BP:122:PRO:HD2	2.02	0.41
40:BT:11:GLU:OE1	40:BT:57:PHE:HB3	2.19	0.41
40:BT:73:GLU:OE1	40:BT:103:ARG:NE	2.41	0.41
45:BY:7:VAL:HG21	45:BY:72:VAL:HG12	2.02	0.41
45:BY:86:ARG:HH11	45:BY:100:ALA:HB1	1.85	0.41
1:CA:1039:C:C4	1:CA:1040:U:C4	3.07	0.41
1:CA:998:G:C6	1:CA:999:C:C4	3.08	0.41
4:CD:17:VAL:HG12	4:CD:18:LYS:N	2.35	0.41
23:CW:76:31M:N3'	26:DA:2585:U:O4	2.53	0.41
26:DA:1720:U:H2'	26:DA:1721:G:O4'	2.20	0.41
26:DA:1843:C:H5'	28:DD:253:GLN:NE2	2.34	0.41
26:DA:2512:C:H2'	26:DA:2513:G:O4'	2.20	0.41
26:DA:2505:G:O6	26:DA:2576:G:H2'	2.20	0.41
26:DA:2788:C:C4	26:DA:2789:C:N4	2.88	0.41
26:DA:2815:C:H2'	26:DA:2816:C:H6	1.85	0.41
26:DA:569:U:H5''	61:DA:4096:HOH:O	2.20	0.41
26:DA:776:G:C8	26:DA:793:A:C2	3.08	0.41
26:DA:867:C:C2'	26:DA:868:U:H5'	2.50	0.41
26:DA:994:C:O2'	26:DA:996:A:OP1	2.16	0.41
44:DX:88:LYS:NZ	44:DX:90:GLU:HG2	2.34	0.41
46:DZ:166:SER:O	46:DZ:169:GLU:HB2	2.20	0.41
46:DZ:67:LEU:HA	46:DZ:68:PRO:HD3	1.93	0.41
1:AA:1128:C:H4'	1:AA:1148:U:O2	2.19	0.41
1:AA:1296:C:H4'	1:AA:1302:U:C4	2.55	0.41
1:AA:1417:G:H22	1:AA:1482:G:H2'	1.84	0.41
1:AA:309:G:H1'	1:AA:608:A:C2	2.55	0.41
1:AA:765:G:N1	1:AA:812:C:O2'	2.43	0.41
1:AA:890:G:O2'	1:AA:906:G:O6	2.24	0.41
2:AB:27:LYS:HB2	2:AB:194:PRO:HD2	2.01	0.41
4:AD:178:VAL:C	4:AD:180:GLY:H	2.23	0.41
5:AE:6:PHE:HB3	5:AE:35:GLY:C	2.40	0.41
10:AJ:6:ILE:HA	10:AJ:97:GLU:O	2.21	0.41
11:AK:59:TYR:CZ	11:AK:63:LEU:HD11	2.55	0.41
12:AL:42:THR:OG1	12:AL:52:LEU:HD13	2.20	0.41
19:AS:27:GLU:HB3	19:AS:28:LYS:HA	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:AS:38:SER:HB2	19:AS:71:LEU:HD12	2.01	0.41
19:AS:3:ARG:NH1	19:AS:10:PHE:HB2	2.35	0.41
23:AW:25:C:H2'	23:AW:26:A:H5'	2.02	0.41
25:AY:22:G:C2	25:AY:23:A:C5	3.08	0.41
25:AY:39:PSU:H5'	25:AY:39:PSU:H6	1.86	0.41
26:BA:1530:C:HO2'	26:BA:1531:C:P	2.37	0.41
26:BA:2012:G:OP1	43:BW:11:ARG:NH2	2.45	0.41
26:BA:355:G:H2'	26:BA:356:G:O4'	2.20	0.41
26:BA:479:A:N3	26:BA:481:G:H5''	2.35	0.41
26:BA:954:G:H5''	37:BQ:13:GLN:HB3	2.01	0.41
32:BH:96:ALA:HB2	32:BH:105:LEU:HD13	2.02	0.41
34:BN:33:LEU:HD12	34:BN:33:LEU:HA	1.84	0.41
39:BS:10:ARG:HG3	39:BS:13:ARG:NH2	2.35	0.41
41:BU:17:ILE:HG13	41:BU:32:PHE:HE1	1.84	0.41
46:BZ:104:PHE:CD2	46:BZ:139:VAL:HB	2.55	0.41
1:CA:1135:U:HO2'	1:CA:1136:U:H5	1.66	0.41
1:CA:1178:G:N2	1:CA:1181:G:OP2	2.49	0.41
1:CA:1346:A:N1	1:CA:1374:A:H5''	2.34	0.41
1:CA:791:G:N2	1:CA:1497:G:O3'	2.50	0.41
1:CA:434:U:H2'	1:CA:435:C:C6	2.55	0.41
1:CA:657:G:H1'	1:CA:750:G:N2	2.35	0.41
1:CA:814:A:N7	1:CA:816:A:C4	2.88	0.41
1:CA:971:G:H22	1:CA:1363(A):A:P	2.42	0.41
1:CA:986:A:N3	19:CS:52:TYR:OH	2.42	0.41
3:CC:116:VAL:HG13	3:CC:119:ARG:HD3	2.02	0.41
3:CC:82:GLU:O	3:CC:85:ARG:HB2	2.20	0.41
4:CD:112:VAL:HG13	4:CD:161:ASN:OD1	2.20	0.41
8:CH:72:PRO:O	8:CH:73:ASP:HB3	2.20	0.41
13:CM:56:LEU:HD23	13:CM:57:ARG:N	2.35	0.41
13:CM:92:HIS:CE1	13:CM:98:VAL:HG21	2.55	0.41
17:CQ:65:ILE:HB	17:CQ:69:LYS:HB3	2.03	0.41
25:CY:5:G:N2	25:CY:68:C:N3	2.63	0.41
26:DA:1885:A:H2'	26:DA:1886:C:O4'	2.20	0.41
26:DA:1905:C:H1'	26:DA:1928:A:H2	1.85	0.41
26:DA:2124:G:N1	26:DA:2174:C:N4	2.34	0.41
26:DA:2519:U:C4	26:DA:2542:A:C5	3.08	0.41
26:DA:27:G:O2'	26:DA:28:A:OP2	2.36	0.41
27:DB:108:U:H2'	27:DB:109:C:H5''	2.03	0.41
31:DG:86:MET:HA	31:DG:87:PRO:HD3	1.97	0.41
32:DH:40:GLU:OE1	32:DH:61:HIS:NE2	2.52	0.41
38:DR:26:LYS:HE2	38:DR:70:LEU:O	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:DZ:158:PRO:HA	46:DZ:159:PRO:HD3	1.69	0.41
1:AA:1027:C:C2	1:AA:1034:G:C6	3.07	0.41
1:AA:295:C:H2'	1:AA:296:U:O4'	2.21	0.41
1:AA:663:A:H5'	1:AA:836:G:OP1	2.19	0.41
1:AA:977:A:H1'	1:AA:982:U:O4	2.20	0.41
2:AB:48:MET:HA	2:AB:51:LEU:HD12	2.03	0.41
4:AD:190:ASP:H	4:AD:193:ASP:HB2	1.86	0.41
1:AA:589:C:H5''	8:AH:29:SER:OG	2.20	0.41
9:AI:127:LYS:O	9:AI:128:ARG:HG2	2.20	0.41
10:AJ:47:PHE:N	10:AJ:63:PHE:O	2.47	0.41
17:AQ:31:LEU:HD23	17:AQ:32:TYR:CZ	2.56	0.41
24:AX:15:G:H21	24:AX:21:A:H1'	1.84	0.41
25:AY:19:G:C4'	25:AY:57:G:H22	2.33	0.41
52:B5:35:GLU:HG3	52:B5:51:TYR:CG	2.55	0.41
26:BA:1963:U:H4'	26:BA:1964:G:OP1	2.20	0.41
23:AW:76:31M:HD2	26:BA:2506:U:O4'	2.20	0.41
26:BA:2698:U:H2'	26:BA:2699:C:C6	2.55	0.41
26:BA:303:U:H2'	26:BA:304:G:C8	2.55	0.41
26:BA:528:A:C8	26:BA:528:A:H3'	2.54	0.41
26:BA:615:G:OP1	30:BF:40:GLN:NE2	2.53	0.41
27:BB:110:G:O2'	27:BB:111:G:H5'	2.20	0.41
32:BH:88:LEU:HD23	32:BH:165:ALA:HA	2.01	0.41
38:BR:57:ARG:HH21	38:BR:62:ALA:HB2	1.85	0.41
46:BZ:105:VAL:O	46:BZ:140:ASP:HA	2.20	0.41
1:CA:1118:C:H2'	1:CA:1119:C:C6	2.56	0.41
1:CA:250:A:H4'	1:CA:251:G:O5'	2.18	0.41
1:CA:714:G:H2'	1:CA:715:A:C8	2.55	0.41
1:CA:741:G:H2'	1:CA:742:G:O4'	2.20	0.41
5:CE:41:VAL:O	5:CE:66:MET:HA	2.20	0.41
1:CA:1240:U:OP2	7:CG:115:ARG:HA	2.19	0.41
9:CI:77:ILE:O	9:CI:81:ILE:HG22	2.21	0.41
17:CQ:3:LYS:HD3	17:CQ:61:GLU:O	2.20	0.41
26:DA:1248:G:C5	41:DU:3:ARG:HB2	2.55	0.41
26:DA:1372:U:O5'	26:DA:1372:U:H6	2.03	0.41
26:DA:2172:U:O2'	26:DA:2173:A:P	2.78	0.41
26:DA:2541:A:N7	61:DA:3999:HOH:O	2.37	0.41
26:DA:275:G:H2'	26:DA:276:A:O4'	2.20	0.41
26:DA:784:A:N6	28:DD:229:VAL:HG11	2.35	0.41
32:DH:13:LYS:HA	32:DH:14:GLY:HA2	1.67	0.41
32:DH:86:GLU:CD	32:DH:130:ARG:HD3	2.40	0.41
37:DQ:45:GLN:CD	37:DQ:45:GLN:H	2.23	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:DS:83:LYS:HE2	39:DS:83:LYS:HB3	1.90	0.41
26:DA:1008:C:H4'	41:DU:59:ARG:NH2	2.35	0.41
42:DV:46:VAL:HG23	42:DV:52:VAL:HG11	2.01	0.41
46:DZ:126:VAL:HG11	46:DZ:161:VAL:CG2	2.41	0.41
1:AA:103:C:OP2	20:AT:14:LYS:NZ	2.44	0.41
1:AA:1122:U:H2'	1:AA:1123:A:O4'	2.21	0.41
1:AA:382:A:H2'	1:AA:383:A:H8	1.85	0.41
1:AA:826:C:H2'	1:AA:827:U:C6	2.56	0.41
2:AB:218:ALA:O	2:AB:222:ILE:HG13	2.20	0.41
4:AD:173:TRP:CE3	4:AD:174:LEU:HG	2.54	0.41
4:AD:64:LEU:HB2	4:AD:198:VAL:HG11	2.03	0.41
10:AJ:81:THR:HA	10:AJ:84:GLN:HB3	2.02	0.41
11:AK:62:GLN:O	11:AK:66:LEU:HG	2.21	0.41
12:AL:34:ARG:HG2	12:AL:35:GLY:N	2.34	0.41
13:AM:91:ARG:HB2	13:AM:98:VAL:HG13	2.03	0.41
19:AS:80:TYR:CZ	19:AS:82:GLY:HA2	2.56	0.41
25:AY:19:G:H4'	25:AY:20:U:OP2	2.19	0.41
25:AY:57:G:N3	25:AY:58:A:H5'	2.35	0.41
49:B2:35:LEU:HB3	49:B2:50:ILE:HG12	2.01	0.41
26:BA:1266:G:O4'	43:BW:15:ARG:NH2	2.50	0.41
26:BA:1403:C:H5''	26:BA:1471:A:H1'	2.01	0.41
26:BA:2119:A:C5	26:BA:2171:A:C6	3.08	0.41
26:BA:2564:A:C2	26:BA:2647:U:H4'	2.55	0.41
26:BA:2785:C:H2'	26:BA:2786:U:O4'	2.20	0.41
26:BA:1750:G:O2'	26:BA:2860:A:N1	2.38	0.41
26:BA:443:A:H5''	26:BA:444:C:OP1	2.21	0.41
26:BA:601:C:O2'	26:BA:605:C:H5''	2.20	0.41
26:BA:816:C:H2'	26:BA:817:C:C6	2.55	0.41
29:BE:119:ARG:HG2	29:BE:160:TYR:CG	2.56	0.41
33:BI:93:THR:H	33:BI:96:ASP:CG	2.23	0.41
45:BY:15:VAL:HG21	45:BY:42:VAL:HG11	2.02	0.41
1:CA:1041:A:H2'	1:CA:1042:G:O4'	2.20	0.41
1:CA:336:C:H2'	1:CA:337:C:C6	2.55	0.41
1:CA:501:C:H2'	1:CA:502:G:H8	1.84	0.41
2:CB:12:GLU:O	2:CB:15:VAL:N	2.50	0.41
2:CB:158:LEU:HA	2:CB:159:PRO:HD3	1.76	0.41
3:CC:28:GLN:HE21	3:CC:28:GLN:HB2	1.59	0.41
7:CG:23:VAL:HG13	7:CG:43:PHE:CE2	2.55	0.41
8:CH:51:VAL:HG12	8:CH:52:ASP:N	2.35	0.41
1:CA:562:C:H1'	12:CL:15:ARG:HB3	2.02	0.41
14:CN:45:ARG:O	14:CN:49:HIS:HD2	2.04	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:D0:50:ASN:HB3	47:D0:63:VAL:HG22	2.03	0.41
26:DA:1127:A:N7	26:DA:2488:A:O2'	2.47	0.41
26:DA:2867:G:OP2	40:DT:119:LYS:NZ	2.50	0.41
26:DA:752:A:OP1	54:D7:3:ARG:NH2	2.50	0.41
26:DA:8:A:H2'	26:DA:9:U:C6	2.55	0.41
32:DH:27:LYS:HB3	32:DH:27:LYS:HE3	1.82	0.41
33:DI:110:ASP:OD1	33:DI:111:PRO:HD2	2.21	0.41
34:DN:39:ARG:HA	34:DN:40:PRO:HD3	1.80	0.41
35:DO:120:GLU:HG2	35:DO:122:LEU:HG	2.02	0.41
38:DR:21:TYR:OH	38:DR:43:GLU:HG2	2.21	0.41
41:DU:81:HIS:O	41:DU:84:LYS:HB3	2.20	0.41
42:DV:29:PRO:HA	42:DV:61:VAL:HG22	2.02	0.41
1:AA:103:C:OP2	20:AT:17:ARG:NH2	2.53	0.41
51:B4:28:LYS:HA	51:B4:29:PRO:HD3	1.84	0.41
26:BA:1456:G:OP2	61:BA:4012:HOH:O	2.21	0.41
26:BA:2283:C:H2'	26:BA:2284:C:O4'	2.20	0.41
26:BA:465:G:H2'	26:BA:466:A:C8	2.55	0.41
26:BA:634:C:H2'	26:BA:635:C:C6	2.56	0.41
33:BI:109:ILE:HG23	33:BI:110:ASP:N	2.35	0.41
1:CA:1173:G:H2'	1:CA:1174:G:C8	2.55	0.41
1:CA:971:G:N2	1:CA:1363(A):A:OP2	2.51	0.41
1:CA:29:G:O2'	1:CA:295:C:H4'	2.20	0.41
1:CA:723:U:HO2'	1:CA:724:G:H5'	1.85	0.41
1:CA:730:G:C5	1:CA:731:G:H1'	2.55	0.41
1:CA:978:A:C6	1:CA:1319:A:C5	3.08	0.41
6:CF:94:GLN:HE22	18:CR:72:ARG:HH12	1.69	0.41
20:CT:72:LEU:HA	20:CT:72:LEU:HD23	1.84	0.41
26:DA:1024:G:C6	26:DA:1025:G:C6	3.08	0.41
26:DA:1127:A:C2'	26:DA:1128:A:H5''	2.50	0.41
26:DA:1580:A:OP2	26:DA:1580:A:H8	2.03	0.41
26:DA:1882:C:H3'	26:DA:1883:G:H8	1.85	0.41
26:DA:2169:A:C2	26:DA:2170:A:C2	3.08	0.41
26:DA:2550:G:C6	26:DA:2551:C:C4	3.08	0.41
26:DA:2683:C:OP1	40:DT:53:ARG:NH2	2.49	0.41
26:DA:2693:A:H2'	26:DA:2694:G:H8	1.85	0.41
26:DA:324:A:N6	26:DA:338:G:O2'	2.49	0.41
26:DA:932:G:H4'	26:DA:933:A:O5'	2.19	0.41
29:DE:169:ASN:HB2	29:DE:203:LYS:HG3	2.03	0.41
30:DF:135:LYS:HE2	30:DF:135:LYS:HA	2.02	0.41
37:DQ:109:VAL:HG13	37:DQ:113:GLN:HB3	2.02	0.41
40:DT:6:LEU:O	40:DT:10:VAL:HG23	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:DA:996:A:H4'	41:DU:91:ASP:OD2	2.19	0.41
1:AA:600:C:H2'	1:AA:601:C:H6	1.85	0.41
2:AB:33:TYR:HB2	2:AB:43:ASP:HB2	2.02	0.41
2:AB:77:ALA:CB	2:AB:165:VAL:HG11	2.51	0.41
3:AC:27:LYS:HA	3:AC:27:LYS:HD2	1.76	0.41
4:AD:138:TYR:CE1	4:AD:140:VAL:HA	2.56	0.41
8:AH:33:GLU:HG2	8:AH:48:TYR:CZ	2.56	0.41
10:AJ:27:ALA:HA	10:AJ:81:THR:HG21	2.03	0.41
20:AT:57:ARG:HH22	20:AT:100:ILE:HD12	1.86	0.41
21:AU:6:ARG:O	21:AU:12:LYS:HD2	2.21	0.41
53:B6:9:LEU:HD11	53:B6:23:THR:HG23	2.03	0.41
26:BA:1756:G:H4'	26:BA:1758:G:O4'	2.21	0.41
26:BA:2639:A:OP2	61:BA:4129:HOH:O	2.22	0.41
26:BA:719:C:H2'	26:BA:720:C:H6	1.85	0.41
27:BB:6:C:H2'	27:BB:7:G:H5''	2.02	0.41
28:BD:142:VAL:HG13	28:BD:191:ALA:HB1	2.01	0.41
30:BF:183:VAL:O	30:BF:187:VAL:HG23	2.21	0.41
32:BH:13:LYS:HA	32:BH:14:GLY:HA2	1.68	0.41
33:BI:103:ARG:HE	33:BI:103:ARG:HB3	1.53	0.41
34:BN:48:MET:H	34:BN:48:MET:HG3	1.78	0.41
1:CA:983:A:O2'	1:CA:1050:G:OP2	2.33	0.41
1:CA:942:G:C2	1:CA:1342:C:C2	3.09	0.41
1:CA:513:C:H2'	1:CA:514:C:O4'	2.19	0.41
1:CA:722:A:C8	1:CA:724:G:H1'	2.55	0.41
1:CA:857:C:H2'	1:CA:858:G:O4'	2.21	0.41
1:CA:998:G:H2'	1:CA:999:C:O4'	2.20	0.41
2:CB:130:ARG:HA	2:CB:131:PRO:HD3	1.88	0.41
4:CD:163:GLU:O	4:CD:166:LYS:HG2	2.21	0.41
4:CD:208:SER:OG	5:CE:101:ILE:HD12	2.20	0.41
14:CN:37:PHE:HB3	14:CN:39:LEU:HG	2.03	0.41
20:CT:86:ARG:CZ	20:CT:86:ARG:HB3	2.49	0.41
23:CW:23:A:H2'	23:CW:24:G:C8	2.56	0.41
26:DA:1021:A:C3'	26:DA:1021:A:C8	3.02	0.41
26:DA:1766:U:H2'	26:DA:1767:C:H6	1.85	0.41
26:DA:2114:A:N1	26:DA:2117:A:N6	2.69	0.41
26:DA:2154:G:N1	26:DA:2155:G:N7	2.69	0.41
26:DA:775:G:O3'	61:DA:4253:HOH:O	2.21	0.41
26:DA:869:G:C6	26:DA:870:A:C5	3.08	0.41
27:DB:8:U:H3	27:DB:113:G:H1	1.69	0.41
30:DF:184:TYR:O	30:DF:188:ARG:HG3	2.21	0.41
32:DH:54:ARG:HD3	32:DH:65:HIS:ND1	2.34	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:DI:43:ASN:C	33:DI:43:ASN:HD22	2.24	0.41
35:DO:20:MET:HE3	35:DO:44:LYS:HE3	2.02	0.41
39:DS:65:VAL:O	39:DS:69:VAL:HG12	2.20	0.41
1:AA:1286:A:H2'	1:AA:1287:A:H4'	2.01	0.41
1:AA:161:A:O5'	1:AA:161:A:H8	2.02	0.41
1:AA:37:U:O2'	1:AA:500:G:H4'	2.20	0.41
1:AA:993:G:N3	1:AA:993:G:H2'	2.36	0.41
3:AC:15:THR:CG2	3:AC:181:ASN:HA	2.44	0.41
9:AI:26:VAL:HG22	9:AI:61:ALA:HB3	2.02	0.41
20:AT:46:GLU:HG2	20:AT:46:GLU:O	2.20	0.41
23:AW:13:C:O2'	23:AW:14:A:O5'	2.37	0.41
24:AX:31:G:C8	24:AX:32:5MC:HM52	2.56	0.41
25:AY:38:A:H3'	25:AY:39:PSU:H5'	2.02	0.41
52:B5:16:ARG:NH1	52:B5:17:ASP:OD1	2.50	0.41
26:BA:1338:G:N7	44:BX:62:LYS:NZ	2.65	0.41
26:BA:271(A):A:N1	26:BA:272(D):G:O2'	2.47	0.41
30:BF:101:LEU:HA	30:BF:101:LEU:HD12	1.84	0.41
30:BF:157:VAL:HG21	30:BF:181:LEU:HD13	2.02	0.41
33:BI:9:LEU:HD22	33:BI:9:LEU:HA	1.79	0.41
36:BP:6:LEU:HA	36:BP:6:LEU:HD23	1.80	0.41
45:BY:5:MET:HE1	45:BY:32:PRO:HA	2.03	0.41
1:CA:176:C:H2'	1:CA:177:C:C6	2.55	0.41
3:CC:26:LYS:HE3	3:CC:26:LYS:HB3	1.88	0.41
15:CO:18:PHE:CE2	15:CO:21:ASP:HB2	2.56	0.41
16:CP:17:TYR:HE2	16:CP:41:PRO:HG3	1.86	0.41
23:CW:34:G:H2'	23:CW:35:A:C8	2.56	0.41
26:DA:1498:C:O4'	26:DA:1577:C:H4'	2.21	0.41
26:DA:2025:C:H2'	26:DA:2026:C:C6	2.56	0.41
26:DA:2026:C:H2'	26:DA:2027:G:O4'	2.21	0.41
26:DA:2152:G:C2	26:DA:2153:G:H1'	2.54	0.41
26:DA:2228:G:C6	26:DA:2229:C:C4	3.09	0.41
26:DA:2314:C:H2'	26:DA:2315:G:C8	2.56	0.41
26:DA:2432:A:C6	26:DA:2433:A:C6	3.09	0.41
26:DA:2445:G:OP1	30:DF:74:ARG:NH2	2.45	0.41
26:DA:340:A:H2'	26:DA:341:G:O4'	2.20	0.41
26:DA:62:C:N4	26:DA:93:G:H1	2.19	0.41
27:DB:119:G:C6	27:DB:120:A:C6	3.09	0.41
27:DB:42:C:C4	27:DB:43:C:C4	3.09	0.41
27:DB:33:G:C2	27:DB:50:G:C2	3.08	0.41
31:DG:3:LEU:HD12	31:DG:5:VAL:HG12	2.02	0.41
34:DN:42:TRP:HD1	34:DN:48:MET:HE2	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:DP:55:ARG:HA	61:DP:309:HOH:O	2.21	0.41
39:DS:28:VAL:HG13	39:DS:35:ILE:HD11	2.03	0.41
39:DS:67:ARG:HG2	39:DS:71:ARG:HH11	1.85	0.41
45:DY:65:ALA:HA	45:DY:66:PRO:HD3	1.92	0.41
46:DZ:121:HIS:HB3	46:DZ:123:ASP:O	2.20	0.41
1:AA:109:A:H2'	1:AA:326:G:N2	2.35	0.41
1:AA:1256:A:N6	1:AA:1278:U:O4'	2.52	0.41
1:AA:1376:U:H2'	1:AA:1377:A:H8	1.86	0.41
1:AA:358:U:H2'	1:AA:359:U:C6	2.56	0.41
1:AA:519:C:OP2	12:AL:50:SER:OG	2.26	0.41
2:AB:103:THR:HG23	2:AB:176:GLU:OE1	2.21	0.41
6:AF:97:PHE:HB3	18:AR:32:ARG:HD3	2.01	0.41
15:AO:71:GLN:HA	15:AO:71:GLN:HE21	1.85	0.41
15:AO:7:GLU:H	15:AO:7:GLU:HG3	1.65	0.41
20:AT:54:LYS:HB2	20:AT:100:ILE:HD11	2.03	0.41
25:AY:20:U:H4'	25:AY:21:A:OP1	2.20	0.41
25:AY:59:U:H3'	25:AY:60:U:C5	2.56	0.41
25:AY:70:G:C6	25:AY:71:G:C5	3.09	0.41
48:B1:23:LYS:HB3	48:B1:29:GLY:HA3	2.02	0.41
48:B1:64:ALA:HA	48:B1:67:ILE:HG13	2.02	0.41
54:B7:24:THR:HG22	54:B7:27:GLY:N	2.30	0.41
26:BA:1203:G:OP2	26:BA:1204:A:O2'	2.28	0.41
26:BA:2061:G:H5''	26:BA:2503:A:C2	2.56	0.41
26:BA:2418:A:H2'	26:BA:2419:U:C6	2.55	0.41
31:BG:14:GLU:O	31:BG:17:PRO:HD2	2.21	0.41
32:BH:3:ARG:HD3	32:BH:54:ARG:HH12	1.85	0.41
36:BP:65:ARG:HD3	36:BP:66:GLY:N	2.36	0.41
1:CA:1102:A:O3'	2:CB:96:ARG:NH1	2.47	0.41
1:CA:1315:U:H2'	1:CA:1316:G:O4'	2.21	0.41
2:CB:145:LEU:O	2:CB:149:LEU:HB2	2.21	0.41
2:CB:78:GLN:NE2	2:CB:95:GLN:OE1	2.54	0.41
1:CA:8:A:C6	4:CD:209:ARG:HG3	2.56	0.41
10:CJ:77:PRO:O	10:CJ:81:THR:OG1	2.39	0.41
18:CR:76:LEU:HA	18:CR:76:LEU:HD12	1.81	0.41
23:CW:21:A:N6	23:CW:46:7MG:C4	2.89	0.41
25:CY:64:A:H2'	25:CY:65:G:C8	2.56	0.41
26:DA:2395:C:O2'	48:D1:30:VAL:HG22	2.21	0.41
51:D4:62:ARG:HB2	51:D4:63:TYR:CE1	2.55	0.41
52:D5:47:PRO:HG2	52:D5:48:GLU:OE1	2.21	0.41
26:DA:117:G:C6	26:DA:119:A:C6	3.09	0.41
26:DA:1449:A:C2	26:DA:1529:G:H1'	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:DA:2070:G:H2'	26:DA:2071:A:C8	2.56	0.41
26:DA:2185:C:H2'	26:DA:2186:G:O4'	2.20	0.41
26:DA:674:G:H1'	30:DF:74:ARG:HD3	2.03	0.41
31:DG:58:GLN:OE1	31:DG:58:GLN:HA	2.21	0.41
37:DQ:58:PHE:CZ	37:DQ:109:VAL:HG21	2.55	0.41
41:DU:85:LYS:HE2	41:DU:85:LYS:HB3	1.77	0.41
1:AA:1278:U:H6	1:AA:1278:U:H3'	1.85	0.41
1:AA:551:U:H2'	1:AA:552:U:C6	2.55	0.41
4:AD:157:LEU:HD23	4:AD:161:ASN:HD21	1.85	0.41
4:AD:88:VAL:HG22	5:AE:97:GLY:HA2	2.01	0.41
6:AF:97:PHE:CB	18:AR:32:ARG:HD3	2.51	0.41
20:AT:10:LEU:HD13	20:AT:12:ALA:HB2	2.01	0.41
24:AX:76:A:OP2	61:AX:3106:HOH:O	2.20	0.41
25:AY:21:A:H4'	25:AY:22:G:OP1	2.21	0.41
25:AY:58:A:H2'	25:AY:58:A:H8	1.72	0.41
26:BA:100:G:H3'	26:BA:102:G:C5'	2.50	0.41
26:BA:1170:G:C2	26:BA:1171:G:H1'	2.55	0.41
26:BA:1550:C:H4'	26:BA:1743:C:O2	2.21	0.41
26:BA:2065:C:H2'	26:BA:2066:C:C6	2.56	0.41
26:BA:2114:A:H2'	26:BA:2115:G:O4'	2.20	0.41
26:BA:2570:G:H2'	26:BA:2571:C:O4'	2.21	0.41
26:BA:2857:G:N2	26:BA:2860:A:OP2	2.43	0.41
26:BA:687:C:H42	26:BA:787:U:H4'	1.86	0.41
26:BA:86:C:H4'	26:BA:104:U:H1'	2.03	0.41
26:BA:947:G:H2'	26:BA:948:G:C8	2.56	0.41
28:BD:121:PRO:HB3	28:BD:135:PHE:CE2	2.56	0.41
28:BD:264:LYS:HA	28:BD:265:PRO:HD3	1.92	0.41
30:BF:11:VAL:HB	30:BF:18:ARG:HB3	2.03	0.41
1:CA:1002:G:C2	1:CA:1003:G:C8	3.09	0.41
1:CA:1133:G:H2'	1:CA:1134:G:O4'	2.20	0.41
1:CA:1198:G:H2'	1:CA:1199:U:C6	2.56	0.41
1:CA:1492:A:H2'	1:CA:1493:A:C5	2.55	0.41
1:CA:1511:G:H2'	1:CA:1512:U:O4'	2.21	0.41
1:CA:429:U:H1'	1:CA:430:A:H5''	2.03	0.41
1:CA:447:G:O6	1:CA:485:G:O2'	2.19	0.41
2:CB:112:VAL:O	2:CB:116:GLU:HB2	2.21	0.41
2:CB:188:ALA:HB1	2:CB:192:SER:OG	2.21	0.41
9:CI:56:LEU:HD23	9:CI:56:LEU:HA	1.86	0.41
26:DA:1283:G:O2'	26:DA:1285:G:N7	2.44	0.41
26:DA:2275:C:H5'	26:DA:2275:C:H6	1.86	0.41
26:DA:2803:C:H2'	26:DA:2804:C:C6	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:DA:821:A:H2'	26:DA:946:G:H5''	2.02	0.41
27:DB:24:G:H4'	27:DB:25:A:N7	2.36	0.41
32:DH:95:ARG:HB3	32:DH:95:ARG:HE	1.77	0.41
37:DQ:29:PHE:HB2	37:DQ:105:GLU:OE2	2.21	0.41
38:DR:28:LEU:HD23	38:DR:28:LEU:HA	1.93	0.41
39:DS:4:LEU:HD23	39:DS:4:LEU:HA	1.76	0.41
44:DX:57:LEU:HD22	44:DX:78:LYS:HG2	2.03	0.41
1:AA:115:G:H4'	1:AA:116:A:O5'	2.20	0.41
1:AA:1324:A:O4'	1:AA:1362:C:H4'	2.21	0.41
1:AA:192:U:O3'	20:AT:57:ARG:HD2	2.20	0.41
1:AA:277:C:H5''	17:AQ:68:ARG:HH22	1.86	0.41
6:AF:36:ARG:NH1	6:AF:36:ARG:HB3	2.36	0.41
7:AG:104:LEU:HD13	7:AG:104:LEU:HA	1.96	0.41
9:AI:49:PRO:HG3	9:AI:101:PHE:HD2	1.86	0.41
25:AY:69:G:H2'	25:AY:70:G:O4'	2.21	0.41
26:BA:1033:U:OP1	56:B9:9:ARG:NH2	2.54	0.41
26:BA:1047:G:O2'	26:BA:1048:A:H8	2.03	0.41
26:BA:2729:G:H2'	26:BA:2730:C:O4'	2.21	0.41
26:BA:528:A:C3'	26:BA:529:A:H5''	2.51	0.41
1:AA:1422:G:C5'	35:BO:48:PRO:HB3	2.44	0.41
35:BO:86:ILE:HG22	35:BO:94:ARG:HG3	2.03	0.41
41:BU:58:ARG:HA	41:BU:61:TRP:CE3	2.56	0.41
1:CA:1003:G:C6	1:CA:1004:A:C2	3.09	0.41
1:CA:1015:A:H2'	1:CA:1016:A:C8	2.56	0.41
1:CA:1029:C:N3	1:CA:1032:G:C2	2.89	0.41
1:CA:1243:C:H2'	1:CA:1244:C:H6	1.85	0.41
2:CB:100:GLY:O	2:CB:104:ASN:N	2.49	0.41
2:CB:48:MET:O	2:CB:52:GLU:N	2.37	0.41
24:CX:31:G:C8	24:CX:32:5MC:HM52	2.56	0.41
25:CY:8:4SU:S4	25:CY:14:A:C8	3.13	0.41
26:DA:1910:G:H2'	26:DA:1911:U:H6	1.85	0.41
26:DA:1268:A:C2	26:DA:2013:A:C4	3.09	0.41
26:DA:2113:U:N3	26:DA:2114:A:N7	2.69	0.41
26:DA:2133:G:O2'	26:DA:2134:A:P	2.79	0.41
26:DA:2761:G:N3	26:DA:2761:G:H2'	2.35	0.41
26:DA:446:G:OP1	41:DU:3:ARG:NH1	2.52	0.41
26:DA:516:C:H1'	26:DA:1261:C:O2'	2.21	0.41
26:DA:571:A:H5'	26:DA:2030:A:N7	2.36	0.41
26:DA:921:G:C6	26:DA:922:U:C4	3.09	0.41
29:DE:46:ALA:HB2	29:DE:82:ARG:HA	2.02	0.41
31:DG:101:ILE:O	31:DG:104:GLU:HB3	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:DG:108:ASN:O	31:DG:112:PRO:HG2	2.21	0.41
41:DU:61:TRP:CH2	41:DU:93:LYS:HB2	2.56	0.41
46:DZ:138:GLU:H	46:DZ:156:LYS:HE2	1.85	0.41
1:AA:1003:G:N2	1:AA:1004:A:N3	2.69	0.41
1:AA:1075:C:C2'	1:AA:1076:C:H5''	2.51	0.41
6:AF:19:LEU:HD11	6:AF:59:TYR:CZ	2.56	0.41
25:AY:21:A:H8	25:AY:21:A:OP2	2.04	0.41
26:BA:1359:A:C2	26:BA:1372:U:O4	2.74	0.41
26:BA:2893:G:H4'	26:BA:2894:G:O5'	2.21	0.41
26:BA:719:C:H2'	26:BA:720:C:C6	2.56	0.41
26:BA:887:A:H4'	26:BA:888:C:H5	1.82	0.41
31:BG:125:PHE:HB3	31:BG:166:ASP:OD1	2.20	0.41
34:BN:138:LEU:HA	34:BN:138:LEU:HD23	1.81	0.41
44:BX:88:LYS:HE3	44:BX:88:LYS:HB3	1.87	0.41
1:CA:1030(A):G:N2	1:CA:1030(C):G:H8	2.19	0.41
1:CA:1030(A):G:H2'	1:CA:1030(C):G:OP2	2.20	0.41
1:CA:1053:G:H4'	1:CA:1054:C:H5'	2.03	0.41
1:CA:344:A:H4'	1:CA:345:C:OP2	2.21	0.41
1:CA:436:C:H2'	1:CA:437:U:H6	1.86	0.41
1:CA:609:A:C5	1:CA:610:G:C8	3.09	0.41
1:CA:946:A:H2'	1:CA:947:G:C8	2.56	0.41
4:CD:18:LYS:HE3	4:CD:20:TYR:CE1	2.55	0.41
4:CD:33:MET:O	4:CD:37:PRO:HB3	2.20	0.41
7:CG:24:THR:O	7:CG:27:ILE:HB	2.21	0.41
10:CJ:6:ILE:N	10:CJ:72:VAL:O	2.36	0.41
14:CN:37:PHE:CE2	14:CN:53:LEU:HD22	2.56	0.41
6:CF:100:ASN:ND2	18:CR:23:LYS:HE3	2.36	0.41
26:DA:649:G:H4'	55:D8:46:ARG:HH22	1.86	0.41
56:D9:17:ILE:HD12	56:D9:17:ILE:HA	1.92	0.41
26:DA:1161:C:H2'	26:DA:1162:G:H8	1.86	0.41
26:DA:2193:G:H2'	26:DA:2194:G:C8	2.56	0.41
26:DA:2706:G:H2'	26:DA:2707:G:O4'	2.21	0.41
26:DA:41:C:H2'	26:DA:42:G:C8	2.56	0.41
26:DA:753:C:H6	26:DA:753:C:OP2	2.03	0.41
26:DA:966:G:H2'	26:DA:967:C:C6	2.55	0.41
33:DI:83:ALA:CB	33:DI:123:LEU:HD21	2.50	0.41
33:DI:86:THR:O	33:DI:123:LEU:HD23	2.21	0.41
35:DO:98:VAL:HG11	35:DO:114:ILE:HG23	2.02	0.41
36:DP:47:ASP:HA	36:DP:48:PRO:HD3	1.85	0.41
38:DR:38:VAL:HG12	38:DR:42:LYS:HE3	2.03	0.41
38:DR:38:VAL:HB	38:DR:39:PRO:HD3	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:DX:35:THR:HG22	44:DX:37:THR:N	2.36	0.41
46:DZ:120:ILE:HD11	46:DZ:173:ALA:CB	2.51	0.41
1:AA:1020:U:H2'	1:AA:1021:G:C8	2.56	0.40
1:AA:1152:A:OP1	10:AJ:68:HIS:ND1	2.52	0.40
1:AA:319:G:H1	1:AA:334:C:H42	1.69	0.40
2:AB:21:ARG:NH2	2:AB:23:ARG:HE	2.19	0.40
3:AC:52:LEU:HD11	3:AC:55:VAL:HG23	2.02	0.40
4:AD:120:LEU:HA	4:AD:120:LEU:HD23	1.82	0.40
4:AD:178:VAL:HG12	4:AD:179:GLU:H	1.86	0.40
25:AY:6:G:C6	25:AY:7:A:C5	3.08	0.40
26:BA:1185:C:H5''	26:BA:1186:G:OP1	2.20	0.40
26:BA:1266:G:O5'	43:BW:15:ARG:NH2	2.54	0.40
26:BA:2113:U:C4	26:BA:2114:A:N7	2.89	0.40
26:BA:2282:G:OP1	26:BA:2283:C:H1'	2.21	0.40
26:BA:2804:C:H2'	26:BA:2805:G:O4'	2.21	0.40
26:BA:614:U:H5'	26:BA:614(C):A:N6	2.35	0.40
31:BG:14:GLU:C	31:BG:17:PRO:HD2	2.42	0.40
46:BZ:146:ILE:HA	46:BZ:147:GLY:HA2	1.77	0.40
46:BZ:92:SER:OG	46:BZ:93:ASP:N	2.55	0.40
1:CA:1134:G:N3	1:CA:1134:G:H2'	2.35	0.40
1:CA:1243:C:H2'	1:CA:1244:C:C6	2.56	0.40
1:CA:1497:G:HO2'	1:CA:1518:A:H2	1.62	0.40
1:CA:64:G:H4'	1:CA:65:U:H3'	2.02	0.40
1:CA:690:G:H8	1:CA:690:G:O5'	2.04	0.40
1:CA:861:G:OP1	8:CH:75:ARG:NH2	2.54	0.40
5:CE:31:LEU:HA	5:CE:31:LEU:HD23	1.86	0.40
1:CA:19:C:H5''	5:CE:86:ALA:HB3	2.03	0.40
7:CG:14:PRO:HG3	7:CG:21:VAL:HG13	2.03	0.40
11:CK:93:GLN:HA	11:CK:93:GLN:HE21	1.86	0.40
23:CW:27:G:H2'	23:CW:28:G:C8	2.56	0.40
26:DA:1309:G:H3'	54:D7:9:ARG:NH1	2.36	0.40
26:DA:1336:A:H2'	26:DA:1337:G:C8	2.56	0.40
26:DA:1853:A:N1	26:DA:2087:G:H1'	2.37	0.40
26:DA:225:A:N6	26:DA:226:G:C2	2.89	0.40
26:DA:2262:U:H4'	26:DA:2328:A:C2	2.57	0.40
26:DA:2849:U:O4	40:DT:23:ARG:NH2	2.43	0.40
26:DA:2849:U:H4'	26:DA:2868:A:C2	2.55	0.40
26:DA:478:A:N1	26:DA:500:G:H4'	2.35	0.40
27:DB:78:A:C2	27:DB:100:A:C4	3.09	0.40
40:DT:108:ARG:HG2	40:DT:111:ARG:NH1	2.32	0.40
42:DV:52:VAL:CG2	42:DV:55:ALA:HB3	2.51	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:DA:299:A:H5''	45:DY:86:ARG:NH2	2.36	0.40
46:DZ:161:VAL:O	46:DZ:161:VAL:HG13	2.20	0.40
1:AA:1223:C:P	19:AS:78:ARG:HH21	2.44	0.40
1:AA:613:C:H2'	1:AA:614:A:C8	2.55	0.40
2:AB:118:LEU:HA	2:AB:118:LEU:HD23	1.84	0.40
8:AH:39:LEU:HD12	8:AH:39:LEU:HA	1.86	0.40
9:AI:50:LEU:HB2	9:AI:55:ALA:HB3	2.04	0.40
15:AO:7:GLU:O	15:AO:11:VAL:HG23	2.21	0.40
18:AR:59:SER:OG	18:AR:62:GLU:HG2	2.22	0.40
1:AA:955:U:O2'	19:AS:83:HIS:HD2	2.03	0.40
20:AT:92:LEU:O	20:AT:96:GLY:HA2	2.22	0.40
25:AY:36:A:C6	25:AY:37:MIA:C5	3.03	0.40
49:B2:23:LYS:O	49:B2:27:GLU:HG3	2.21	0.40
51:B4:16:CYS:SG	51:B4:17:GLY:N	2.94	0.40
53:B6:14:THR:HB	53:B6:48:VAL:O	2.22	0.40
54:B7:8:ASN:HB3	54:B7:11:LYS:HB3	2.02	0.40
26:BA:1223:G:N2	26:BA:1226:A:OP2	2.47	0.40
26:BA:1805:U:O2	28:BD:50:THR:HB	2.21	0.40
26:BA:828:U:C5	26:BA:2247:A:H4'	2.56	0.40
26:BA:817:C:H4'	26:BA:932:G:C5	2.56	0.40
28:BD:180:GLY:HA3	28:BD:275:LYS:HB2	2.03	0.40
30:BF:150:GLY:HA2	30:BF:172:TRP:CE3	2.56	0.40
26:BA:2278:A:OP1	37:BQ:11:LYS:HD2	2.22	0.40
26:BA:1161:C:O2'	42:BV:8:GLY:HA2	2.21	0.40
1:CA:1277:C:O2'	1:CA:1279:A:C8	2.66	0.40
1:CA:1414:U:H3	1:CA:1486:G:H1	1.68	0.40
1:CA:149:A:H2'	1:CA:150:C:C6	2.56	0.40
1:CA:993:G:O2'	1:CA:994:A:N7	2.51	0.40
2:CB:219:VAL:O	2:CB:222:ILE:HG12	2.21	0.40
4:CD:22:LYS:HB2	4:CD:26:CYS:SG	2.60	0.40
7:CG:65:ALA:HB1	7:CG:127:ALA:HB3	2.02	0.40
8:CH:69:ARG:NH2	8:CH:75:ARG:O	2.53	0.40
14:CN:23:ARG:HG3	14:CN:28:GLY:O	2.21	0.40
19:CS:69:HIS:HD2	19:CS:73:GLU:OE1	2.05	0.40
22:CV:14:A:C2	25:CY:34:G:C2	3.10	0.40
23:CW:9:A:OP2	23:CW:13:C:N4	2.47	0.40
24:CX:2:G:H5'	57:CX:3002:MG:MG	1.46	0.40
24:CX:43:A:H2'	24:CX:44:A:C8	2.56	0.40
26:DA:1394:U:C4	26:DA:1395:A:C5	3.10	0.40
26:DA:565:C:H2'	26:DA:566:U:O4'	2.20	0.40
26:DA:820:A:N3	26:DA:943:U:H4'	2.36	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:DB:110:G:O2'	27:DB:111:G:H5'	2.21	0.40
27:DB:33:G:C6	27:DB:34:U:N3	2.89	0.40
27:DB:42:C:O2'	31:DG:66:GLN:HG2	2.21	0.40
29:DE:30:PRO:HD3	29:DE:180:ASN:ND2	2.35	0.40
30:DF:59:TYR:HE2	30:DF:85:GLY:O	2.04	0.40
30:DF:93:LYS:HD3	30:DF:93:LYS:HA	1.86	0.40
31:DG:125:PHE:HB3	31:DG:166:ASP:CG	2.42	0.40
35:DO:47:ILE:HB	35:DO:48:PRO:HD2	2.04	0.40
38:DR:38:VAL:HG22	38:DR:112:ALA:HB2	2.03	0.40
38:DR:63:ARG:O	38:DR:67:LEU:HB2	2.22	0.40
1:AA:1272:G:H2'	1:AA:1273:G:O4'	2.22	0.40
1:AA:271:C:H2'	1:AA:272:C:H6	1.87	0.40
1:AA:542:G:O3'	4:AD:14:ARG:NH2	2.53	0.40
1:AA:936:C:H2'	1:AA:937:A:O4'	2.20	0.40
3:AC:121:ALA:HB1	3:AC:189:ALA:HB2	2.04	0.40
4:AD:11:LEU:HG	4:AD:66:ARG:HD3	2.03	0.40
9:AI:33:PHE:HD1	9:AI:34:ASN:ND2	2.20	0.40
10:AJ:90:LEU:HA	10:AJ:91:PRO:HD3	1.92	0.40
1:AA:189(F):U:C2	17:AQ:72:ARG:NH2	2.90	0.40
20:AT:56:MET:HE3	20:AT:88:VAL:HG21	2.03	0.40
25:AY:58:A:O2'	25:AY:60:U:OP2	2.29	0.40
47:B0:50:ASN:HB3	47:B0:63:VAL:HG22	2.02	0.40
26:BA:1174:A:H1'	26:BA:1175:U:C5'	2.50	0.40
26:BA:570:G:H2'	26:BA:2030:A:N7	2.37	0.40
26:BA:2274:A:C5	26:BA:2276:G:C8	3.10	0.40
26:BA:2615:U:H2'	26:BA:2616:C:C6	2.56	0.40
26:BA:923:C:H2'	26:BA:924:C:C6	2.56	0.40
28:BD:4:LYS:HB3	28:BD:18:VAL:HG23	2.04	0.40
1:CA:1084:G:H1'	1:CA:1102:A:N7	2.36	0.40
1:CA:1286:A:H3'	1:CA:1286:A:H8	1.85	0.40
1:CA:453:A:H4'	16:CP:72:ARG:HG3	2.02	0.40
1:CA:630:G:O2'	1:CA:631:G:H5'	2.21	0.40
1:CA:697:U:H2'	1:CA:698:G:H5'	2.04	0.40
1:CA:828:A:H4'	1:CA:828:A:OP1	2.21	0.40
2:CB:28:PHE:O	2:CB:32:ILE:HG13	2.21	0.40
4:CD:108:LEU:HB3	4:CD:110:PHE:CE1	2.56	0.40
7:CG:26:PHE:HE1	7:CG:30:ILE:HD11	1.87	0.40
12:CL:27:LEU:HD23	12:CL:30:ALA:O	2.22	0.40
3:CC:29:TYR:CZ	14:CN:54:PRO:HG2	2.57	0.40
51:D4:62:ARG:N	51:D4:62:ARG:HD3	2.35	0.40
26:DA:2022:U:OP2	52:D5:15:ARG:NH2	2.54	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:D5:49:CYS:SG	52:D5:51:TYR:HB2	2.61	0.40
26:DA:1014:U:H2'	26:DA:1015:G:C8	2.55	0.40
26:DA:1611:C:C2'	26:DA:1612:C:H5'	2.50	0.40
26:DA:2155:G:C2'	26:DA:2156:G:H5'	2.52	0.40
26:DA:234:C:H2'	26:DA:235:U:H6	1.87	0.40
26:DA:1669:A:H5''	26:DA:2550:G:OP1	2.21	0.40
26:DA:856:C:H2'	26:DA:857:C:C6	2.56	0.40
26:DA:866:A:C6	26:DA:914:C:C5	3.10	0.40
29:DE:85:ASN:HA	29:DE:86:PRO:HD2	1.84	0.40
31:DG:115:ARG:HG2	31:DG:136:ARG:HH21	1.85	0.40
33:DI:92:VAL:HG22	33:DI:120:ILE:HB	2.03	0.40
34:DN:60:ILE:HG13	34:DN:61:ARG:N	2.36	0.40
42:DV:24:LYS:HA	42:DV:92:THR:OG1	2.21	0.40
46:DZ:79:ARG:HB2	46:DZ:80:ARG:NH1	2.36	0.40
1:AA:1024:G:H2'	1:AA:1025:U:H5'	2.04	0.40
1:AA:148:G:H2'	1:AA:149:A:C8	2.50	0.40
1:AA:390:C:H2'	1:AA:391:G:C8	2.56	0.40
1:AA:933:G:O6	7:AG:3:ARG:NH2	2.52	0.40
2:AB:19:HIS:CG	2:AB:20:GLU:H	2.39	0.40
2:AB:8:LYS:HG2	2:AB:8:LYS:H	1.51	0.40
7:AG:14:PRO:HG3	7:AG:21:VAL:HG13	2.03	0.40
10:AJ:26:ALA:O	10:AJ:30:SER:OG	2.39	0.40
13:AM:97:PRO:HG2	13:AM:103:THR:HG22	2.04	0.40
13:AM:88:ARG:HG3	13:AM:98:VAL:CG1	2.52	0.40
19:AS:15:LEU:O	19:AS:19:VAL:HG23	2.21	0.40
19:AS:69:HIS:HD2	19:AS:73:GLU:OE1	2.05	0.40
24:AX:19:G:H5''	24:AX:60:U:O4	2.21	0.40
52:B5:35:GLU:HG3	52:B5:51:TYR:CD2	2.57	0.40
26:BA:1406:U:H2'	26:BA:1407:C:H6	1.86	0.40
26:BA:2070:G:H2'	26:BA:2071:A:C8	2.57	0.40
26:BA:2355:C:H5'	61:BA:3944:HOH:O	2.22	0.40
26:BA:2398:U:H2'	26:BA:2399:G:C8	2.57	0.40
26:BA:589:C:H2'	26:BA:590:A:C8	2.56	0.40
28:BD:19:ALA:HB3	28:BD:21:PHE:CE1	2.56	0.40
30:BF:64:ILE:HG13	30:BF:65:TRP:N	2.37	0.40
42:BV:49:THR:HG22	42:BV:49:THR:O	2.21	0.40
44:BX:94:GLY:N	44:BX:95:LEU:HA	2.36	0.40
45:BY:83:THR:HG21	45:BY:99:CYS:HB2	2.02	0.40
1:CA:1075:C:H42	1:CA:1082:G:H1	1.68	0.40
1:CA:1164:G:O2'	1:CA:1165:C:H5'	2.22	0.40
1:CA:1360:A:H2'	1:CA:1361:G:O4'	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:1429:C:H2'	1:CA:1430:C:C6	2.57	0.40
1:CA:1479:C:H2'	1:CA:1480:G:C8	2.56	0.40
1:CA:57:G:H2'	1:CA:58:C:C6	2.57	0.40
2:CB:16:HIS:ND1	2:CB:17:PHE:N	2.68	0.40
2:CB:53:ARG:CZ	2:CB:53:ARG:HB3	2.50	0.40
3:CC:109:PRO:HB3	3:CC:115:LEU:HD23	2.03	0.40
3:CC:178:LEU:HA	3:CC:178:LEU:HD13	1.93	0.40
8:CH:119:LEU:HB3	8:CH:123:GLU:CB	2.51	0.40
8:CH:25:ASP:N	8:CH:25:ASP:OD1	2.55	0.40
9:CI:23:ASN:HD22	9:CI:24:GLY:N	2.20	0.40
1:CA:1226:C:H4'	19:CS:80:TYR:CZ	2.57	0.40
48:D1:5:CYS:SG	48:D1:62:VAL:HG23	2.62	0.40
49:D2:64:LEU:O	49:D2:68:ARG:HG3	2.22	0.40
50:D3:23:LEU:HD13	50:D3:50:VAL:HG11	2.02	0.40
26:DA:1486:A:O2'	26:DA:1487:G:H5'	2.21	0.40
24:CX:12:G:H4'	26:DA:1908:C:O2	2.21	0.40
26:DA:2174:C:H2'	26:DA:2174:C:O2	2.21	0.40
26:DA:2462:U:H2'	26:DA:2463:C:C6	2.56	0.40
26:DA:2741:A:H2'	26:DA:2742:C:O4'	2.21	0.40
26:DA:2756:U:H1'	26:DA:2757:A:H5''	2.02	0.40
26:DA:335:C:H4'	45:DY:73:ARG:NE	2.37	0.40
26:DA:428:A:H3'	26:DA:429:A:H8	1.87	0.40
26:DA:443:A:H5''	26:DA:444:C:OP1	2.21	0.40
26:DA:570:G:H2'	26:DA:2030:A:C5	2.56	0.40
26:DA:892:G:H2'	26:DA:893:C:C4'	2.52	0.40
31:DG:31:VAL:HA	31:DG:32:PRO:HD2	1.72	0.40
36:DP:84:ASN:OD1	36:DP:117:GLU:HB2	2.20	0.40
40:DT:94:ALA:HB1	40:DT:99:LEU:HD21	2.02	0.40
26:DA:996:A:O3'	41:DU:91:ASP:HB2	2.22	0.40
1:AA:1002:G:C6	1:AA:1003:G:C2	3.10	0.40
1:AA:1151:A:O2'	1:AA:1152:A:H8	2.05	0.40
1:AA:512:U:H2'	1:AA:513:C:C6	2.56	0.40
2:AB:215:LEU:HD23	2:AB:215:LEU:HA	1.79	0.40
3:AC:82:GLU:HA	3:AC:85:ARG:CZ	2.51	0.40
4:AD:18:LYS:HE3	4:AD:20:TYR:CZ	2.56	0.40
6:AF:22:GLU:O	6:AF:26:ILE:HG13	2.22	0.40
6:AF:55:ASP:HA	6:AF:56:PRO:HD2	1.98	0.40
13:AM:39:ILE:HG13	13:AM:56:LEU:HD12	2.03	0.40
25:AY:26:A:N1	25:AY:44:G:N2	2.54	0.40
26:BA:370:G:H4'	26:BA:371:A:OP2	2.21	0.40
30:BF:106:ARG:HG2	30:BF:106:ARG:H	1.70	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:BA:674:G:O2'	30:BF:74:ARG:HD3	2.22	0.40
1:CA:1154:G:O6	1:CA:1155:G:C6	2.75	0.40
1:CA:1367:C:O2'	10:CJ:62:HIS:HE1	2.04	0.40
1:CA:1496:C:H2'	1:CA:1497:G:O4'	2.20	0.40
1:CA:243:A:C2	1:CA:246:A:C8	3.10	0.40
2:CB:28:PHE:CD2	2:CB:190:THR:HA	2.56	0.40
7:CG:52:GLU:H	7:CG:52:GLU:HG2	1.62	0.40
1:CA:1350:A:OP1	9:CI:121:ARG:HD3	2.21	0.40
14:CN:9:LYS:HG3	14:CN:12:ARG:HH11	1.86	0.40
24:CX:66:C:H2'	24:CX:67:C:O4'	2.22	0.40
25:CY:29:G:N1	25:CY:41:C:N4	2.69	0.40
50:D3:10:LYS:HB3	50:D3:53:LEU:HA	2.02	0.40
51:D4:28:LYS:HA	51:D4:29:PRO:HD3	1.84	0.40
26:DA:1001:A:H2'	26:DA:1002:G:O4'	2.21	0.40
26:DA:1221(A):C:C2	26:DA:1229:G:C2	3.09	0.40
26:DA:1241:A:O2'	26:DA:1242:A:H5'	2.21	0.40
26:DA:2507:C:H2'	26:DA:2508:G:O4'	2.22	0.40
26:DA:305:U:H2'	26:DA:306:U:C6	2.56	0.40
26:DA:56:A:H2'	26:DA:57:C:O4'	2.22	0.40
26:DA:832:G:H5'	36:DP:45:LEU:HD21	2.04	0.40
26:DA:933:A:H2'	26:DA:934:G:O4'	2.22	0.40
34:DN:115:ARG:HA	34:DN:118:LYS:HE3	2.02	0.40
26:DA:2294:C:P	39:DS:89:ARG:HH22	2.44	0.40
46:DZ:171:ILE:HG13	46:DZ:171:ILE:H	1.65	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	AB	229/256 (90%)	208 (91%)	14 (6%)	7 (3%)	4 3

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	CB	229/256 (90%)	206 (90%)	16 (7%)	7 (3%)	4	3
3	AC	204/239 (85%)	195 (96%)	8 (4%)	1 (0%)	29	40
3	CC	204/239 (85%)	189 (93%)	15 (7%)	0	100	100
4	AD	206/209 (99%)	197 (96%)	7 (3%)	2 (1%)	15	22
4	CD	206/209 (99%)	196 (95%)	9 (4%)	1 (0%)	29	40
5	AE	146/162 (90%)	142 (97%)	4 (3%)	0	100	100
5	CE	146/162 (90%)	140 (96%)	6 (4%)	0	100	100
6	AF	98/101 (97%)	97 (99%)	1 (1%)	0	100	100
6	CF	98/101 (97%)	97 (99%)	1 (1%)	0	100	100
7	AG	153/156 (98%)	144 (94%)	5 (3%)	4 (3%)	5	5
7	CG	153/156 (98%)	144 (94%)	8 (5%)	1 (1%)	22	30
8	AH	135/138 (98%)	134 (99%)	1 (1%)	0	100	100
8	CH	135/138 (98%)	132 (98%)	3 (2%)	0	100	100
9	AI	125/128 (98%)	117 (94%)	8 (6%)	0	100	100
9	CI	125/128 (98%)	119 (95%)	5 (4%)	1 (1%)	19	27
10	AJ	95/105 (90%)	85 (90%)	6 (6%)	4 (4%)	3	1
10	CJ	94/105 (90%)	85 (90%)	4 (4%)	5 (5%)	2	0
11	AK	112/129 (87%)	104 (93%)	6 (5%)	2 (2%)	8	10
11	CK	112/129 (87%)	103 (92%)	7 (6%)	2 (2%)	8	10
12	AL	120/132 (91%)	117 (98%)	3 (2%)	0	100	100
12	CL	120/132 (91%)	118 (98%)	2 (2%)	0	100	100
13	AM	121/126 (96%)	116 (96%)	5 (4%)	0	100	100
13	CM	120/126 (95%)	113 (94%)	7 (6%)	0	100	100
14	AN	58/61 (95%)	56 (97%)	2 (3%)	0	100	100
14	CN	58/61 (95%)	56 (97%)	2 (3%)	0	100	100
15	AO	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
15	CO	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
16	AP	80/88 (91%)	79 (99%)	1 (1%)	0	100	100
16	CP	80/88 (91%)	78 (98%)	1 (1%)	1 (1%)	12	16
17	AQ	97/105 (92%)	93 (96%)	4 (4%)	0	100	100
17	CQ	97/105 (92%)	93 (96%)	4 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	AR	66/88 (75%)	65 (98%)	1 (2%)	0	100	100
18	CR	66/88 (75%)	65 (98%)	1 (2%)	0	100	100
19	AS	81/93 (87%)	73 (90%)	7 (9%)	1 (1%)	13	17
19	CS	81/93 (87%)	72 (89%)	9 (11%)	0	100	100
20	AT	94/106 (89%)	87 (93%)	3 (3%)	4 (4%)	2	1
20	CT	94/106 (89%)	88 (94%)	3 (3%)	3 (3%)	4	3
21	AU	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
21	CU	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
28	BD	273/276 (99%)	264 (97%)	8 (3%)	1 (0%)	34	46
28	DD	273/276 (99%)	263 (96%)	8 (3%)	2 (1%)	22	30
29	BE	202/206 (98%)	196 (97%)	5 (2%)	1 (0%)	29	40
29	DE	202/206 (98%)	196 (97%)	4 (2%)	2 (1%)	15	22
30	BF	201/210 (96%)	200 (100%)	0	1 (0%)	29	40
30	DF	201/210 (96%)	199 (99%)	0	2 (1%)	15	22
31	BG	179/182 (98%)	170 (95%)	8 (4%)	1 (1%)	25	34
31	DG	179/182 (98%)	171 (96%)	5 (3%)	3 (2%)	9	11
32	BH	172/180 (96%)	168 (98%)	3 (2%)	1 (1%)	25	34
32	DH	172/180 (96%)	166 (96%)	5 (3%)	1 (1%)	25	34
33	BI	144/148 (97%)	130 (90%)	11 (8%)	3 (2%)	7	7
33	DI	144/148 (97%)	133 (92%)	10 (7%)	1 (1%)	22	30
34	BN	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
34	DN	138/140 (99%)	135 (98%)	2 (1%)	1 (1%)	22	30
35	BO	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
35	DO	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
36	BP	147/150 (98%)	140 (95%)	6 (4%)	1 (1%)	22	30
36	DP	147/150 (98%)	138 (94%)	7 (5%)	2 (1%)	11	15
37	BQ	139/141 (99%)	135 (97%)	4 (3%)	0	100	100
37	DQ	139/141 (99%)	134 (96%)	4 (3%)	1 (1%)	22	30
38	BR	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
38	DR	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
39	BS	108/112 (96%)	104 (96%)	3 (3%)	1 (1%)	17	24

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	DS	108/112 (96%)	105 (97%)	2 (2%)	1 (1%)	17	24
40	BT	129/146 (88%)	122 (95%)	7 (5%)	0	100	100
40	DT	129/146 (88%)	127 (98%)	2 (2%)	0	100	100
41	BU	114/118 (97%)	114 (100%)	0	0	100	100
41	DU	114/118 (97%)	114 (100%)	0	0	100	100
42	BV	99/101 (98%)	93 (94%)	6 (6%)	0	100	100
42	DV	99/101 (98%)	95 (96%)	3 (3%)	1 (1%)	15	22
43	BW	110/113 (97%)	110 (100%)	0	0	100	100
43	DW	110/113 (97%)	110 (100%)	0	0	100	100
44	BX	93/96 (97%)	89 (96%)	4 (4%)	0	100	100
44	DX	93/96 (97%)	89 (96%)	4 (4%)	0	100	100
45	BY	105/110 (96%)	98 (93%)	7 (7%)	0	100	100
45	DY	105/110 (96%)	101 (96%)	4 (4%)	0	100	100
46	BZ	169/206 (82%)	153 (90%)	15 (9%)	1 (1%)	25	34
46	DZ	172/206 (84%)	161 (94%)	11 (6%)	0	100	100
47	B0	81/85 (95%)	81 (100%)	0	0	100	100
47	D0	81/85 (95%)	79 (98%)	2 (2%)	0	100	100
48	B1	95/98 (97%)	94 (99%)	0	1 (1%)	14	19
48	D1	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	14	19
49	B2	68/72 (94%)	68 (100%)	0	0	100	100
49	D2	68/72 (94%)	68 (100%)	0	0	100	100
50	B3	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
50	D3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
51	B4	67/71 (94%)	53 (79%)	11 (16%)	3 (4%)	2	1
51	D4	67/71 (94%)	53 (79%)	9 (13%)	5 (8%)	1	0
52	B5	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
52	D5	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
53	B6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
53	D6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
54	B7	46/49 (94%)	46 (100%)	0	0	100	100
54	D7	46/49 (94%)	45 (98%)	0	1 (2%)	6	7

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
55	B8	62/65 (95%)	62 (100%)	0	0	100	100
55	D8	62/65 (95%)	62 (100%)	0	0	100	100
56	B9	35/37 (95%)	35 (100%)	0	0	100	100
56	D9	35/37 (95%)	35 (100%)	0	0	100	100
All	All	11409/12128 (94%)	10908 (96%)	416 (4%)	85 (1%)	22	30

All (85) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	126	GLU
7	AG	80	VAL
20	AT	10	LEU
20	AT	96	GLY
28	BD	275	LYS
29	BE	52	LEU
30	BF	130	ALA
33	BI	107	VAL
51	B4	55	ARG
2	CB	16	HIS
2	CB	20	GLU
2	CB	126	GLU
4	CD	46	LYS
9	CI	54	ASP
10	CJ	79	ARG
20	CT	99	LEU
30	DF	21	ALA
30	DF	130	ALA
33	DI	10	GLU
36	DP	29	LYS
51	D4	39	CYS
51	D4	63	TYR
54	D7	46	VAL
2	AB	10	LEU
2	AB	19	HIS
4	AD	166	LYS
7	AG	8	GLU
7	AG	81	GLY
10	AJ	31	GLY
10	AJ	56	HIS
11	AK	49	GLY
20	AT	47	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
33	BI	106	GLY
48	B1	3	LYS
51	B4	54	GLY
51	B4	57	GLU
2	CB	8	LYS
2	CB	9	GLU
10	CJ	56	HIS
10	CJ	77	PRO
11	CK	49	GLY
20	CT	47	GLY
20	CT	95	ALA
29	DE	52	LEU
31	DG	81	LYS
32	DH	126	PRO
37	DQ	28	ALA
51	D4	45	GLY
2	AB	20	GLU
4	AD	164	ALA
10	AJ	79	ARG
19	AS	42	PRO
20	AT	95	ALA
31	BG	47	LYS
32	BH	126	PRO
39	BS	60	GLY
46	BZ	152	ALA
11	CK	105	VAL
28	DD	239	ARG
34	DN	2	LYS
39	DS	84	GLN
33	BI	73	GLU
36	BP	29	LYS
2	CB	10	LEU
10	CJ	55	LYS
28	DD	3	VAL
31	DG	32	PRO
31	DG	47	LYS
36	DP	45	LEU
48	D1	3	LYS
51	D4	55	ARG
10	AJ	91	PRO
29	DE	73	GLU
51	D4	62	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	AB	231	GLU
3	AC	66	VAL
2	CB	231	GLU
7	CG	17	VAL
16	CP	53	VAL
11	AK	105	VAL
2	AB	124	SER
10	CJ	91	PRO
42	DV	79	VAL
7	AG	17	VAL
2	AB	125	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	192/220 (87%)	163 (85%)	29 (15%)	3	2
2	CB	187/220 (85%)	149 (80%)	38 (20%)	1	1
3	AC	143/188 (76%)	121 (85%)	22 (15%)	2	2
3	CC	140/188 (74%)	124 (89%)	16 (11%)	5	5
4	AD	170/181 (94%)	152 (89%)	18 (11%)	6	7
4	CD	173/181 (96%)	152 (88%)	21 (12%)	5	4
5	AE	113/123 (92%)	105 (93%)	8 (7%)	14	19
5	CE	114/123 (93%)	101 (89%)	13 (11%)	5	5
6	AF	83/90 (92%)	76 (92%)	7 (8%)	11	13
6	CF	85/90 (94%)	80 (94%)	5 (6%)	19	25
7	AG	119/127 (94%)	108 (91%)	11 (9%)	9	11
7	CG	120/127 (94%)	109 (91%)	11 (9%)	9	11
8	AH	114/119 (96%)	105 (92%)	9 (8%)	12	15
8	CH	114/119 (96%)	107 (94%)	7 (6%)	18	24
9	AI	90/99 (91%)	76 (84%)	14 (16%)	2	2

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	CI	89/99 (90%)	76 (85%)	13 (15%)	3	2
10	AJ	66/92 (72%)	58 (88%)	8 (12%)	5	4
10	CJ	69/92 (75%)	63 (91%)	6 (9%)	10	12
11	AK	82/99 (83%)	77 (94%)	5 (6%)	18	24
11	CK	83/99 (84%)	76 (92%)	7 (8%)	11	13
12	AL	97/109 (89%)	93 (96%)	4 (4%)	30	41
12	CL	97/109 (89%)	93 (96%)	4 (4%)	30	41
13	AM	93/101 (92%)	82 (88%)	11 (12%)	5	5
13	CM	92/101 (91%)	80 (87%)	12 (13%)	4	3
14	AN	49/50 (98%)	42 (86%)	7 (14%)	3	3
14	CN	49/50 (98%)	41 (84%)	8 (16%)	2	2
15	AO	78/80 (98%)	64 (82%)	14 (18%)	2	1
15	CO	78/80 (98%)	69 (88%)	9 (12%)	5	5
16	AP	69/74 (93%)	60 (87%)	9 (13%)	4	3
16	CP	68/74 (92%)	61 (90%)	7 (10%)	7	7
17	AQ	94/97 (97%)	85 (90%)	9 (10%)	8	9
17	CQ	94/97 (97%)	87 (93%)	7 (7%)	13	18
18	AR	59/77 (77%)	54 (92%)	5 (8%)	10	13
18	CR	59/77 (77%)	52 (88%)	7 (12%)	5	5
19	AS	69/80 (86%)	64 (93%)	5 (7%)	14	18
19	CS	67/80 (84%)	63 (94%)	4 (6%)	19	25
20	AT	70/82 (85%)	62 (89%)	8 (11%)	5	5
20	CT	70/82 (85%)	62 (89%)	8 (11%)	5	5
21	AU	18/22 (82%)	15 (83%)	3 (17%)	2	2
21	CU	18/22 (82%)	17 (94%)	1 (6%)	21	28
28	BD	215/218 (99%)	195 (91%)	20 (9%)	9	10
28	DD	215/218 (99%)	193 (90%)	22 (10%)	7	8
29	BE	164/166 (99%)	146 (89%)	18 (11%)	6	6
29	DE	164/166 (99%)	145 (88%)	19 (12%)	5	5
30	BF	160/166 (96%)	149 (93%)	11 (7%)	15	20
30	DF	159/166 (96%)	144 (91%)	15 (9%)	8	10

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	BG	143/156 (92%)	128 (90%)	15 (10%)	7	7
31	DG	142/156 (91%)	122 (86%)	20 (14%)	3	3
32	BH	144/148 (97%)	126 (88%)	18 (12%)	4	4
32	DH	144/148 (97%)	126 (88%)	18 (12%)	4	4
33	BI	110/124 (89%)	86 (78%)	24 (22%)	1	1
33	DI	104/124 (84%)	88 (85%)	16 (15%)	2	2
34	BN	118/119 (99%)	103 (87%)	15 (13%)	4	4
34	DN	118/119 (99%)	106 (90%)	12 (10%)	7	8
35	BO	100/100 (100%)	93 (93%)	7 (7%)	15	19
35	DO	100/100 (100%)	93 (93%)	7 (7%)	15	19
36	BP	115/116 (99%)	98 (85%)	17 (15%)	3	2
36	DP	115/116 (99%)	100 (87%)	15 (13%)	4	3
37	BQ	111/111 (100%)	95 (86%)	16 (14%)	3	3
37	DQ	111/111 (100%)	99 (89%)	12 (11%)	6	6
38	BR	101/101 (100%)	82 (81%)	19 (19%)	1	1
38	DR	101/101 (100%)	83 (82%)	18 (18%)	2	1
39	BS	87/88 (99%)	81 (93%)	6 (7%)	15	20
39	DS	85/88 (97%)	75 (88%)	10 (12%)	5	5
40	BT	115/127 (91%)	106 (92%)	9 (8%)	12	16
40	DT	113/127 (89%)	103 (91%)	10 (9%)	10	12
41	BU	93/94 (99%)	84 (90%)	9 (10%)	8	9
41	DU	93/94 (99%)	85 (91%)	8 (9%)	10	13
42	BV	80/82 (98%)	68 (85%)	12 (15%)	3	2
42	DV	80/82 (98%)	67 (84%)	13 (16%)	2	2
43	BW	90/92 (98%)	83 (92%)	7 (8%)	12	16
43	DW	90/92 (98%)	83 (92%)	7 (8%)	12	16
44	BX	77/78 (99%)	71 (92%)	6 (8%)	12	16
44	DX	77/78 (99%)	71 (92%)	6 (8%)	12	16
45	BY	85/91 (93%)	75 (88%)	10 (12%)	5	5
45	DY	85/91 (93%)	79 (93%)	6 (7%)	14	19
46	BZ	145/179 (81%)	133 (92%)	12 (8%)	11	14

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	DZ	145/179 (81%)	129 (89%)	16 (11%)	6	6
47	B0	65/67 (97%)	62 (95%)	3 (5%)	27	36
47	D0	65/67 (97%)	60 (92%)	5 (8%)	13	16
48	B1	80/83 (96%)	73 (91%)	7 (9%)	10	12
48	D1	80/83 (96%)	71 (89%)	9 (11%)	6	5
49	B2	65/67 (97%)	57 (88%)	8 (12%)	4	4
49	D2	65/67 (97%)	59 (91%)	6 (9%)	9	11
50	B3	51/52 (98%)	46 (90%)	5 (10%)	8	9
50	D3	50/52 (96%)	44 (88%)	6 (12%)	5	5
51	B4	60/63 (95%)	47 (78%)	13 (22%)	1	1
51	D4	53/63 (84%)	43 (81%)	10 (19%)	1	1
52	B5	50/52 (96%)	45 (90%)	5 (10%)	7	8
52	D5	50/52 (96%)	46 (92%)	4 (8%)	12	15
53	B6	51/52 (98%)	44 (86%)	7 (14%)	3	3
53	D6	50/52 (96%)	48 (96%)	2 (4%)	31	43
54	B7	41/42 (98%)	38 (93%)	3 (7%)	14	18
54	D7	41/42 (98%)	38 (93%)	3 (7%)	14	18
55	B8	53/55 (96%)	49 (92%)	4 (8%)	13	17
55	D8	54/55 (98%)	51 (94%)	3 (6%)	21	28
56	B9	34/34 (100%)	34 (100%)	0	100	100
56	D9	34/34 (100%)	32 (94%)	2 (6%)	19	25
All	All	9320/10066 (93%)	8304 (89%)	1016 (11%)	6	6

All (1016) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	AB	8	LYS
2	AB	10	LEU
2	AB	11	LEU
2	AB	15	VAL
2	AB	17	PHE
2	AB	21	ARG
2	AB	23	ARG
2	AB	24	TRP
2	AB	49	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	AB	64	ARG
2	AB	67	THR
2	AB	76	GLN
2	AB	94	ASN
2	AB	108	ILE
2	AB	111	ARG
2	AB	114	ARG
2	AB	127	ILE
2	AB	144	ARG
2	AB	145	LEU
2	AB	153	ARG
2	AB	155	LEU
2	AB	156	LYS
2	AB	157	ARG
2	AB	160	ASP
2	AB	170	GLU
2	AB	187	LEU
2	AB	200	ILE
2	AB	221	LEU
2	AB	230	VAL
3	AC	3	ASN
3	AC	26	LYS
3	AC	27	LYS
3	AC	28	GLN
3	AC	32	LEU
3	AC	37	GLN
3	AC	45	LYS
3	AC	49	SER
3	AC	70	VAL
3	AC	77	ILE
3	AC	97	LYS
3	AC	98	ASN
3	AC	104	GLN
3	AC	115	LEU
3	AC	118	GLN
3	AC	119	ARG
3	AC	127	ARG
3	AC	140	ARG
3	AC	144	SER
3	AC	181	ASN
3	AC	196	LEU
3	AC	198	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	AD	5	ILE
4	AD	31	CYS
4	AD	49	ARG
4	AD	52	SER
4	AD	53	ASP
4	AD	58	LEU
4	AD	63	LYS
4	AD	86	LYS
4	AD	108	LEU
4	AD	122	ARG
4	AD	127	THR
4	AD	135	LEU
4	AD	139	ARG
4	AD	141	ARG
4	AD	144	ASP
4	AD	158	ILE
4	AD	168	ARG
4	AD	188	LEU
5	AE	6	PHE
5	AE	12	LEU
5	AE	31	LEU
5	AE	38	GLN
5	AE	41	VAL
5	AE	47	LYS
5	AE	73	ASN
5	AE	145	LYS
6	AF	36	ARG
6	AF	40	VAL
6	AF	55	ASP
6	AF	69	GLU
6	AF	74	ASP
6	AF	75	LEU
6	AF	82	ARG
7	AG	8	GLU
7	AG	12	LEU
7	AG	50	ILE
7	AG	51	GLN
7	AG	52	GLU
7	AG	53	LYS
7	AG	76	ARG
7	AG	79	ARG
7	AG	104	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	AG	113	GLU
7	AG	155	ARG
8	AH	21	LYS
8	AH	29	SER
8	AH	39	LEU
8	AH	52	ASP
8	AH	78	GLN
8	AH	84	ARG
8	AH	109	ILE
8	AH	112	LEU
8	AH	127	LEU
9	AI	14	VAL
9	AI	17	VAL
9	AI	23	ASN
9	AI	42	ARG
9	AI	53	VAL
9	AI	56	LEU
9	AI	81	ILE
9	AI	86	VAL
9	AI	89	ASN
9	AI	103	THR
9	AI	108	VAL
9	AI	121	ARG
9	AI	127	LYS
9	AI	128	ARG
10	AJ	16	LEU
10	AJ	17	ASP
10	AJ	43	ARG
10	AJ	66	ARG
10	AJ	81	THR
10	AJ	84	GLN
10	AJ	94	VAL
10	AJ	100	THR
11	AK	14	VAL
11	AK	16	SER
11	AK	31	THR
11	AK	48	ILE
11	AK	96	ARG
12	AL	33	ARG
12	AL	46	LYS
12	AL	52	LEU
12	AL	83	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	AM	4	ILE
13	AM	15	VAL
13	AM	27	LYS
13	AM	43	THR
13	AM	49	THR
13	AM	52	GLU
13	AM	70	LEU
13	AM	73	GLU
13	AM	84	ILE
13	AM	110	ARG
13	AM	121	LYS
14	AN	3	ARG
14	AN	7	ILE
14	AN	18	VAL
14	AN	23	ARG
14	AN	26	ARG
14	AN	32	SER
14	AN	50	LYS
15	AO	3	ILE
15	AO	5	LYS
15	AO	21	ASP
15	AO	22	THR
15	AO	26	GLU
15	AO	39	LEU
15	AO	41	GLU
15	AO	47	LYS
15	AO	64	ARG
15	AO	66	LEU
15	AO	71	GLN
15	AO	76	GLU
15	AO	83	GLU
15	AO	84	LYS
16	AP	1	MET
16	AP	2	VAL
16	AP	19	ILE
16	AP	20	VAL
16	AP	50	LYS
16	AP	54	GLU
16	AP	60	LEU
16	AP	62	VAL
16	AP	67	THR
17	AQ	14	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
17	AQ	19	VAL
17	AQ	24	GLU
17	AQ	60	ILE
17	AQ	63	ARG
17	AQ	72	ARG
17	AQ	74	LEU
17	AQ	91	ARG
17	AQ	98	LEU
18	AR	31	LEU
18	AR	37	VAL
18	AR	38	GLU
18	AR	46	GLU
18	AR	76	LEU
19	AS	12	ASP
19	AS	28	LYS
19	AS	37	ARG
19	AS	65	ASN
19	AS	66	MET
20	AT	8	ARG
20	AT	9	ASN
20	AT	13	LEU
20	AT	24	LEU
20	AT	30	LYS
20	AT	45	GLN
20	AT	54	LYS
20	AT	62	LEU
21	AU	9	ARG
21	AU	10	ARG
21	AU	12	LYS
28	BD	12	SER
28	BD	13	ARG
28	BD	61	LEU
28	BD	88	ARG
28	BD	94	LEU
28	BD	99	ASP
28	BD	103	ARG
28	BD	113	VAL
28	BD	126	GLN
28	BD	138	VAL
28	BD	142	VAL
28	BD	155	LEU
28	BD	211	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
28	BD	217	ARG
28	BD	221	VAL
28	BD	229	VAL
28	BD	242	ARG
28	BD	257	LEU
28	BD	259	THR
28	BD	260	ARG
29	BE	1	MET
29	BE	14	ILE
29	BE	24	THR
29	BE	33	VAL
29	BE	49	LEU
29	BE	52	LEU
29	BE	73	GLU
29	BE	75	VAL
29	BE	77	ILE
29	BE	82	ARG
29	BE	97	LYS
29	BE	116	VAL
29	BE	119	ARG
29	BE	144	ARG
29	BE	154	LYS
29	BE	163	GLU
29	BE	175	VAL
29	BE	203	LYS
30	BF	19	GLU
30	BF	24	LEU
30	BF	53	THR
30	BF	57	VAL
30	BF	74	ARG
30	BF	88	VAL
30	BF	106	ARG
30	BF	125	LEU
30	BF	170	LEU
30	BF	192	LEU
30	BF	200	GLU
31	BG	7	LEU
31	BG	43	LEU
31	BG	45	GLU
31	BG	60	LEU
31	BG	81	LYS
31	BG	82	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
31	BG	86	MET
31	BG	133	LEU
31	BG	135	LEU
31	BG	140	ILE
31	BG	143	GLU
31	BG	146	TYR
31	BG	148	MET
31	BG	170	ARG
31	BG	175	LEU
32	BH	6	ARG
32	BH	15	VAL
32	BH	33	LEU
32	BH	41	MET
32	BH	44	VAL
32	BH	45	VAL
32	BH	57	ASP
32	BH	59	ARG
32	BH	69	ARG
32	BH	71	LEU
32	BH	86	GLU
32	BH	95	ARG
32	BH	116	GLU
32	BH	119	GLU
32	BH	124	GLU
32	BH	125	VAL
32	BH	129	THR
32	BH	134	SER
33	BI	5	LEU
33	BI	9	LEU
33	BI	10	GLU
33	BI	38	LEU
33	BI	43	ASN
33	BI	47	LEU
33	BI	50	ARG
33	BI	57	ARG
33	BI	60	GLU
33	BI	61	ARG
33	BI	62	LYS
33	BI	66	GLU
33	BI	68	LEU
33	BI	75	LEU
33	BI	77	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
33	BI	78	THR
33	BI	85	GLU
33	BI	92	VAL
33	BI	96	ASP
33	BI	101	LEU
33	BI	103	ARG
33	BI	117	GLU
33	BI	140	LEU
33	BI	142	VAL
34	BN	28	THR
34	BN	33	LEU
34	BN	34	LEU
34	BN	46	VAL
34	BN	48	MET
34	BN	58	ASP
34	BN	61	ARG
34	BN	67	LEU
34	BN	73	THR
34	BN	83	LYS
34	BN	87	LEU
34	BN	99	LEU
34	BN	120	LEU
34	BN	133	GLN
34	BN	139	GLU
35	BO	8	LEU
35	BO	23	ARG
35	BO	24	VAL
35	BO	69	ILE
35	BO	92	GLU
35	BO	94	ARG
35	BO	108	GLU
36	BP	1	MET
36	BP	2	LYS
36	BP	55	ARG
36	BP	59	LEU
36	BP	65	ARG
36	BP	70	GLN
36	BP	76	LYS
36	BP	77	ARG
36	BP	83	VAL
36	BP	95	VAL
36	BP	98	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	BP	106	LEU
36	BP	112	LEU
36	BP	119	GLU
36	BP	126	VAL
36	BP	148	LEU
36	BP	149	GLU
37	BQ	1	MET
37	BQ	5	ARG
37	BQ	7	MET
37	BQ	10	ARG
37	BQ	16	ARG
37	BQ	21	THR
37	BQ	35	VAL
37	BQ	45	GLN
37	BQ	54	MET
37	BQ	56	ARG
37	BQ	59	ARG
37	BQ	60	ARG
37	BQ	75	THR
37	BQ	85	LYS
37	BQ	109	VAL
37	BQ	110	THR
38	BR	1	MET
38	BR	6	SER
38	BR	15	SER
38	BR	18	LEU
38	BR	24	GLN
38	BR	28	LEU
38	BR	29	LEU
38	BR	33	ARG
38	BR	36	THR
38	BR	44	LEU
38	BR	60	LEU
38	BR	65	LEU
38	BR	67	LEU
38	BR	75	LEU
38	BR	79	LEU
38	BR	100	LEU
38	BR	102	GLU
38	BR	111	LEU
38	BR	114	VAL
39	BS	20	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
39	BS	57	LYS
39	BS	59	LYS
39	BS	67	ARG
39	BS	83	LYS
39	BS	110	LEU
40	BT	17	THR
40	BT	28	VAL
40	BT	34	VAL
40	BT	49	VAL
40	BT	53	ARG
40	BT	78	LEU
40	BT	96	ARG
40	BT	108	ARG
40	BT	118	ARG
41	BU	8	VAL
41	BU	31	SER
41	BU	36	ARG
41	BU	74	LEU
41	BU	83	LEU
41	BU	92	ARG
41	BU	95	LEU
41	BU	104	GLN
41	BU	117	GLN
42	BV	28	GLU
42	BV	43	GLU
42	BV	46	VAL
42	BV	51	VAL
42	BV	52	VAL
42	BV	61	VAL
42	BV	62	LEU
42	BV	72	VAL
42	BV	79	VAL
42	BV	85	LYS
42	BV	95	LEU
42	BV	100	ARG
43	BW	4	LYS
43	BW	11	ARG
43	BW	15	ARG
43	BW	17	VAL
43	BW	51	LEU
43	BW	67	ASP
43	BW	100	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
44	BX	35	THR
44	BX	45	THR
44	BX	57	LEU
44	BX	66	LEU
44	BX	72	LYS
44	BX	88	LYS
45	BY	1	MET
45	BY	2	ARG
45	BY	23	ARG
45	BY	34	LYS
45	BY	43	ASN
45	BY	55	TYR
45	BY	72	VAL
45	BY	90	LEU
45	BY	91	GLU
45	BY	99	CYS
46	BZ	5	LEU
46	BZ	19	ARG
46	BZ	40	ASP
46	BZ	72	ARG
46	BZ	86	VAL
46	BZ	91	LEU
46	BZ	120	ILE
46	BZ	136	PHE
46	BZ	153	SER
46	BZ	154	ASP
46	BZ	155	LEU
46	BZ	170	THR
47	B0	20	ARG
47	B0	55	ARG
47	B0	82	ARG
48	B1	21	ARG
48	B1	40	ARG
48	B1	52	ARG
48	B1	59	THR
48	B1	78	LYS
48	B1	95	LEU
48	B1	98	LEU
49	B2	3	LEU
49	B2	28	LYS
49	B2	30	ARG
49	B2	32	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
49	B2	45	SER
49	B2	55	ARG
49	B2	64	LEU
49	B2	70	GLN
50	B3	8	LEU
50	B3	23	LEU
50	B3	29	ARG
50	B3	32	GLN
50	B3	55	ARG
51	B4	28	LYS
51	B4	34	GLU
51	B4	46	GLN
51	B4	49	PHE
51	B4	50	VAL
51	B4	53	GLU
51	B4	55	ARG
51	B4	56	VAL
51	B4	58	ARG
51	B4	59	PHE
51	B4	61	ARG
51	B4	63	TYR
51	B4	68	ARG
52	B5	16	ARG
52	B5	29	THR
52	B5	40	LYS
52	B5	55	ARG
52	B5	60	VAL
53	B6	4	GLU
53	B6	6	ARG
53	B6	14	THR
53	B6	28	ARG
53	B6	38	LYS
53	B6	48	VAL
53	B6	52	VAL
54	B7	1	MET
54	B7	24	THR
54	B7	43	THR
55	B8	13	ARG
55	B8	14	VAL
55	B8	31	HIS
55	B8	34	TRP
2	CB	11	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	CB	16	HIS
2	CB	17	PHE
2	CB	24	TRP
2	CB	35	GLU
2	CB	39	ILE
2	CB	50	GLU
2	CB	55	PHE
2	CB	67	THR
2	CB	71	VAL
2	CB	76	GLN
2	CB	82	ARG
2	CB	87	ARG
2	CB	96	ARG
2	CB	97	TRP
2	CB	98	LEU
2	CB	114	ARG
2	CB	115	LEU
2	CB	117	GLU
2	CB	124	SER
2	CB	126	GLU
2	CB	128	GLU
2	CB	142	LEU
2	CB	144	ARG
2	CB	154	LEU
2	CB	155	LEU
2	CB	157	ARG
2	CB	160	ASP
2	CB	163	PHE
2	CB	185	ILE
2	CB	187	LEU
2	CB	200	ILE
2	CB	209	ARG
2	CB	210	SER
2	CB	217	ARG
2	CB	221	LEU
2	CB	224	GLN
2	CB	230	VAL
3	CC	3	ASN
3	CC	21	ARG
3	CC	35	GLU
3	CC	49	SER
3	CC	70	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	CC	91	LEU
3	CC	98	ASN
3	CC	101	LEU
3	CC	104	GLN
3	CC	105	GLU
3	CC	118	GLN
3	CC	140	ARG
3	CC	152	ILE
3	CC	179	ARG
3	CC	196	LEU
3	CC	198	VAL
4	CD	10	ARG
4	CD	15	GLU
4	CD	31	CYS
4	CD	34	GLU
4	CD	47	ARG
4	CD	58	LEU
4	CD	61	LYS
4	CD	86	LYS
4	CD	96	LEU
4	CD	108	LEU
4	CD	115	ARG
4	CD	127	THR
4	CD	135	LEU
4	CD	155	LEU
4	CD	157	LEU
4	CD	168	ARG
4	CD	170	VAL
4	CD	181	MET
4	CD	187	ARG
4	CD	188	LEU
4	CD	194	LEU
5	CE	6	PHE
5	CE	10	MET
5	CE	12	LEU
5	CE	27	ARG
5	CE	31	LEU
5	CE	38	GLN
5	CE	41	VAL
5	CE	47	LYS
5	CE	60	TYR
5	CE	67	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	CE	79	GLU
5	CE	137	GLU
5	CE	150	ARG
6	CF	28	ARG
6	CF	40	VAL
6	CF	41	GLU
6	CF	46	ARG
6	CF	75	LEU
7	CG	9	VAL
7	CG	12	LEU
7	CG	32	ARG
7	CG	33	ASP
7	CG	51	GLN
7	CG	52	GLU
7	CG	72	ARG
7	CG	73	MET
7	CG	76	ARG
7	CG	79	ARG
7	CG	155	ARG
8	CH	21	LYS
8	CH	29	SER
8	CH	39	LEU
8	CH	84	ARG
8	CH	91	ARG
8	CH	98	LYS
8	CH	112	LEU
9	CI	7	THR
9	CI	14	VAL
9	CI	23	ASN
9	CI	50	LEU
9	CI	56	LEU
9	CI	81	ILE
9	CI	89	ASN
9	CI	102	LEU
9	CI	108	VAL
9	CI	112	LYS
9	CI	121	ARG
9	CI	125	TYR
9	CI	128	ARG
10	CJ	7	LYS
10	CJ	19	SER
10	CJ	29	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	CJ	59	SER
10	CJ	67	THR
10	CJ	81	THR
11	CK	24	SER
11	CK	31	THR
11	CK	48	ILE
11	CK	51	LYS
11	CK	54	ARG
11	CK	96	ARG
11	CK	104	GLN
12	CL	38	THR
12	CL	60	LEU
12	CL	83	VAL
12	CL	116	SER
13	CM	3	ARG
13	CM	15	VAL
13	CM	19	LEU
13	CM	47	ASP
13	CM	49	THR
13	CM	56	LEU
13	CM	84	ILE
13	CM	103	THR
13	CM	104	ARG
13	CM	110	ARG
13	CM	117	VAL
13	CM	121	LYS
14	CN	3	ARG
14	CN	7	ILE
14	CN	12	ARG
14	CN	18	VAL
14	CN	23	ARG
14	CN	26	ARG
14	CN	32	SER
14	CN	33	VAL
15	CO	3	ILE
15	CO	5	LYS
15	CO	7	GLU
15	CO	26	GLU
15	CO	38	ARG
15	CO	39	LEU
15	CO	41	GLU
15	CO	48	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
15	CO	54	ARG
16	CP	2	VAL
16	CP	5	ARG
16	CP	27	LYS
16	CP	60	LEU
16	CP	62	VAL
16	CP	67	THR
16	CP	69	THR
17	CQ	6	LEU
17	CQ	19	VAL
17	CQ	36	ILE
17	CQ	60	ILE
17	CQ	63	ARG
17	CQ	74	LEU
17	CQ	96	GLU
18	CR	26	LEU
18	CR	32	ARG
18	CR	35	ARG
18	CR	37	VAL
18	CR	41	LYS
18	CR	46	GLU
18	CR	76	LEU
19	CS	28	LYS
19	CS	37	ARG
19	CS	56	GLN
19	CS	78	ARG
20	CT	24	LEU
20	CT	38	LYS
20	CT	45	GLN
20	CT	56	MET
20	CT	62	LEU
20	CT	71	THR
20	CT	80	ARG
20	CT	90	GLN
21	CU	10	ARG
28	DD	3	VAL
28	DD	13	ARG
28	DD	54	ARG
28	DD	61	LEU
28	DD	88	ARG
28	DD	94	LEU
28	DD	103	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
28	DD	106	ILE
28	DD	113	VAL
28	DD	134	ARG
28	DD	142	VAL
28	DD	155	LEU
28	DD	162	SER
28	DD	193	VAL
28	DD	211	ARG
28	DD	217	ARG
28	DD	221	VAL
28	DD	229	VAL
28	DD	257	LEU
28	DD	259	THR
28	DD	260	ARG
28	DD	276	LYS
29	DE	1	MET
29	DE	12	THR
29	DE	21	VAL
29	DE	24	THR
29	DE	33	VAL
29	DE	40	GLU
29	DE	47	VAL
29	DE	52	LEU
29	DE	73	GLU
29	DE	75	VAL
29	DE	79	ARG
29	DE	82	ARG
29	DE	116	VAL
29	DE	119	ARG
29	DE	144	ARG
29	DE	154	LYS
29	DE	163	GLU
29	DE	175	VAL
29	DE	195	LEU
30	DF	19	GLU
30	DF	20	LEU
30	DF	24	LEU
30	DF	28	ILE
30	DF	38	ARG
30	DF	57	VAL
30	DF	74	ARG
30	DF	82	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	DF	88	VAL
30	DF	106	ARG
30	DF	135	LYS
30	DF	170	LEU
30	DF	192	LEU
30	DF	197	ASP
30	DF	200	GLU
31	DG	16	ARG
31	DG	21	ARG
31	DG	36	LYS
31	DG	43	LEU
31	DG	45	GLU
31	DG	49	ASP
31	DG	58	GLN
31	DG	60	LEU
31	DG	84	LYS
31	DG	98	ARG
31	DG	115	ARG
31	DG	133	LEU
31	DG	135	LEU
31	DG	136	ARG
31	DG	140	ILE
31	DG	143	GLU
31	DG	145	THR
31	DG	148	MET
31	DG	153	ARG
31	DG	170	ARG
32	DH	2	SER
32	DH	3	ARG
32	DH	15	VAL
32	DH	33	LEU
32	DH	43	VAL
32	DH	44	VAL
32	DH	45	VAL
32	DH	57	ASP
32	DH	63	SER
32	DH	69	ARG
32	DH	84	SER
32	DH	86	GLU
32	DH	95	ARG
32	DH	106	THR
32	DH	124	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	DH	134	SER
32	DH	136	ILE
32	DH	172	LYS
33	DI	5	LEU
33	DI	9	LEU
33	DI	19	VAL
33	DI	40	THR
33	DI	43	ASN
33	DI	44	LEU
33	DI	50	ARG
33	DI	68	LEU
33	DI	73	GLU
33	DI	86	THR
33	DI	92	VAL
33	DI	114	LEU
33	DI	121	LYS
33	DI	123	LEU
33	DI	140	LEU
33	DI	142	VAL
34	DN	33	LEU
34	DN	34	LEU
34	DN	38	HIS
34	DN	46	VAL
34	DN	58	ASP
34	DN	62	VAL
34	DN	85	ILE
34	DN	87	LEU
34	DN	99	LEU
34	DN	120	LEU
34	DN	137	LYS
34	DN	139	GLU
35	DO	8	LEU
35	DO	9	GLU
35	DO	23	ARG
35	DO	24	VAL
35	DO	69	ILE
35	DO	92	GLU
35	DO	94	ARG
36	DP	1	MET
36	DP	29	LYS
36	DP	45	LEU
36	DP	50	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	DP	55	ARG
36	DP	65	ARG
36	DP	70	GLN
36	DP	95	VAL
36	DP	96	THR
36	DP	99	LEU
36	DP	106	LEU
36	DP	112	LEU
36	DP	119	GLU
36	DP	131	SER
36	DP	148	LEU
37	DQ	1	MET
37	DQ	16	ARG
37	DQ	21	THR
37	DQ	45	GLN
37	DQ	54	MET
37	DQ	56	ARG
37	DQ	59	ARG
37	DQ	60	ARG
37	DQ	65	PHE
37	DQ	75	THR
37	DQ	85	LYS
37	DQ	110	THR
38	DR	1	MET
38	DR	15	SER
38	DR	18	LEU
38	DR	24	GLN
38	DR	28	LEU
38	DR	29	LEU
38	DR	33	ARG
38	DR	36	THR
38	DR	44	LEU
38	DR	60	LEU
38	DR	65	LEU
38	DR	67	LEU
38	DR	75	LEU
38	DR	79	LEU
38	DR	100	LEU
38	DR	102	GLU
38	DR	111	LEU
38	DR	114	VAL
39	DS	20	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
39	DS	35	ILE
39	DS	57	LYS
39	DS	69	VAL
39	DS	71	ARG
39	DS	75	GLU
39	DS	93	LYS
39	DS	101	LEU
39	DS	103	GLU
39	DS	110	LEU
40	DT	6	LEU
40	DT	16	ARG
40	DT	17	THR
40	DT	23	ARG
40	DT	49	VAL
40	DT	53	ARG
40	DT	78	LEU
40	DT	96	ARG
40	DT	113	LYS
40	DT	118	ARG
41	DU	8	VAL
41	DU	36	ARG
41	DU	74	LEU
41	DU	83	LEU
41	DU	89	GLU
41	DU	92	ARG
41	DU	104	GLN
41	DU	108	GLU
42	DV	6	LYS
42	DV	15	GLU
42	DV	18	LEU
42	DV	38	LEU
42	DV	46	VAL
42	DV	51	VAL
42	DV	57	VAL
42	DV	61	VAL
42	DV	62	LEU
42	DV	72	VAL
42	DV	79	VAL
42	DV	95	LEU
42	DV	100	ARG
43	DW	11	ARG
43	DW	15	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
43	DW	17	VAL
43	DW	51	LEU
43	DW	52	GLU
43	DW	60	ASN
43	DW	100	THR
44	DX	57	LEU
44	DX	70	LEU
44	DX	72	LYS
44	DX	88	LYS
44	DX	90	GLU
44	DX	92	LEU
45	DY	11	ASP
45	DY	23	ARG
45	DY	90	LEU
45	DY	91	GLU
45	DY	99	CYS
45	DY	107	ASP
46	DZ	5	LEU
46	DZ	18	LEU
46	DZ	35	ARG
46	DZ	40	ASP
46	DZ	41	LEU
46	DZ	72	ARG
46	DZ	86	VAL
46	DZ	97	GLU
46	DZ	102	LEU
46	DZ	119	GLU
46	DZ	136	PHE
46	DZ	144	LEU
46	DZ	153	SER
46	DZ	154	ASP
46	DZ	155	LEU
46	DZ	159	PRO
47	D0	10	THR
47	D0	19	LYS
47	D0	20	ARG
47	D0	24	LYS
47	D0	55	ARG
48	D1	4	VAL
48	D1	21	ARG
48	D1	30	VAL
48	D1	40	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
48	D1	52	ARG
48	D1	59	THR
48	D1	95	LEU
48	D1	97	LEU
48	D1	98	LEU
49	D2	21	LEU
49	D2	28	LYS
49	D2	30	ARG
49	D2	45	SER
49	D2	55	ARG
49	D2	70	GLN
50	D3	3	ARG
50	D3	8	LEU
50	D3	24	LYS
50	D3	30	ARG
50	D3	44	ARG
50	D3	55	ARG
51	D4	24	THR
51	D4	34	GLU
51	D4	44	THR
51	D4	50	VAL
51	D4	56	VAL
51	D4	58	ARG
51	D4	61	ARG
51	D4	63	TYR
51	D4	67	TYR
51	D4	68	ARG
52	D5	29	THR
52	D5	40	LYS
52	D5	55	ARG
52	D5	60	VAL
53	D6	6	ARG
53	D6	38	LYS
54	D7	1	MET
54	D7	14	LYS
54	D7	23	ARG
55	D8	13	ARG
55	D8	14	VAL
55	D8	34	TRP
56	D9	7	VAL
56	D9	26	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (130) such

sidechains are listed below:

Mol	Chain	Res	Type
2	AB	16	HIS
2	AB	94	ASN
3	AC	6	HIS
3	AC	28	GLN
3	AC	104	GLN
3	AC	123	GLN
3	AC	136	GLN
3	AC	162	GLN
3	AC	181	ASN
4	AD	45	GLN
4	AD	77	ASN
4	AD	123	HIS
4	AD	125	HIS
4	AD	161	ASN
5	AE	20	GLN
5	AE	38	GLN
6	AF	94	GLN
6	AF	100	ASN
7	AG	13	GLN
7	AG	28	ASN
9	AI	23	ASN
9	AI	31	GLN
9	AI	34	ASN
9	AI	73	GLN
9	AI	89	ASN
9	AI	124	GLN
10	AJ	56	HIS
11	AK	93	GLN
11	AK	104	GLN
12	AL	78	GLN
12	AL	99	HIS
13	AM	92	HIS
15	AO	9	GLN
15	AO	28	GLN
15	AO	46	HIS
15	AO	71	GLN
16	AP	76	GLN
19	AS	65	ASN
19	AS	69	HIS
19	AS	83	HIS
20	AT	9	ASN
20	AT	90	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
28	BD	87	ASN
28	BD	164	GLN
28	BD	166	GLN
28	BD	253	GLN
30	BF	69	HIS
30	BF	169	ASN
30	BF	203	GLN
31	BG	26	GLN
31	BG	40	ASN
33	BI	43	ASN
33	BI	54	GLN
35	BO	5	GLN
36	BP	38	GLN
38	BR	71	GLN
40	BT	43	GLN
40	BT	58	ASN
40	BT	123	GLN
41	BU	94	ASN
44	BX	31	HIS
44	BX	82	GLN
45	BY	6	HIS
45	BY	43	ASN
49	B2	9	GLN
49	B2	70	GLN
51	B4	46	GLN
56	B9	36	GLN
2	CB	40	HIS
2	CB	94	ASN
2	CB	224	GLN
3	CC	6	HIS
3	CC	28	GLN
3	CC	69	HIS
3	CC	104	GLN
3	CC	118	GLN
3	CC	123	GLN
3	CC	136	GLN
4	CD	77	ASN
4	CD	119	GLN
4	CD	123	HIS
4	CD	125	HIS
4	CD	161	ASN
5	CE	20	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	CE	141	GLN
6	CF	94	GLN
7	CG	28	ASN
7	CG	51	GLN
9	CI	23	ASN
9	CI	31	GLN
9	CI	58	HIS
9	CI	89	ASN
9	CI	124	GLN
10	CJ	62	HIS
11	CK	93	GLN
12	CL	78	GLN
12	CL	99	HIS
13	CM	77	ASN
13	CM	92	HIS
15	CO	28	GLN
15	CO	62	GLN
19	CS	56	GLN
19	CS	57	HIS
19	CS	65	ASN
19	CS	69	HIS
19	CS	83	HIS
28	DD	96	HIS
28	DD	164	GLN
28	DD	166	GLN
28	DD	253	GLN
29	DE	85	ASN
30	DF	69	HIS
30	DF	169	ASN
30	DF	203	GLN
31	DG	26	GLN
31	DG	40	ASN
33	DI	43	ASN
38	DR	71	GLN
39	DS	68	GLN
40	DT	58	ASN
40	DT	123	GLN
41	DU	117	GLN
42	DV	64	HIS
44	DX	31	HIS
44	DX	82	GLN
45	DY	43	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
46	DZ	55	HIS
46	DZ	151	HIS
56	D9	20	HIS
56	D9	36	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1495/1521 (98%)	304 (20%)	25 (1%)
1	CA	1501/1521 (98%)	316 (21%)	28 (1%)
22	AV	12/24 (50%)	3 (25%)	0
22	CV	11/24 (45%)	2 (18%)	0
23	AW	70/76 (92%)	30 (42%)	2 (2%)
23	CW	67/76 (88%)	32 (47%)	2 (2%)
24	AX	75/77 (97%)	16 (21%)	0
24	CX	75/77 (97%)	21 (28%)	0
25	AY	71/76 (93%)	35 (49%)	4 (5%)
25	CY	69/76 (90%)	32 (46%)	1 (1%)
26	BA	2811/2915 (96%)	450 (16%)	34 (1%)
26	DA	2791/2915 (95%)	552 (19%)	30 (1%)
27	BB	119/121 (98%)	14 (11%)	0
27	DB	119/121 (98%)	17 (14%)	0
All	All	9286/9620 (96%)	1824 (19%)	126 (1%)

All (1824) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	6	G
1	AA	7	G
1	AA	9	G
1	AA	22	G
1	AA	29	G
1	AA	32	A
1	AA	39	G
1	AA	47	C
1	AA	48	C
1	AA	51	A
1	AA	59	A
1	AA	61	G
1	AA	65	U
1	AA	73	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	AA	77	G
1	AA	78	G
1	AA	79	G
1	AA	91	C
1	AA	96	U
1	AA	97	G
1	AA	98	G
1	AA	101	A
1	AA	111	G
1	AA	112	G
1	AA	116	A
1	AA	121	C
1	AA	131	C
1	AA	146	G
1	AA	155	C
1	AA	163	C
1	AA	166	G
1	AA	173	U
1	AA	174	C
1	AA	180	U
1	AA	182	U
1	AA	189(D)	C
1	AA	189(F)	U
1	AA	189(H)	G
1	AA	189(I)	G
1	AA	189(K)	U
1	AA	190	U
1	AA	195	A
1	AA	197	A
1	AA	201	C
1	AA	202	U
1	AA	203	U
1	AA	204	U
1	AA	216	G
1	AA	221	C
1	AA	247	G
1	AA	251	G
1	AA	258	G
1	AA	266	G
1	AA	267	C
1	AA	279	A
1	AA	289	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	AA	301	G
1	AA	321	A
1	AA	328	C
1	AA	332	G
1	AA	342	C
1	AA	346	G
1	AA	347	G
1	AA	348	G
1	AA	352	C
1	AA	353	A
1	AA	354	G
1	AA	355	C
1	AA	367	U
1	AA	372	C
1	AA	373	A
1	AA	382	A
1	AA	384	G
1	AA	397	A
1	AA	398	C
1	AA	406	G
1	AA	412	A
1	AA	414	A
1	AA	421	U
1	AA	424	G
1	AA	429	U
1	AA	430	A
1	AA	439	A
1	AA	442	C
1	AA	443	C
1	AA	452	A
1	AA	461	A
1	AA	470	C
1	AA	471	G
1	AA	484	G
1	AA	485	G
1	AA	496	A
1	AA	498	U
1	AA	505	G
1	AA	509	A
1	AA	510	A
1	AA	511	C
1	AA	513	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	AA	518	C
1	AA	527	G
1	AA	531	U
1	AA	532	A
1	AA	533	A
1	AA	545	C
1	AA	547	A
1	AA	559	A
1	AA	560	U
1	AA	561	U
1	AA	572	A
1	AA	573	A
1	AA	576	G
1	AA	592	G
1	AA	596	C
1	AA	629	G
1	AA	630	G
1	AA	632	A
1	AA	633	G
1	AA	649	G
1	AA	653	A
1	AA	665	A
1	AA	673	G
1	AA	680	C
1	AA	687	A
1	AA	688	G
1	AA	695	A
1	AA	711	G
1	AA	712	A
1	AA	721	G
1	AA	723	U
1	AA	724	G
1	AA	731	G
1	AA	749	C
1	AA	753	A
1	AA	755	G
1	AA	774	G
1	AA	777	A
1	AA	792	A
1	AA	793	U
1	AA	794	A
1	AA	815	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	AA	816	A
1	AA	817	C
1	AA	821	G
1	AA	828	A
1	AA	833	U
1	AA	840	C
1	AA	841	U
1	AA	851	G
1	AA	853	G
1	AA	859	A
1	AA	874	G
1	AA	902	G
1	AA	914	A
1	AA	922	G
1	AA	926	G
1	AA	927	G
1	AA	932	C
1	AA	934	C
1	AA	935	A
1	AA	960	U
1	AA	961	U
1	AA	968	A
1	AA	969	A
1	AA	971	G
1	AA	972	C
1	AA	974	A
1	AA	975	A
1	AA	976	G
1	AA	977	A
1	AA	989	C
1	AA	992	U
1	AA	993	G
1	AA	996	A
1	AA	1000	U
1	AA	1001(A)	G
1	AA	1002	G
1	AA	1003	G
1	AA	1004	A
1	AA	1005	A
1	AA	1008	C
1	AA	1009	G
1	AA	1019	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	AA	1021	G
1	AA	1022	G
1	AA	1023	G
1	AA	1025	U
1	AA	1026	G
1	AA	1027	C
1	AA	1028	C
1	AA	1029	C
1	AA	1030	C
1	AA	1030(A)	G
1	AA	1030(B)	C
1	AA	1030(C)	G
1	AA	1030(D)	A
1	AA	1031	G
1	AA	1033	G
1	AA	1037	C
1	AA	1039	C
1	AA	1043	C
1	AA	1044	A
1	AA	1045	C
1	AA	1052	U
1	AA	1054	C
1	AA	1055	A
1	AA	1065	U
1	AA	1066	C
1	AA	1068	G
1	AA	1076	C
1	AA	1081	G
1	AA	1088	G
1	AA	1094	G
1	AA	1095	U
1	AA	1096	C
1	AA	1097	C
1	AA	1101	A
1	AA	1104	G
1	AA	1108	G
1	AA	1110	A
1	AA	1113	C
1	AA	1124	G
1	AA	1126	U
1	AA	1130	A
1	AA	1132	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	AA	1135	U
1	AA	1136	U
1	AA	1137	C
1	AA	1138	G
1	AA	1139	G
1	AA	1140	C
1	AA	1141	C
1	AA	1146	A
1	AA	1152	A
1	AA	1154	G
1	AA	1157	A
1	AA	1158	C
1	AA	1159	U
1	AA	1183	A
1	AA	1184	G
1	AA	1196	U
1	AA	1197	G
1	AA	1202	G
1	AA	1212	U
1	AA	1213	A
1	AA	1224	G
1	AA	1227	A
1	AA	1228	C
1	AA	1236	A
1	AA	1238	A
1	AA	1240	U
1	AA	1244	C
1	AA	1256	A
1	AA	1257	U
1	AA	1258	G
1	AA	1260	C
1	AA	1270	C
1	AA	1273	G
1	AA	1278	U
1	AA	1279	A
1	AA	1280	A
1	AA	1281	U
1	AA	1286	A
1	AA	1287	A
1	AA	1299	A
1	AA	1300	G
1	AA	1302	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	AA	1305	G
1	AA	1314	C
1	AA	1317	C
1	AA	1322	C
1	AA	1338	G
1	AA	1340	A
1	AA	1346	A
1	AA	1347	G
1	AA	1353	G
1	AA	1355	G
1	AA	1360	A
1	AA	1363	C
1	AA	1364	U
1	AA	1370	G
1	AA	1397	C
1	AA	1402	C
1	AA	1419	G
1	AA	1422	G
1	AA	1442	G
1	AA	1442(A)	G
1	AA	1442(B)	A
1	AA	1446	U
1	AA	1447	A
1	AA	1452	C
1	AA	1487	G
1	AA	1492	A
1	AA	1493	A
1	AA	1494	G
1	AA	1503	A
1	AA	1504	G
1	AA	1506	U
1	AA	1517	G
1	AA	1519	A
1	AA	1520	G
1	AA	1529	G
1	AA	1530	G
1	AA	1531	A
1	AA	1532	U
22	AV	13	A
22	AV	14	A
22	AV	24	A
23	AW	2	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
23	AW	3	C
23	AW	4	C
23	AW	8	4SU
23	AW	12	U
23	AW	14	A
23	AW	19	G
23	AW	20	U
23	AW	21	A
23	AW	22	G
23	AW	23	A
23	AW	24	G
23	AW	26	A
23	AW	27	G
23	AW	30	G
23	AW	42	C
23	AW	43	C
23	AW	45	U
23	AW	46	7MG
23	AW	47	U
23	AW	48	C
23	AW	49	C
23	AW	52	G
23	AW	53	G
23	AW	59	U
23	AW	61	C
23	AW	68	C
23	AW	70	G
23	AW	73	A
23	AW	74	C
24	AX	3	C
24	AX	9	G
24	AX	13	C
24	AX	19	G
24	AX	20	U
24	AX	21	A
24	AX	31	G
24	AX	42	G
24	AX	48	C
24	AX	56	C
24	AX	59	A
24	AX	63	G
24	AX	67	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
24	AX	68	C
24	AX	70	G
24	AX	76	A
25	AY	2	C
25	AY	5	G
25	AY	9	A
25	AY	11	C
25	AY	13	C
25	AY	15	G
25	AY	19	G
25	AY	20	U
25	AY	21	A
25	AY	22	G
25	AY	26	A
25	AY	29	G
25	AY	30	G
25	AY	33	U
25	AY	34	G
25	AY	35	A
25	AY	36	A
25	AY	39	PSU
25	AY	41	C
25	AY	44	G
25	AY	45	U
25	AY	46	7MG
25	AY	47	U
25	AY	48	C
25	AY	49	C
25	AY	54	5MU
25	AY	57	G
25	AY	58	A
25	AY	59	U
25	AY	60	U
25	AY	62	C
25	AY	65	G
25	AY	67	C
25	AY	70	G
25	AY	73	A
26	BA	12	U
26	BA	34	C
26	BA	36	G
26	BA	45	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	BA	64	A
26	BA	71	A
26	BA	72	U
26	BA	74	A
26	BA	75	G
26	BA	84	A
26	BA	95	G
26	BA	99	U
26	BA	100	G
26	BA	102	G
26	BA	118	A
26	BA	119	A
26	BA	120	U
26	BA	151	C
26	BA	154(A)	C
26	BA	172	C
26	BA	181	A
26	BA	182	A
26	BA	188	G
26	BA	196	A
26	BA	197	A
26	BA	199	A
26	BA	205	G
26	BA	215	G
26	BA	216	A
26	BA	221	A
26	BA	222	A
26	BA	223	A
26	BA	229	A
26	BA	233	A
26	BA	248	G
26	BA	271(E)	U
26	BA	271(I)	G
26	BA	271(K)	U
26	BA	271(L)	U
26	BA	271(M)	G
26	BA	271(N)	U
26	BA	271(S)	G
26	BA	272(A)	U
26	BA	272(B)	G
26	BA	272(G)	C
26	BA	272(I)	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	BA	279	C
26	BA	282	A
26	BA	283	A
26	BA	311	A
26	BA	329	G
26	BA	330	A
26	BA	352	G
26	BA	363	G
26	BA	363(B)	G
26	BA	372	G
26	BA	380	U
26	BA	386	G
26	BA	396	G
26	BA	405	U
26	BA	411	G
26	BA	428	A
26	BA	443	A
26	BA	444	C
26	BA	448	U
26	BA	454	A
26	BA	456	C
26	BA	470	A
26	BA	479	A
26	BA	481	G
26	BA	504	U
26	BA	505	A
26	BA	509	C
26	BA	528	A
26	BA	529	A
26	BA	530	G
26	BA	531	C
26	BA	532	A
26	BA	533	G
26	BA	545	G
26	BA	549	G
26	BA	563	G
26	BA	573	G
26	BA	575	A
26	BA	592	G
26	BA	603	A
26	BA	604	G
26	BA	607	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	BA	614(A)	U
26	BA	614(B)	G
26	BA	615	G
26	BA	616	G
26	BA	627	A
26	BA	637	A
26	BA	645	C
26	BA	646	A
26	BA	652(F)	G
26	BA	652(T)	C
26	BA	652(U)	G
26	BA	669	G
26	BA	677	A
26	BA	686	G
26	BA	730	C
26	BA	732	C
26	BA	764	A
26	BA	765	G
26	BA	775	G
26	BA	776	G
26	BA	782	A
26	BA	784	A
26	BA	785	G
26	BA	792	G
26	BA	805	G
26	BA	812	C
26	BA	819	A
26	BA	824	A
26	BA	827	U
26	BA	828	U
26	BA	830	G
26	BA	855	G
26	BA	859	G
26	BA	862	G
26	BA	866	A
26	BA	877	U
26	BA	879	G
26	BA	880	G
26	BA	882	G
26	BA	884	C
26	BA	885	C
26	BA	886	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	BA	887	A
26	BA	888	C
26	BA	889	C
26	BA	890	A
26	BA	892	G
26	BA	893	C
26	BA	894	C
26	BA	895	U
26	BA	896	A
26	BA	897	C
26	BA	898	C
26	BA	899	A
26	BA	900	A
26	BA	901	A
26	BA	907	U
26	BA	910	A
26	BA	932	G
26	BA	941	A
26	BA	945	A
26	BA	946	G
26	BA	958	U
26	BA	959	A
26	BA	961	C
26	BA	974	G
26	BA	975	C
26	BA	983	A
26	BA	996	A
26	BA	1012	U
26	BA	1013	C
26	BA	1022	G
26	BA	1033	U
26	BA	1038	C
26	BA	1041	C
26	BA	1045	A
26	BA	1046	A
26	BA	1047	G
26	BA	1048	A
26	BA	1051	G
26	BA	1107	G
26	BA	1108	U
26	BA	1110	G
26	BA	1112	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	BA	1128	A
26	BA	1130	U
26	BA	1135	C
26	BA	1136	G
26	BA	1170	G
26	BA	1171	G
26	BA	1173	G
26	BA	1174	A
26	BA	1175	U
26	BA	1176	G
26	BA	1177	A
26	BA	1178	C
26	BA	1210	A
26	BA	1211	U
26	BA	1220	A
26	BA	1244	G
26	BA	1248	G
26	BA	1253	A
26	BA	1256	G
26	BA	1271	G
26	BA	1272	A
26	BA	1273	U
26	BA	1289	C
26	BA	1300	U
26	BA	1301	A
26	BA	1303	G
26	BA	1314	C
26	BA	1319	G
26	BA	1352	U
26	BA	1359	A
26	BA	1360	A
26	BA	1365	A
26	BA	1370	C
26	BA	1380	G
26	BA	1384	A
26	BA	1385	G
26	BA	1416	G
26	BA	1417	C
26	BA	1420	U
26	BA	1421	G
26	BA	1428	C
26	BA	1445	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	BA	1449	A
26	BA	1450	G
26	BA	1459	G
26	BA	1467	C
26	BA	1471	A
26	BA	1478	G
26	BA	1482	G
26	BA	1484	G
26	BA	1493	C
26	BA	1507	A
26	BA	1508	A
26	BA	1509	C
26	BA	1509(A)	A
26	BA	1531	C
26	BA	1538	G
26	BA	1543	C
26	BA	1558	A
26	BA	1566	A
26	BA	1569	A
26	BA	1578	U
26	BA	1580	A
26	BA	1581	G
26	BA	1584	C
26	BA	1586	A
26	BA	1608	A
26	BA	1610	A
26	BA	1648	C
26	BA	1654	A
26	BA	1664	A
26	BA	1674	G
26	BA	1694	C
26	BA	1700	A
26	BA	1701	A
26	BA	1703	G
26	BA	1722	A
26	BA	1739	U
26	BA	1746	G
26	BA	1748	G
26	BA	1756	G
26	BA	1759	A
26	BA	1762	A
26	BA	1763	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	BA	1764	G
26	BA	1773	A
26	BA	1780	A
26	BA	1782	C
26	BA	1786	A
26	BA	1791	A
26	BA	1800	C
26	BA	1816	G
26	BA	1839	G
26	BA	1847	A
26	BA	1848	A
26	BA	1861	G
26	BA	1877	A
26	BA	1878	G
26	BA	1886	C
26	BA	1889	A
26	BA	1900	A
26	BA	1906	G
26	BA	1915	U
26	BA	1919	A
26	BA	1924	C
26	BA	1927	A
26	BA	1929	G
26	BA	1930	G
26	BA	1937	A
26	BA	1938	A
26	BA	1955	U
26	BA	1963	U
26	BA	1967	C
26	BA	1970	A
26	BA	1971	A
26	BA	1972	A
26	BA	1992	G
26	BA	1993	U
26	BA	1997	G
26	BA	2020	A
26	BA	2023	G
26	BA	2031	A
26	BA	2032	G
26	BA	2033	A
26	BA	2043	C
26	BA	2055	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	BA	2056	G
26	BA	2060	A
26	BA	2061	G
26	BA	2062	A
26	BA	2069	G
26	BA	2098	U
26	BA	2102	U
26	BA	2110	G
26	BA	2111	C
26	BA	2119	A
26	BA	2120	G
26	BA	2121	G
26	BA	2125	G
26	BA	2126	A
26	BA	2127	G
26	BA	2128	C
26	BA	2129	C
26	BA	2132	U
26	BA	2133	G
26	BA	2134	A
26	BA	2135	A
26	BA	2136	C
26	BA	2138	C
26	BA	2140	C
26	BA	2141	G
26	BA	2142	C
26	BA	2143	C
26	BA	2145	C
26	BA	2146	C
26	BA	2147	G
26	BA	2149	G
26	BA	2157	G
26	BA	2158	A
26	BA	2159	G
26	BA	2160	G
26	BA	2165	G
26	BA	2167	U
26	BA	2168	G
26	BA	2169	A
26	BA	2171	A
26	BA	2172	U
26	BA	2173	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	BA	2174	C
26	BA	2178	C
26	BA	2181	G
26	BA	2182	G
26	BA	2184	G
26	BA	2188	C
26	BA	2189	U
26	BA	2192	G
26	BA	2198	A
26	BA	2199	A
26	BA	2206	G
26	BA	2207	G
26	BA	2208	A
26	BA	2218	U
26	BA	2225	A
26	BA	2238	G
26	BA	2239	G
26	BA	2268	A
26	BA	2269	A
26	BA	2275	C
26	BA	2283	C
26	BA	2287	A
26	BA	2289	G
26	BA	2305	A
26	BA	2308	G
26	BA	2320	A
26	BA	2325	G
26	BA	2334	G
26	BA	2336	A
26	BA	2343	C
26	BA	2347	C
26	BA	2350	C
26	BA	2361	A
26	BA	2383	G
26	BA	2385	C
26	BA	2393	A
26	BA	2400	G
26	BA	2406	U
26	BA	2414	G
26	BA	2419	U
26	BA	2425	A
26	BA	2429	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	BA	2430	A
26	BA	2435	A
26	BA	2439	A
26	BA	2441	C
26	BA	2448	A
26	BA	2464	C
26	BA	2468	G
26	BA	2469	A
26	BA	2471	C
26	BA	2474	C
26	BA	2476	A
26	BA	2487	G
26	BA	2490	G
26	BA	2502	G
26	BA	2505	G
26	BA	2518	A
26	BA	2529	G
26	BA	2535	G
26	BA	2549	G
26	BA	2554	U
26	BA	2566	A
26	BA	2567	G
26	BA	2573	C
26	BA	2574	G
26	BA	2602	A
26	BA	2609	U
26	BA	2611	U
26	BA	2612	C
26	BA	2629	A
26	BA	2630	G
26	BA	2654	A
26	BA	2669	G
26	BA	2689	U
26	BA	2690	C
26	BA	2691	C
26	BA	2702	U
26	BA	2712(A)	A
26	BA	2713	A
26	BA	2726	U
26	BA	2733	A
26	BA	2757	A
26	BA	2758	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	BA	2761	G
26	BA	2764	A
26	BA	2765	A
26	BA	2766	G
26	BA	2778	A
26	BA	2790	A
26	BA	2791	C
26	BA	2792	G
26	BA	2793	G
26	BA	2802	G
26	BA	2805	G
26	BA	2808	U
26	BA	2818	G
26	BA	2820	A
26	BA	2821	A
26	BA	2833	G
26	BA	2834	G
26	BA	2835	A
26	BA	2872	G
26	BA	2873	A
26	BA	2876	G
26	BA	2880	C
26	BA	2882	A
26	BA	2883	A
26	BA	2892	A
26	BA	2894	G
27	BB	2	C
27	BB	7	G
27	BB	34	U
27	BB	42	C
27	BB	56	G
27	BB	73	A
27	BB	75	G
27	BB	85	G
27	BB	93	G
27	BB	106	G
27	BB	110	G
27	BB	111	G
27	BB	112	U
27	BB	120	A
1	CA	5	U
1	CA	6	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	CA	7	G
1	CA	9	G
1	CA	13	U
1	CA	22	G
1	CA	29	G
1	CA	32	A
1	CA	39	G
1	CA	47	C
1	CA	48	C
1	CA	51	A
1	CA	59	A
1	CA	61	G
1	CA	65	U
1	CA	66	G
1	CA	77	G
1	CA	79	G
1	CA	80	G
1	CA	88	A
1	CA	89	C
1	CA	91	C
1	CA	96	U
1	CA	97	G
1	CA	98	G
1	CA	100	C
1	CA	101	A
1	CA	111	G
1	CA	112	G
1	CA	116	A
1	CA	121	C
1	CA	131	C
1	CA	146	G
1	CA	155	C
1	CA	163	C
1	CA	166	G
1	CA	173	U
1	CA	174	C
1	CA	180	U
1	CA	182	U
1	CA	189(D)	C
1	CA	189(K)	U
1	CA	190	U
1	CA	195	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	CA	197	A
1	CA	201	C
1	CA	202	U
1	CA	203	U
1	CA	204	U
1	CA	216	G
1	CA	221	C
1	CA	247	G
1	CA	251	G
1	CA	258	G
1	CA	266	G
1	CA	267	C
1	CA	279	A
1	CA	289	G
1	CA	301	G
1	CA	321	A
1	CA	328	C
1	CA	332	G
1	CA	342	C
1	CA	344	A
1	CA	346	G
1	CA	350	G
1	CA	352	C
1	CA	353	A
1	CA	354	G
1	CA	355	C
1	CA	367	U
1	CA	372	C
1	CA	373	A
1	CA	382	A
1	CA	384	G
1	CA	397	A
1	CA	398	C
1	CA	406	G
1	CA	412	A
1	CA	413	G
1	CA	414	A
1	CA	421	U
1	CA	424	G
1	CA	429	U
1	CA	430	A
1	CA	439	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	CA	442	C
1	CA	443	C
1	CA	452	A
1	CA	461	A
1	CA	471	G
1	CA	484	G
1	CA	485	G
1	CA	496	A
1	CA	498	U
1	CA	505	G
1	CA	509	A
1	CA	510	A
1	CA	511	C
1	CA	513	C
1	CA	518	C
1	CA	521	G
1	CA	528	C
1	CA	531	U
1	CA	532	A
1	CA	533	A
1	CA	545	C
1	CA	547	A
1	CA	559	A
1	CA	561	U
1	CA	572	A
1	CA	573	A
1	CA	576	G
1	CA	592	G
1	CA	596	C
1	CA	629	G
1	CA	630	G
1	CA	632	A
1	CA	633	G
1	CA	649	G
1	CA	650	G
1	CA	653	A
1	CA	664	G
1	CA	665	A
1	CA	673	G
1	CA	680	C
1	CA	687	A
1	CA	688	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	CA	693	G
1	CA	695	A
1	CA	711	G
1	CA	712	A
1	CA	721	G
1	CA	723	U
1	CA	724	G
1	CA	731	G
1	CA	749	C
1	CA	753	A
1	CA	755	G
1	CA	774	G
1	CA	777	A
1	CA	792	A
1	CA	793	U
1	CA	794	A
1	CA	815	A
1	CA	817	C
1	CA	821	G
1	CA	828	A
1	CA	833	U
1	CA	840	C
1	CA	841	U
1	CA	851	G
1	CA	853	G
1	CA	859	A
1	CA	874	G
1	CA	902	G
1	CA	914	A
1	CA	926	G
1	CA	927	G
1	CA	932	C
1	CA	934	C
1	CA	935	A
1	CA	960	U
1	CA	961	U
1	CA	968	A
1	CA	969	A
1	CA	971	G
1	CA	972	C
1	CA	974	A
1	CA	975	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	CA	976	G
1	CA	977	A
1	CA	989	C
1	CA	992	U
1	CA	993	G
1	CA	996	A
1	CA	997	U
1	CA	1000	U
1	CA	1001(A)	G
1	CA	1002	G
1	CA	1003	G
1	CA	1004	A
1	CA	1005	A
1	CA	1006	C
1	CA	1009	G
1	CA	1019	C
1	CA	1021	G
1	CA	1022	G
1	CA	1023	G
1	CA	1024	G
1	CA	1025	U
1	CA	1026	G
1	CA	1027	C
1	CA	1028	C
1	CA	1030	C
1	CA	1030(A)	G
1	CA	1030(C)	G
1	CA	1030(D)	A
1	CA	1031	G
1	CA	1032	G
1	CA	1037	C
1	CA	1039	C
1	CA	1041	A
1	CA	1043	C
1	CA	1052	U
1	CA	1054	C
1	CA	1055	A
1	CA	1065	U
1	CA	1066	C
1	CA	1068	G
1	CA	1076	C
1	CA	1081	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	CA	1088	G
1	CA	1094	G
1	CA	1095	U
1	CA	1096	C
1	CA	1097	C
1	CA	1101	A
1	CA	1104	G
1	CA	1108	G
1	CA	1109	C
1	CA	1110	A
1	CA	1113	C
1	CA	1117	G
1	CA	1124	G
1	CA	1125	U
1	CA	1126	U
1	CA	1129	C
1	CA	1130	A
1	CA	1131	G
1	CA	1132	C
1	CA	1135	U
1	CA	1136	U
1	CA	1137	C
1	CA	1138	G
1	CA	1139	G
1	CA	1140	C
1	CA	1141	C
1	CA	1146	A
1	CA	1147	C
1	CA	1152	A
1	CA	1154	G
1	CA	1157	A
1	CA	1158	C
1	CA	1159	U
1	CA	1183	A
1	CA	1184	G
1	CA	1196	U
1	CA	1197	G
1	CA	1202	G
1	CA	1211	U
1	CA	1212	U
1	CA	1213	A
1	CA	1224	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	CA	1227	A
1	CA	1228	C
1	CA	1236	A
1	CA	1238	A
1	CA	1240	U
1	CA	1244	C
1	CA	1256	A
1	CA	1257	U
1	CA	1258	G
1	CA	1260	C
1	CA	1262	C
1	CA	1270	C
1	CA	1273	G
1	CA	1278	U
1	CA	1279	A
1	CA	1280	A
1	CA	1281	U
1	CA	1282	C
1	CA	1286	A
1	CA	1287	A
1	CA	1299	A
1	CA	1300	G
1	CA	1305	G
1	CA	1314	C
1	CA	1317	C
1	CA	1322	C
1	CA	1338	G
1	CA	1340	A
1	CA	1346	A
1	CA	1347	G
1	CA	1353	G
1	CA	1355	G
1	CA	1363	C
1	CA	1364	U
1	CA	1370	G
1	CA	1397	C
1	CA	1402	C
1	CA	1419	G
1	CA	1422	G
1	CA	1442	G
1	CA	1442(A)	G
1	CA	1442(B)	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	CA	1446	U
1	CA	1447	A
1	CA	1452	C
1	CA	1456	G
1	CA	1487	G
1	CA	1492	A
1	CA	1493	A
1	CA	1494	G
1	CA	1497	G
1	CA	1502	A
1	CA	1503	A
1	CA	1504	G
1	CA	1506	U
1	CA	1517	G
1	CA	1519	A
1	CA	1520	G
1	CA	1529	G
1	CA	1530	G
1	CA	1531	A
1	CA	1532	U
22	CV	14	A
22	CV	24	A
23	CW	3	C
23	CW	4	C
23	CW	5	G
23	CW	6	G
23	CW	8	4SU
23	CW	9	A
23	CW	12	U
23	CW	14	A
23	CW	19	G
23	CW	22	G
23	CW	23	A
23	CW	25	C
23	CW	26	A
23	CW	27	G
23	CW	30	G
23	CW	42	C
23	CW	43	C
23	CW	45	U
23	CW	46	7MG
23	CW	47	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
23	CW	48	C
23	CW	49	C
23	CW	52	G
23	CW	53	G
23	CW	61	C
23	CW	62	C
23	CW	64	A
23	CW	66	U
23	CW	67	C
23	CW	68	C
23	CW	70	G
23	CW	74	C
24	CX	8	4SU
24	CX	9	G
24	CX	13	C
24	CX	16	C
24	CX	19	G
24	CX	20	U
24	CX	21	A
24	CX	31	G
24	CX	42	G
24	CX	47	U
24	CX	48	C
24	CX	50	U
24	CX	52	G
24	CX	56	C
24	CX	59	A
24	CX	60	U
24	CX	61	C
24	CX	63	G
24	CX	67	C
24	CX	68	C
24	CX	76	A
25	CY	2	C
25	CY	8	4SU
25	CY	9	A
25	CY	11	C
25	CY	13	C
25	CY	15	G
25	CY	19	G
25	CY	23	A
25	CY	27	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
25	CY	29	G
25	CY	30	G
25	CY	33	U
25	CY	34	G
25	CY	35	A
25	CY	36	A
25	CY	39	PSU
25	CY	41	C
25	CY	45	U
25	CY	46	7MG
25	CY	47	U
25	CY	49	C
25	CY	52	G
25	CY	54	5MU
25	CY	56	C
25	CY	57	G
25	CY	58	A
25	CY	59	U
25	CY	62	C
25	CY	65	G
25	CY	67	C
25	CY	70	G
25	CY	73	A
26	DA	10	G
26	DA	12	U
26	DA	15	G
26	DA	16	G
26	DA	34	C
26	DA	35	G
26	DA	45	C
26	DA	51	G
26	DA	61	G
26	DA	71	A
26	DA	74	A
26	DA	75	G
26	DA	78	A
26	DA	83	G
26	DA	84	A
26	DA	90	U
26	DA	95	G
26	DA	100	G
26	DA	102	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	DA	118	A
26	DA	119	A
26	DA	120	U
26	DA	141	A
26	DA	154(A)	C
26	DA	157	U
26	DA	173	G
26	DA	181	A
26	DA	182	A
26	DA	196	A
26	DA	199	A
26	DA	205	G
26	DA	214	G
26	DA	215	G
26	DA	216	A
26	DA	221	A
26	DA	222	A
26	DA	225	A
26	DA	228	A
26	DA	229	A
26	DA	233	A
26	DA	248	G
26	DA	266	G
26	DA	271(I)	G
26	DA	271(K)	U
26	DA	271(L)	U
26	DA	271(M)	G
26	DA	271(N)	U
26	DA	271(V)	G
26	DA	271(W)	G
26	DA	272(A)	U
26	DA	272(B)	G
26	DA	272(C)	G
26	DA	272(J)	C
26	DA	274	G
26	DA	277	C
26	DA	278	A
26	DA	285	C
26	DA	288	C
26	DA	292	C
26	DA	294	A
26	DA	311	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	DA	324	A
26	DA	327	G
26	DA	329	G
26	DA	330	A
26	DA	333	G
26	DA	352	G
26	DA	363	G
26	DA	372	G
26	DA	386	G
26	DA	389	G
26	DA	396	G
26	DA	399	G
26	DA	405	U
26	DA	407	G
26	DA	411	G
26	DA	412	A
26	DA	415	A
26	DA	421	U
26	DA	428	A
26	DA	442	G
26	DA	443	A
26	DA	444	C
26	DA	447	A
26	DA	454	A
26	DA	455	C
26	DA	457	A
26	DA	470	A
26	DA	481	G
26	DA	485	C
26	DA	494	G
26	DA	498	G
26	DA	504	U
26	DA	505	A
26	DA	509	C
26	DA	521	G
26	DA	530	G
26	DA	531	C
26	DA	532	A
26	DA	533	G
26	DA	545	G
26	DA	563	G
26	DA	568	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	DA	573	G
26	DA	574	C
26	DA	575	A
26	DA	586	A
26	DA	587	C
26	DA	588	U
26	DA	592	G
26	DA	603	A
26	DA	604	G
26	DA	607	U
26	DA	614(B)	G
26	DA	614(C)	A
26	DA	615	G
26	DA	616	G
26	DA	620	G
26	DA	627	A
26	DA	637	A
26	DA	645	C
26	DA	646	A
26	DA	652(B)	A
26	DA	652(C)	G
26	DA	652(D)	C
26	DA	652(U)	G
26	DA	656	G
26	DA	668	G
26	DA	669	G
26	DA	686	G
26	DA	698	C
26	DA	699	A
26	DA	715	G
26	DA	726	G
26	DA	730	C
26	DA	752	A
26	DA	753	C
26	DA	765	G
26	DA	775	G
26	DA	776	G
26	DA	782	A
26	DA	783	A
26	DA	784	A
26	DA	785	G
26	DA	790	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	DA	792	G
26	DA	794	G
26	DA	803	U
26	DA	805	G
26	DA	812	C
26	DA	819	A
26	DA	827	U
26	DA	851	U
26	DA	852	G
26	DA	854	G
26	DA	857	C
26	DA	859	G
26	DA	866	A
26	DA	868	U
26	DA	874	G
26	DA	879	G
26	DA	880	G
26	DA	882	G
26	DA	884	C
26	DA	886	C
26	DA	887	A
26	DA	888	C
26	DA	889	C
26	DA	890	A
26	DA	893	C
26	DA	896	A
26	DA	897	C
26	DA	898	C
26	DA	900	A
26	DA	901	A
26	DA	903	C
26	DA	910	A
26	DA	917	A
26	DA	932	G
26	DA	938	G
26	DA	941	A
26	DA	945	A
26	DA	946	G
26	DA	950	G
26	DA	952	G
26	DA	953	A
26	DA	958	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	DA	959	A
26	DA	961	C
26	DA	974	G
26	DA	975	C
26	DA	983	A
26	DA	996	A
26	DA	1005	C
26	DA	1006	C
26	DA	1012	U
26	DA	1013	C
26	DA	1017	G
26	DA	1022	G
26	DA	1025	G
26	DA	1026	U
26	DA	1033	U
26	DA	1034	G
26	DA	1038	C
26	DA	1039	G
26	DA	1042	G
26	DA	1043	C
26	DA	1114	G
26	DA	1118	C
26	DA	1126	A
26	DA	1128	A
26	DA	1130	U
26	DA	1135	C
26	DA	1136	G
26	DA	1139	G
26	DA	1142(A)	A
26	DA	1144	G
26	DA	1171	G
26	DA	1180	C
26	DA	1196	C
26	DA	1205	U
26	DA	1210	A
26	DA	1211	U
26	DA	1220	A
26	DA	1221	C
26	DA	1229	G
26	DA	1242	A
26	DA	1247	A
26	DA	1253	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	DA	1256	G
26	DA	1271	G
26	DA	1272	A
26	DA	1273	U
26	DA	1287	A
26	DA	1300	U
26	DA	1301	A
26	DA	1303	G
26	DA	1305	C
26	DA	1314	C
26	DA	1332	G
26	DA	1352	U
26	DA	1359	A
26	DA	1360	A
26	DA	1365	A
26	DA	1368	G
26	DA	1370	C
26	DA	1380	G
26	DA	1384	A
26	DA	1385	G
26	DA	1412	A
26	DA	1416	G
26	DA	1417	C
26	DA	1419	A
26	DA	1420	U
26	DA	1421	G
26	DA	1428	C
26	DA	1437	C
26	DA	1445	A
26	DA	1445(A)	C
26	DA	1449	A
26	DA	1450	G
26	DA	1459	G
26	DA	1467	C
26	DA	1471	A
26	DA	1482	G
26	DA	1490	A
26	DA	1493	C
26	DA	1494	A
26	DA	1495	A
26	DA	1496	A
26	DA	1497	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	DA	1508	A
26	DA	1509	C
26	DA	1509(A)	A
26	DA	1523	U
26	DA	1525	G
26	DA	1531	C
26	DA	1541	G
26	DA	1542	A
26	DA	1543	C
26	DA	1547	C
26	DA	1554	A
26	DA	1558	A
26	DA	1559	G
26	DA	1566	A
26	DA	1569	A
26	DA	1578	U
26	DA	1580	A
26	DA	1583	A
26	DA	1584	C
26	DA	1586	A
26	DA	1595	G
26	DA	1598	C
26	DA	1608	A
26	DA	1609	A
26	DA	1610	A
26	DA	1612	C
26	DA	1639	U
26	DA	1640	C
26	DA	1647	G
26	DA	1648	C
26	DA	1654	A
26	DA	1674	G
26	DA	1696	G
26	DA	1700	A
26	DA	1703	G
26	DA	1721	G
26	DA	1722	A
26	DA	1740	G
26	DA	1756	G
26	DA	1758	G
26	DA	1763	G
26	DA	1764	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	DA	1773	A
26	DA	1780	A
26	DA	1782	C
26	DA	1791	A
26	DA	1800	C
26	DA	1801	G
26	DA	1812	A
26	DA	1816	G
26	DA	1835	G
26	DA	1836	C
26	DA	1847	A
26	DA	1848	A
26	DA	1866	C
26	DA	1877	A
26	DA	1887	C
26	DA	1889	A
26	DA	1895	C
26	DA	1900	A
26	DA	1906	G
26	DA	1914	C
26	DA	1929	G
26	DA	1930	G
26	DA	1931	U
26	DA	1936	A
26	DA	1937	A
26	DA	1938	A
26	DA	1955	U
26	DA	1963	U
26	DA	1964	G
26	DA	1967	C
26	DA	1970	A
26	DA	1971	A
26	DA	1972	A
26	DA	1993	U
26	DA	1997	G
26	DA	2020	A
26	DA	2023	G
26	DA	2031	A
26	DA	2032	G
26	DA	2033	A
26	DA	2043	C
26	DA	2046	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	DA	2055	C
26	DA	2056	G
26	DA	2060	A
26	DA	2061	G
26	DA	2062	A
26	DA	2069	G
26	DA	2082	A
26	DA	2093	G
26	DA	2095	C
26	DA	2096	U
26	DA	2099	U
26	DA	2101	G
26	DA	2102	U
26	DA	2103	C
26	DA	2104	G
26	DA	2105	C
26	DA	2108	C
26	DA	2111	C
26	DA	2112	G
26	DA	2113	U
26	DA	2115	G
26	DA	2116	G
26	DA	2117	A
26	DA	2119	A
26	DA	2122	U
26	DA	2124	G
26	DA	2125	G
26	DA	2126	A
26	DA	2127	G
26	DA	2129	C
26	DA	2130	U
26	DA	2131	G
26	DA	2132	U
26	DA	2133	G
26	DA	2134	A
26	DA	2135	A
26	DA	2136	C
26	DA	2137	C
26	DA	2138	C
26	DA	2139	C
26	DA	2143	C
26	DA	2145	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	DA	2146	C
26	DA	2148	G
26	DA	2150	U
26	DA	2151	G
26	DA	2153	G
26	DA	2154	G
26	DA	2155	G
26	DA	2157	G
26	DA	2158	A
26	DA	2159	G
26	DA	2160	G
26	DA	2163	C
26	DA	2164	C
26	DA	2165	G
26	DA	2167	U
26	DA	2168	G
26	DA	2169	A
26	DA	2170	A
26	DA	2172	U
26	DA	2173	A
26	DA	2174	C
26	DA	2177	C
26	DA	2178	C
26	DA	2181	G
26	DA	2184	G
26	DA	2185	C
26	DA	2186	G
26	DA	2189	U
26	DA	2192	G
26	DA	2193	G
26	DA	2198	A
26	DA	2206	G
26	DA	2207	G
26	DA	2208	A
26	DA	2218	U
26	DA	2219	G
26	DA	2225	A
26	DA	2235	G
26	DA	2238	G
26	DA	2239	G
26	DA	2259	G
26	DA	2273	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	DA	2275	C
26	DA	2278	A
26	DA	2280	G
26	DA	2283	C
26	DA	2287	A
26	DA	2288	A
26	DA	2294	C
26	DA	2299	G
26	DA	2302	G
26	DA	2303	G
26	DA	2305	A
26	DA	2308	G
26	DA	2312	U
26	DA	2318	G
26	DA	2319	G
26	DA	2320	A
26	DA	2321	G
26	DA	2325	G
26	DA	2327	A
26	DA	2328	A
26	DA	2334	G
26	DA	2336	A
26	DA	2339	G
26	DA	2343	C
26	DA	2347	C
26	DA	2350	C
26	DA	2354	G
26	DA	2366	A
26	DA	2376	A
26	DA	2383	G
26	DA	2385	C
26	DA	2388	A
26	DA	2400	G
26	DA	2406	U
26	DA	2410	G
26	DA	2422	A
26	DA	2425	A
26	DA	2429	G
26	DA	2430	A
26	DA	2435	A
26	DA	2439	A
26	DA	2441	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	DA	2445	G
26	DA	2448	A
26	DA	2465	C
26	DA	2468	G
26	DA	2469	A
26	DA	2474	C
26	DA	2476	A
26	DA	2478	A
26	DA	2490	G
26	DA	2494	G
26	DA	2497	A
26	DA	2502	G
26	DA	2505	G
26	DA	2506	U
26	DA	2518	A
26	DA	2529	G
26	DA	2549	G
26	DA	2554	U
26	DA	2555	U
26	DA	2566	A
26	DA	2567	G
26	DA	2573	C
26	DA	2586	C
26	DA	2602	A
26	DA	2603	G
26	DA	2609	U
26	DA	2611	U
26	DA	2612	C
26	DA	2615	U
26	DA	2629	A
26	DA	2630	G
26	DA	2652	C
26	DA	2654	A
26	DA	2663	G
26	DA	2669	G
26	DA	2689	U
26	DA	2690	C
26	DA	2691	C
26	DA	2703	C
26	DA	2712(A)	A
26	DA	2713	A
26	DA	2714	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	DA	2726	U
26	DA	2733	A
26	DA	2734	A
26	DA	2751	G
26	DA	2757	A
26	DA	2758	A
26	DA	2760	C
26	DA	2764	A
26	DA	2765	A
26	DA	2766	G
26	DA	2778	A
26	DA	2784	C
26	DA	2793	G
26	DA	2794	C
26	DA	2809	A
26	DA	2818	G
26	DA	2820	A
26	DA	2821	A
26	DA	2833	G
26	DA	2834	G
26	DA	2835	A
26	DA	2872	G
26	DA	2873	A
26	DA	2879	C
26	DA	2880	C
26	DA	2892	A
26	DA	2894	G
26	DA	2895	U
26	DA	2897	U
27	DB	2	C
27	DB	7	G
27	DB	8	U
27	DB	34	U
27	DB	42	C
27	DB	56	G
27	DB	73	A
27	DB	75	G
27	DB	85	G
27	DB	90	A
27	DB	93	G
27	DB	106	G
27	DB	108	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
27	DB	110	G
27	DB	111	G
27	DB	112	U
27	DB	120	A

All (126) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	AA	96	U
1	AA	115	G
1	AA	266	G
1	AA	347	G
1	AA	429	U
1	AA	509	A
1	AA	532	A
1	AA	560	U
1	AA	687	A
1	AA	748	C
1	AA	793	U
1	AA	839	U
1	AA	913	A
1	AA	991	U
1	AA	1026	G
1	AA	1054	C
1	AA	1064	G
1	AA	1065	U
1	AA	1067	A
1	AA	1181	G
1	AA	1201	A
1	AA	1256	A
1	AA	1285	A
1	AA	1442	G
1	AA	1492	A
23	AW	13	C
23	AW	22	G
25	AY	19	G
25	AY	21	A
25	AY	25	C
25	AY	58	A
26	BA	71	A
26	BA	196	A
26	BA	271(J)	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	BA	271(K)	U
26	BA	271(M)	G
26	BA	278	A
26	BA	746	A
26	BA	764	A
26	BA	774	A
26	BA	899	A
26	BA	974	G
26	BA	1047	G
26	BA	1142(A)	A
26	BA	1174	A
26	BA	1175	U
26	BA	1176	G
26	BA	1210	A
26	BA	1300	U
26	BA	1301	A
26	BA	1379	A
26	BA	1420	U
26	BA	1530	C
26	BA	1653	G
26	BA	1992	G
26	BA	2110	G
26	BA	2126	A
26	BA	2181	G
26	BA	2183	C
26	BA	2187	G
26	BA	2406	U
26	BA	2430	A
26	BA	2689	U
26	BA	2756	U
26	BA	2893	G
1	CA	60	A
1	CA	65	U
1	CA	115	G
1	CA	266	G
1	CA	429	U
1	CA	509	A
1	CA	532	A
1	CA	560	U
1	CA	687	A
1	CA	748	C
1	CA	840	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	CA	913	A
1	CA	991	U
1	CA	992	U
1	CA	1027	C
1	CA	1054	C
1	CA	1064	G
1	CA	1065	U
1	CA	1067	A
1	CA	1128	C
1	CA	1181	G
1	CA	1183	A
1	CA	1201	A
1	CA	1212	U
1	CA	1256	A
1	CA	1299	A
1	CA	1442	G
1	CA	1492	A
23	CW	4	C
23	CW	13	C
25	CY	46	7MG
26	DA	271(K)	U
26	DA	271(M)	G
26	DA	277	C
26	DA	587	C
26	DA	752	A
26	DA	764	A
26	DA	774	A
26	DA	827	U
26	DA	856	C
26	DA	900	A
26	DA	1210	A
26	DA	1300	U
26	DA	1379	A
26	DA	1420	U
26	DA	1427	A
26	DA	1493	C
26	DA	1530	C
26	DA	1558	A
26	DA	1653	G
26	DA	1913	A
26	DA	1992	G
26	DA	2110	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	DA	2126	A
26	DA	2136	C
26	DA	2169	A
26	DA	2177	C
26	DA	2318	G
26	DA	2689	U
26	DA	2756	U
26	DA	2893	G

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

38 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	5MU	CW	54	23	15,22,23	1.08	1 (6%)	16,32,35	1.92	1 (6%)
24	5MC	AX	32	24	15,22,23	1.35	1 (6%)	19,32,35	1.36	3 (15%)
23	MIA	AW	37	23	24,31,32	2.19	4 (16%)	26,44,47	2.60	10 (38%)
25	PSU	CY	55	25	17,21,22	1.46	4 (23%)	20,30,33	3.47	7 (35%)
23	4SU	AW	8	23	14,21,22	1.26	1 (7%)	15,30,33	1.43	2 (13%)
23	PSU	CW	39	23	17,21,22	1.64	3 (17%)	20,30,33	3.37	6 (30%)
25	MIA	CY	37	25	18,24,32	1.16	2 (11%)	18,35,47	1.25	3 (16%)
24	5MC	CX	32	24	15,22,23	1.30	1 (6%)	19,32,35	1.34	3 (15%)
23	PSU	AW	32	23	17,21,22	1.53	2 (11%)	20,30,33	3.22	6 (30%)
23	PSU	CW	32	23	17,21,22	1.58	3 (17%)	20,30,33	3.09	5 (25%)
25	7MG	CY	46	25	22,26,27	1.80	4 (18%)	28,39,42	2.76	10 (35%)
23	31M	CW	76	23	38,44,45	1.41	5 (13%)	38,61,64	1.23	3 (7%)
25	4SU	AY	8	25	14,21,22	1.31	2 (14%)	15,30,33	1.61	2 (13%)
23	PSU	AW	55	23	17,21,22	1.54	2 (11%)	20,30,33	3.34	6 (30%)
24	PSU	AX	55	24,57	17,21,22	1.66	3 (17%)	20,30,33	3.16	7 (35%)
25	PSU	AY	55	25	17,21,22	1.81	3 (17%)	20,30,33	3.00	8 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	PSU	CY	32	25	17,21,22	1.47	3 (17%)	20,30,33	3.22	7 (35%)
23	PSU	CW	55	23	17,21,22	1.42	2 (11%)	20,30,33	3.17	6 (30%)
24	5MU	CX	54	24	15,22,23	1.10	1 (6%)	16,32,35	1.70	2 (12%)
24	4SU	CX	8	24	14,21,22	1.25	2 (14%)	15,30,33	2.36	2 (13%)
25	PSU	AY	32	25	17,21,22	1.45	2 (11%)	20,30,33	3.18	7 (35%)
24	4SU	AX	8	24	14,21,22	1.50	2 (14%)	15,30,33	2.68	2 (13%)
23	MIA	CW	37	23	18,24,32	1.12	2 (11%)	18,35,47	1.19	2 (11%)
23	5MU	AW	54	23	15,22,23	1.04	1 (6%)	16,32,35	2.02	2 (12%)
23	7MG	AW	46	23	22,26,27	1.78	4 (18%)	28,39,42	2.85	9 (32%)
24	PSU	CX	55	24	17,21,22	1.54	3 (17%)	20,30,33	3.11	6 (30%)
23	7MG	CW	46	23	22,26,27	1.81	4 (18%)	28,39,42	2.62	8 (28%)
25	PSU	CY	39	25	17,21,22	1.66	4 (23%)	20,30,33	2.88	6 (30%)
23	PSU	AW	39	23	17,21,22	1.63	3 (17%)	20,30,33	3.32	6 (30%)
25	MIA	AY	37	25	18,24,32	1.14	2 (11%)	18,35,47	1.22	2 (11%)
23	31M	AW	76	23	38,44,45	1.40	5 (13%)	38,61,64	1.39	4 (10%)
25	5MU	AY	54	25	15,22,23	1.15	1 (6%)	16,32,35	1.81	2 (12%)
25	4SU	CY	8	25	14,21,22	1.32	1 (7%)	15,30,33	1.17	1 (6%)
25	5MU	CY	54	25	15,22,23	1.05	2 (13%)	16,32,35	1.85	2 (12%)
25	PSU	AY	39	25	17,21,22	1.58	4 (23%)	20,30,33	3.80	5 (25%)
25	7MG	AY	46	25	22,26,27	1.72	3 (13%)	28,39,42	3.02	9 (32%)
24	5MU	AX	54	24,57	15,22,23	1.07	1 (6%)	16,32,35	1.94	2 (12%)
23	4SU	CW	8	23	14,21,22	1.27	1 (7%)	15,30,33	1.32	2 (13%)

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
23	5MU	CW	54	23	-	0/5/25/26	0/2/2/2
24	5MC	AX	32	24	-	0/5/25/26	0/2/2/2
23	MIA	AW	37	23	-	1/11/33/34	0/3/3/3
25	PSU	CY	55	25	-	1/7/25/26	0/2/2/2
23	4SU	AW	8	23	-	0/5/25/26	0/2/2/2
23	PSU	CW	39	23	-	0/7/25/26	0/2/2/2
25	MIA	CY	37	25	-	3/3/25/34	0/3/3/3
24	5MC	CX	32	24	-	0/5/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	PSU	AW	32	23	-	0/7/25/26	0/2/2/2
23	PSU	CW	32	23	-	0/7/25/26	0/2/2/2
25	7MG	CY	46	25	-	5/7/37/38	0/3/3/3
23	31M	CW	76	23	-	11/27/49/50	0/4/4/4
25	4SU	AY	8	25	-	1/5/25/26	0/2/2/2
23	PSU	AW	55	23	-	0/7/25/26	0/2/2/2
24	PSU	AX	55	24,57	-	0/7/25/26	0/2/2/2
25	PSU	AY	55	25	-	1/7/25/26	0/2/2/2
25	PSU	CY	32	25	-	1/7/25/26	0/2/2/2
23	PSU	CW	55	23	-	0/7/25/26	0/2/2/2
24	5MU	CX	54	24	-	0/5/25/26	0/2/2/2
24	4SU	CX	8	24	-	0/5/25/26	0/2/2/2
25	PSU	AY	32	25	-	1/7/25/26	0/2/2/2
24	4SU	AX	8	24	-	0/5/25/26	0/2/2/2
23	MIA	CW	37	23	-	0/3/25/34	0/3/3/3
23	5MU	AW	54	23	-	0/5/25/26	0/2/2/2
23	7MG	AW	46	23	-	3/7/37/38	0/3/3/3
24	PSU	CX	55	24	-	1/7/25/26	0/2/2/2
23	7MG	CW	46	23	-	3/7/37/38	0/3/3/3
25	PSU	CY	39	25	-	2/7/25/26	0/2/2/2
23	PSU	AW	39	23	-	0/7/25/26	0/2/2/2
25	MIA	AY	37	25	-	3/3/25/34	0/3/3/3
23	31M	AW	76	23	-	9/27/49/50	0/4/4/4
25	5MU	AY	54	25	-	2/5/25/26	0/2/2/2
25	4SU	CY	8	25	-	2/5/25/26	0/2/2/2
25	5MU	CY	54	25	-	2/5/25/26	0/2/2/2
25	PSU	AY	39	25	-	2/7/25/26	0/2/2/2
25	7MG	AY	46	25	-	2/7/37/38	0/3/3/3
24	5MU	AX	54	24,57	-	0/5/25/26	0/2/2/2
23	4SU	CW	8	23	-	0/5/25/26	0/2/2/2

All (94) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AW	37	MIA	C13-C14	7.24	1.53	1.32
23	AW	37	MIA	C2-S10	-6.30	1.70	1.75
25	AY	55	PSU	C5-C1'	-5.84	1.47	1.52
25	CY	46	7MG	C6-C5	5.43	1.48	1.41
23	CW	46	7MG	C6-C5	5.07	1.48	1.41
23	AW	76	31M	CB-CG	-5.03	1.39	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	CW	39	PSU	C5-C1'	-4.98	1.48	1.52
24	AX	55	PSU	C5-C1'	-4.88	1.48	1.52
23	CW	76	31M	CB-CG	-4.85	1.39	1.51
23	AW	39	PSU	C5-C1'	-4.83	1.48	1.52
24	AX	32	5MC	C5-C4	4.77	1.48	1.41
24	CX	32	5MC	C5-C4	4.66	1.48	1.41
23	AW	46	7MG	C6-C5	4.63	1.47	1.41
23	AW	46	7MG	C5-C4	4.55	1.48	1.39
23	CW	46	7MG	C5-C4	4.50	1.48	1.39
25	AY	46	7MG	C6-C5	4.48	1.47	1.41
25	AY	46	7MG	C5-C4	4.47	1.47	1.39
25	CY	46	7MG	C5-C4	4.39	1.47	1.39
23	CW	32	PSU	C5-C1'	-4.37	1.48	1.52
25	CY	8	4SU	C4-S4	-4.33	1.59	1.67
23	AW	55	PSU	C5-C1'	-4.26	1.48	1.52
25	CY	55	PSU	C4-C5	4.20	1.50	1.41
25	AY	8	4SU	C4-S4	-4.07	1.60	1.67
23	AW	8	4SU	C4-S4	-4.02	1.60	1.67
24	AX	8	4SU	C4-S4	-3.99	1.60	1.67
25	CY	39	PSU	C5-C1'	-3.99	1.48	1.52
23	CW	8	4SU	C4-S4	-3.92	1.60	1.67
24	CX	8	4SU	C4-S4	-3.91	1.60	1.67
24	CX	55	PSU	C5-C1'	-3.89	1.48	1.52
23	AW	32	PSU	C5-C1'	-3.88	1.48	1.52
25	CY	39	PSU	C4-C5	3.82	1.49	1.41
25	AY	39	PSU	C5-C1'	-3.74	1.49	1.52
24	CX	55	PSU	C4-C5	3.70	1.49	1.41
25	AY	32	PSU	C4-C5	3.69	1.49	1.41
24	AX	8	4SU	C2-N3	-3.65	1.30	1.38
25	AY	54	5MU	C4-C5	3.65	1.49	1.41
25	CY	32	PSU	C4-C5	3.56	1.49	1.41
23	AW	32	PSU	C4-C5	3.54	1.49	1.41
25	AY	46	7MG	C5-N7	-3.45	1.33	1.39
23	CW	55	PSU	C4-C5	3.44	1.48	1.41
23	CW	54	5MU	C4-C5	3.44	1.48	1.41
24	CX	54	5MU	C4-C5	3.41	1.48	1.41
25	CY	32	PSU	C5-C1'	-3.41	1.49	1.52
23	CW	76	31M	O4'-C1'	3.40	1.45	1.41
23	CW	55	PSU	C5-C1'	-3.39	1.49	1.52
23	CW	32	PSU	C4-C5	3.39	1.48	1.41
23	CW	46	7MG	C5-N7	-3.35	1.34	1.39
23	AW	55	PSU	C4-C5	3.31	1.48	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AW	46	7MG	C5-N7	-3.31	1.34	1.39
24	AX	54	5MU	C4-C5	3.30	1.48	1.41
23	AW	76	31M	O4'-C1'	3.28	1.45	1.41
23	AW	54	5MU	C4-C5	3.21	1.48	1.41
25	AY	32	PSU	C5-C1'	-3.21	1.49	1.52
25	AY	39	PSU	C4-C5	3.10	1.48	1.41
23	AW	76	31M	C5-C4	-3.07	1.32	1.40
23	CW	39	PSU	C4-C5	3.07	1.48	1.41
25	CY	54	5MU	C4-C5	3.07	1.48	1.41
23	AW	39	PSU	C4-C5	3.06	1.48	1.41
23	CW	76	31M	C5-C4	-3.03	1.32	1.40
24	AX	55	PSU	C4-C5	2.96	1.47	1.41
25	CY	46	7MG	C5-N7	-2.91	1.34	1.39
25	CY	37	MIA	C5-C4	2.89	1.48	1.40
25	AY	55	PSU	C4-C5	2.75	1.47	1.41
23	CW	37	MIA	C2-N3	2.75	1.36	1.32
25	AY	37	MIA	C5-C4	2.73	1.48	1.40
25	AY	55	PSU	O4'-C1'	-2.73	1.40	1.44
23	AW	76	31M	C6-C5	-2.73	1.33	1.43
23	CW	37	MIA	C5-C4	2.69	1.48	1.40
25	AY	37	MIA	C2-N3	2.66	1.36	1.32
25	AY	39	PSU	O4'-C1'	-2.65	1.40	1.44
25	CY	37	MIA	C2-N3	2.63	1.36	1.32
25	CY	46	7MG	C4-N9	-2.56	1.33	1.38
23	CW	76	31M	C6-C5	-2.55	1.33	1.43
23	AW	37	MIA	C5-C4	2.51	1.47	1.40
23	CW	46	7MG	C4-N9	-2.41	1.33	1.38
23	AW	76	31M	C2-N1	2.36	1.38	1.33
25	CY	55	PSU	C2-N3	-2.33	1.33	1.38
25	CY	55	PSU	C5-C1'	-2.28	1.50	1.52
25	CY	54	5MU	C2-N3	-2.27	1.33	1.38
24	AX	55	PSU	O4'-C1'	-2.23	1.41	1.44
25	AY	39	PSU	C2-N1	-2.18	1.33	1.38
23	CW	76	31M	C5-N7	-2.14	1.32	1.39
25	CY	32	PSU	O4'-C1'	-2.12	1.41	1.44
23	AW	46	7MG	C4-N9	-2.12	1.34	1.38
23	AW	37	MIA	C6-N1	2.10	1.35	1.32
25	AY	8	4SU	C2-N3	-2.10	1.34	1.38
25	CY	39	PSU	C2-N1	-2.09	1.34	1.38
23	CW	32	PSU	O4'-C1'	-2.08	1.41	1.44
24	CX	8	4SU	C2-N3	-2.07	1.34	1.38
25	CY	39	PSU	O4'-C1'	-2.07	1.41	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	CW	39	PSU	O4'-C1'	-2.06	1.41	1.44
23	AW	39	PSU	O4'-C1'	-2.02	1.41	1.44
24	CX	55	PSU	O4'-C1'	-2.01	1.41	1.44
25	CY	55	PSU	C2-N1	-2.00	1.34	1.38

All (176) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	AY	46	7MG	N3-C4-N9	10.62	140.54	126.91
25	AY	39	PSU	C4-N3-C2	9.65	123.29	115.14
23	AW	46	7MG	N3-C4-N9	9.26	138.81	126.91
24	AX	8	4SU	C2-N3-C4	9.26	128.58	115.15
25	AY	39	PSU	N1-C2-N3	-9.18	121.13	128.43
23	CW	39	PSU	N1-C2-N3	-9.07	121.22	128.43
23	AW	39	PSU	N1-C2-N3	-8.84	121.40	128.43
25	CY	32	PSU	N1-C2-N3	-8.68	121.53	128.43
23	AW	55	PSU	N1-C2-N3	-8.66	121.55	128.43
25	AY	32	PSU	N1-C2-N3	-8.59	121.60	128.43
23	AW	32	PSU	N1-C2-N3	-8.54	121.64	128.43
24	AX	55	PSU	N1-C2-N3	-8.53	121.65	128.43
23	CW	32	PSU	N1-C2-N3	-8.48	121.69	128.43
23	AW	37	MIA	C12-C13-C14	-8.47	110.65	127.14
24	CX	55	PSU	N1-C2-N3	-8.35	121.79	128.43
23	CW	46	7MG	N3-C4-N9	8.31	137.58	126.91
23	CW	55	PSU	N1-C2-N3	-8.29	121.84	128.43
25	CY	46	7MG	N3-C4-N9	8.10	137.32	126.91
24	CX	8	4SU	C2-N3-C4	7.74	126.36	115.15
25	CY	55	PSU	N1-C2-N3	-7.68	122.33	128.43
23	AW	39	PSU	C4-N3-C2	7.62	121.58	115.14
23	AW	54	5MU	C4-N3-C2	7.46	121.44	115.14
25	AY	55	PSU	N1-C2-N3	-7.34	122.59	128.43
23	CW	54	5MU	C4-N3-C2	7.26	121.27	115.14
25	CY	55	PSU	O4'-C1'-C5	7.24	121.15	109.93
23	AW	55	PSU	C4-N3-C2	7.24	121.25	115.14
23	CW	39	PSU	C4-N3-C2	7.23	121.24	115.14
24	AX	54	5MU	C4-N3-C2	7.22	121.23	115.14
25	CY	32	PSU	C4-N3-C2	7.22	121.23	115.14
25	CY	39	PSU	N1-C2-N3	-7.12	122.77	128.43
23	CW	32	PSU	C4-N3-C2	6.71	120.81	115.14
25	AY	39	PSU	C5-C4-N3	-6.65	116.79	125.36
23	AW	32	PSU	C4-N3-C2	6.60	120.71	115.14
24	CX	55	PSU	C4-N3-C2	6.49	120.62	115.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	AY	54	5MU	C4-N3-C2	6.48	120.61	115.14
23	CW	55	PSU	C4-N3-C2	6.48	120.61	115.14
25	AY	39	PSU	O4'-C1'-C5	-6.45	99.94	109.93
25	CY	54	5MU	C4-N3-C2	6.44	120.58	115.14
24	AX	55	PSU	C4-N3-C2	6.41	120.55	115.14
25	CY	55	PSU	C5-C1'-C2'	-6.37	103.95	115.32
25	AY	32	PSU	C4-N3-C2	6.24	120.41	115.14
25	AY	46	7MG	C5-C4-N3	-6.18	116.40	126.49
25	CY	46	7MG	N7-C8-N9	-5.86	94.99	103.38
25	AY	55	PSU	C4-N3-C2	5.81	120.05	115.14
24	CX	54	5MU	C4-N3-C2	5.75	120.00	115.14
23	AW	39	PSU	C5-C4-N3	-5.72	117.99	125.36
25	CY	39	PSU	C4-N3-C2	5.62	119.89	115.14
25	CY	32	PSU	C5-C4-N3	-5.59	118.16	125.36
25	AY	55	PSU	C5-C4-N3	-5.58	118.18	125.36
23	CW	39	PSU	C5-C4-N3	-5.50	118.27	125.36
23	AW	76	31M	N3-C2-N1	-5.49	120.09	128.68
23	AW	55	PSU	C5-C4-N3	-5.46	118.32	125.36
23	CW	32	PSU	C5-C4-N3	-5.43	118.37	125.36
23	AW	46	7MG	N7-C8-N9	-5.42	95.63	103.38
24	AX	55	PSU	C5-C4-N3	-5.38	118.42	125.36
23	AW	46	7MG	C6-N1-C2	5.36	124.44	115.93
25	CY	39	PSU	C5-C4-N3	-5.34	118.48	125.36
24	CX	55	PSU	C5-C4-N3	-5.33	118.49	125.36
23	CW	76	31M	N3-C2-N1	-5.31	120.38	128.68
23	CW	55	PSU	C5-C4-N3	-5.17	118.70	125.36
23	AW	32	PSU	C5-C4-N3	-5.13	118.76	125.36
23	CW	46	7MG	N7-C8-N9	-5.07	96.12	103.38
23	AW	55	PSU	C5-C1'-C2'	-5.04	106.33	115.32
23	CW	46	7MG	C5-C4-N3	-5.03	118.28	126.49
25	AY	46	7MG	N7-C8-N9	-4.87	96.42	103.38
23	AW	46	7MG	C5-C4-N3	-4.79	118.68	126.49
25	AY	46	7MG	C6-C5-C4	4.77	120.32	115.20
25	CY	55	PSU	C4-N3-C2	4.73	119.14	115.14
25	CY	46	7MG	C6-N1-C2	4.71	123.42	115.93
25	CY	55	PSU	C6-N1-C2	4.71	123.13	115.36
25	AY	8	4SU	C2-N3-C4	4.68	121.93	115.15
25	AY	32	PSU	C5-C4-N3	-4.65	119.37	125.36
25	CY	46	7MG	C5-C4-N3	-4.61	118.96	126.49
24	AX	55	PSU	C5-C6-N1	-4.53	118.87	124.44
25	AY	55	PSU	C5-C6-N1	-4.52	118.88	124.44
25	AY	32	PSU	C5-C6-N1	-4.47	118.95	124.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	AY	32	PSU	C6-N1-C2	4.46	122.71	115.36
24	CX	55	PSU	C5-C6-N1	-4.42	119.00	124.44
25	CY	55	PSU	C5-C6-N1	-4.41	119.03	124.44
23	CW	39	PSU	C5-C1'-C2'	-4.35	107.55	115.32
23	AW	37	MIA	C2-N3-C4	4.33	121.29	115.32
23	AW	8	4SU	C2-N3-C4	4.33	121.43	115.15
23	CW	46	7MG	C6-N1-C2	4.31	122.77	115.93
23	AW	32	PSU	C6-N1-C2	4.29	122.44	115.36
23	AW	32	PSU	C5-C1'-C2'	-4.28	107.69	115.32
24	CX	55	PSU	C6-N1-C2	4.26	122.38	115.36
24	AX	55	PSU	C6-N1-C2	4.24	122.36	115.36
23	AW	32	PSU	C5-C6-N1	-4.22	119.25	124.44
23	CW	39	PSU	C5-C6-N1	-4.19	119.29	124.44
24	CX	8	4SU	C5-C4-N3	-4.19	118.22	123.83
23	AW	39	PSU	C5-C6-N1	-4.19	119.29	124.44
24	AX	8	4SU	C5-C4-N3	-4.18	118.24	123.83
23	CW	55	PSU	C5-C1'-C2'	-4.18	107.87	115.32
23	CW	39	PSU	C6-N1-C2	4.12	122.15	115.36
23	CW	55	PSU	C6-N1-C2	4.07	122.08	115.36
23	CW	32	PSU	C6-N1-C2	4.06	122.06	115.36
23	CW	55	PSU	C5-C6-N1	-4.06	119.45	124.44
23	CW	32	PSU	C5-C6-N1	-4.05	119.47	124.44
25	CY	39	PSU	C6-N1-C2	4.02	121.99	115.36
23	AW	37	MIA	C16-C14-C13	-4.00	111.09	122.65
25	CY	39	PSU	C5-C6-N1	-3.98	119.55	124.44
23	CW	46	7MG	C6-C5-C4	3.97	119.46	115.20
23	AW	39	PSU	C6-N1-C2	3.96	121.90	115.36
23	AW	55	PSU	C6-N1-C2	3.91	121.82	115.36
25	CY	32	PSU	C6-N1-C2	3.91	121.80	115.36
25	CY	55	PSU	C5-C4-N3	-3.84	120.41	125.36
23	AW	37	MIA	C15-C14-C13	-3.83	111.57	122.65
25	AY	46	7MG	C6-N1-C2	3.82	122.00	115.93
23	AW	46	7MG	C5-C6-N1	-3.81	115.31	123.14
23	AW	46	7MG	C6-C5-C4	3.79	119.27	115.20
23	AW	55	PSU	C5-C6-N1	-3.78	119.80	124.44
25	CY	39	PSU	C5-C1'-C2'	-3.77	108.59	115.32
25	AY	32	PSU	O4'-C1'-C5	3.76	115.75	109.93
25	AY	55	PSU	C6-N1-C2	3.68	121.44	115.36
24	CX	32	5MC	C2-N3-C4	3.65	120.42	116.02
23	CW	46	7MG	C5-C6-N1	-3.65	115.65	123.14
23	AW	37	MIA	C5-C6-N1	-3.62	117.80	120.81
25	CY	46	7MG	C5-C6-N1	-3.60	115.75	123.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	CW	8	4SU	C2-N3-C4	3.47	120.18	115.15
25	CY	32	PSU	C5-C6-N1	-3.41	120.25	124.44
23	AW	39	PSU	C5-C1'-C2'	-3.24	109.53	115.32
25	AY	37	MIA	N3-C2-N1	-3.22	123.64	128.68
25	CY	46	7MG	C6-C5-C4	3.19	118.62	115.20
23	CW	37	MIA	N3-C2-N1	-3.15	123.75	128.68
23	AW	76	31M	CAM-CTM-N	3.15	120.52	116.15
24	AX	32	5MC	C2-N3-C4	3.15	119.81	116.02
25	AY	46	7MG	C5-C6-N1	-3.14	116.69	123.14
23	AW	76	31M	OTM-CTM-CAM	-3.13	113.55	120.18
25	CY	37	MIA	N3-C2-N1	-3.12	123.80	128.68
24	AX	55	PSU	C5-C1'-C2'	-3.11	109.77	115.32
23	CW	76	31M	OTM-CTM-CAM	-3.02	113.79	120.18
24	AX	32	5MC	C5-C6-N1	-3.02	118.94	122.19
25	AY	8	4SU	C5-C4-N3	-2.97	119.85	123.83
23	CW	8	4SU	C5-C4-N3	-2.90	119.95	123.83
23	AW	37	MIA	C2-N1-C6	2.90	122.38	117.19
25	CY	46	7MG	C8-N7-C5	2.88	116.43	108.94
25	AY	39	PSU	C6-N1-C2	2.86	120.08	115.36
25	CY	32	PSU	O4'-C1'-C5	-2.85	105.52	109.93
25	AY	55	PSU	C5-C1'-C2'	-2.84	110.26	115.32
25	AY	55	PSU	O4'-C1'-C5	-2.81	105.58	109.93
23	AW	46	7MG	C5-C4-N9	-2.80	102.51	106.44
25	CY	54	5MU	C5-C6-N1	-2.78	119.20	122.19
25	CY	46	7MG	O4'-C1'-N9	-2.77	105.60	109.35
23	AW	8	4SU	C5-C4-N3	-2.76	120.13	123.83
23	AW	37	MIA	C4-C5-N7	-2.73	106.56	109.40
25	AY	37	MIA	C4-C5-N7	-2.72	106.56	109.40
24	AX	32	5MC	N4-C4-N3	2.70	120.84	117.03
23	CW	37	MIA	C4-C5-N7	-2.68	106.61	109.40
23	AW	76	31M	O4'-C4'-C3'	2.68	107.90	104.06
23	CW	46	7MG	C8-N7-C5	2.62	115.75	108.94
23	CW	76	31M	CAM-CTM-N	2.61	119.77	116.15
23	AW	46	7MG	C8-N7-C5	2.60	115.71	108.94
24	CX	32	5MC	N4-C4-N3	2.57	120.67	117.03
23	AW	37	MIA	N3-C2-N1	-2.57	122.26	126.98
25	AY	46	7MG	C8-N7-C5	2.54	115.56	108.94
25	AY	46	7MG	C2-N3-C4	2.53	120.88	113.89
25	CY	8	4SU	C2-N3-C4	2.48	118.75	115.15
24	CX	55	PSU	C5-C1'-C2'	-2.47	110.90	115.32
25	AY	46	7MG	C5-C4-N9	-2.42	103.05	106.44
23	AW	37	MIA	C12-N6-C6	-2.42	118.97	122.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	AY	55	PSU	O4'-C1'-C2'	2.40	108.55	104.66
23	AW	37	MIA	C11-S10-C2	-2.38	100.49	102.27
24	CX	32	5MC	C5-C6-N1	-2.34	119.68	122.19
24	CX	54	5MU	C5-C6-N1	-2.32	119.69	122.19
25	AY	32	PSU	C5-C1'-C2'	-2.30	111.21	115.32
25	CY	46	7MG	C2-N3-C4	2.20	119.98	113.89
25	CY	46	7MG	N2-C2-N1	2.20	120.67	117.25
25	AY	54	5MU	C5-C6-N1	-2.15	119.88	122.19
23	CW	46	7MG	C2-N3-C4	2.13	119.79	113.89
23	AW	54	5MU	C5-C6-N1	-2.12	119.91	122.19
25	CY	32	PSU	O4'-C1'-C2'	2.12	108.09	104.66
23	AW	46	7MG	C2-N3-C4	2.09	119.66	113.89
24	AX	54	5MU	C5-C6-N1	-2.05	119.99	122.19
25	CY	37	MIA	C4-C5-N7	-2.01	107.30	109.40
25	CY	37	MIA	N6-C6-N1	2.01	122.74	118.57
24	AX	55	PSU	O4'-C1'-C2'	2.00	107.91	104.66

There are no chirality outliers.

All (56) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	AW	37	MIA	C12-C13-C14-C16
25	CY	37	MIA	C3'-C4'-C5'-O5'
25	CY	46	7MG	O4'-C4'-C5'-O5'
23	CW	76	31M	C3'-C4'-C5'-O5'
23	CW	76	31M	O4'-C4'-C5'-O5'
23	CW	76	31M	NM-CAM-CTM-N
25	AY	8	4SU	C2'-C1'-N1-C6
23	CW	46	7MG	C2'-C1'-N9-C8
23	AW	76	31M	NM-CAM-CTM-N
23	AW	76	31M	CBM-CAM-CTM-N
23	AW	76	31M	CBM-CAM-CTM-OTM
25	AY	54	5MU	C3'-C4'-C5'-O5'
25	AY	54	5MU	O4'-C4'-C5'-O5'
25	CY	54	5MU	C3'-C4'-C5'-O5'
25	CY	54	5MU	O4'-C4'-C5'-O5'
25	AY	39	PSU	C3'-C4'-C5'-O5'
25	AY	46	7MG	C4'-C5'-O5'-P
23	CW	76	31M	C-CA-CB-CG
23	CW	76	31M	N-CA-CB-CG
25	CY	46	7MG	C3'-C4'-C5'-O5'
25	CY	39	PSU	C3'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	CY	39	PSU	O4'-C4'-C5'-O5'
25	AY	39	PSU	O4'-C4'-C5'-O5'
25	CY	37	MIA	O4'-C4'-C5'-O5'
25	CY	8	4SU	C3'-C4'-C5'-O5'
25	CY	8	4SU	O4'-C4'-C5'-O5'
23	CW	46	7MG	C2'-C1'-N9-C4
23	CW	76	31M	CA-CB-CG-CD1
23	CW	76	31M	CA-CB-CG-CD2
23	CW	76	31M	NM-CAM-CTM-OTM
23	AW	76	31M	NM-CAM-CTM-OTM
23	CW	76	31M	CBM-CAM-CTM-OTM
23	AW	76	31M	CTM-CAM-CBM-CGM
25	CY	46	7MG	C2'-C1'-N9-C8
23	AW	76	31M	CBM-CGM-SDM-CEM
23	AW	76	31M	NM-CAM-CBM-CGM
23	AW	46	7MG	C4'-C5'-O5'-P
23	CW	76	31M	CBM-CGM-SDM-CEM
25	AY	37	MIA	C4'-C5'-O5'-P
23	AW	46	7MG	C3'-C4'-C5'-O5'
25	AY	37	MIA	C3'-C4'-C5'-O5'
25	CY	37	MIA	C4'-C5'-O5'-P
25	AY	32	PSU	O4'-C4'-C5'-O5'
25	AY	46	7MG	C3'-C4'-C5'-O5'
23	CW	46	7MG	C4'-C5'-O5'-P
23	AW	76	31M	C2'-C3'-N3'-C
23	AW	46	7MG	O4'-C4'-C5'-O5'
25	CY	46	7MG	C2'-C1'-N9-C4
25	AY	55	PSU	O4'-C1'-C5-C4
25	CY	32	PSU	O4'-C4'-C5'-O5'
25	CY	46	7MG	O4'-C1'-N9-C8
23	CW	76	31M	CBM-CAM-CTM-N
24	CX	55	PSU	O4'-C4'-C5'-O5'
25	CY	55	PSU	C3'-C4'-C5'-O5'
23	AW	76	31M	C4'-C5'-O5'-P
25	AY	37	MIA	O4'-C4'-C5'-O5'

There are no ring outliers.

28 monomers are involved in 67 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	AX	32	5MC	3	0
23	AW	37	MIA	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	CY	55	PSU	4	0
23	AW	8	4SU	1	0
23	CW	39	PSU	3	0
25	CY	37	MIA	2	0
24	CX	32	5MC	2	0
25	CY	46	7MG	1	0
23	CW	76	31M	7	0
25	AY	8	4SU	1	0
24	AX	55	PSU	1	0
25	AY	55	PSU	4	0
23	CW	55	PSU	1	0
24	CX	54	5MU	2	0
24	CX	8	4SU	2	0
25	AY	32	PSU	2	0
24	AX	8	4SU	2	0
23	AW	46	7MG	1	0
23	CW	46	7MG	1	0
25	CY	39	PSU	4	0
23	AW	39	PSU	1	0
25	AY	37	MIA	3	0
23	AW	76	31M	4	0
25	AY	54	5MU	2	0
25	CY	8	4SU	5	0
25	AY	39	PSU	4	0
25	AY	46	7MG	3	0
23	CW	8	4SU	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 2093 ligands modelled in this entry, 2091 are monoatomic - leaving 2 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
58	SF4	CD	302	4	0,12,12	0.00	-	-		
58	SF4	AD	501	4	0,12,12	0.00	-	-		

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
58	SF4	CD	302	4	-	-	0/6/5/5
58	SF4	AD	501	4	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1498/1521 (98%)	0.35	28 (1%) 66 73	42, 72, 93, 108	0
1	CA	1503/1521 (98%)	0.38	63 (4%) 36 42	44, 74, 94, 109	0
2	AB	231/256 (90%)	0.77	30 (12%) 3 4	72, 82, 90, 94	0
2	CB	231/256 (90%)	1.43	52 (22%) 0 0	73, 84, 90, 95	0
3	AC	206/239 (86%)	0.96	33 (16%) 1 2	68, 79, 87, 94	0
3	CC	206/239 (86%)	1.84	76 (36%) 0 0	71, 81, 89, 94	0
4	AD	208/209 (99%)	0.97	27 (12%) 3 4	57, 72, 81, 90	0
4	CD	208/209 (99%)	0.80	16 (7%) 13 17	58, 71, 80, 91	0
5	AE	148/162 (91%)	1.01	17 (11%) 4 6	58, 71, 80, 85	0
5	CE	148/162 (91%)	1.21	29 (19%) 1 1	60, 73, 81, 86	0
6	AF	100/101 (99%)	0.56	5 (5%) 28 34	56, 69, 78, 82	0
6	CF	100/101 (99%)	0.43	5 (5%) 28 34	57, 70, 78, 82	0
7	AG	155/156 (99%)	0.84	10 (6%) 18 22	65, 75, 83, 91	0
7	CG	155/156 (99%)	1.13	24 (15%) 2 2	66, 76, 84, 92	0
8	AH	137/138 (99%)	0.96	25 (18%) 1 1	62, 72, 79, 87	0
8	CH	137/138 (99%)	1.09	27 (19%) 1 1	64, 74, 80, 87	0
9	AI	127/128 (99%)	1.11	25 (19%) 1 1	65, 80, 86, 89	0
9	CI	127/128 (99%)	2.49	72 (56%) 0 0	68, 82, 88, 91	0
10	AJ	97/105 (92%)	1.18	19 (19%) 1 1	64, 82, 90, 93	0
10	CJ	96/105 (91%)	1.72	35 (36%) 0 0	67, 84, 91, 93	0
11	AK	114/129 (88%)	0.83	8 (7%) 16 19	48, 70, 79, 84	0
11	CK	114/129 (88%)	0.76	8 (7%) 16 19	51, 71, 79, 84	0
12	AL	122/132 (92%)	0.77	5 (4%) 37 44	50, 65, 73, 78	0
12	CL	122/132 (92%)	1.17	24 (19%) 1 1	53, 67, 75, 80	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	123/126 (97%)	0.70	9 (7%) 15 18	55, 70, 81, 89	0
13	CM	122/126 (96%)	2.06	53 (43%) 0 0	70, 84, 91, 99	0
14	AN	60/61 (98%)	1.20	9 (15%) 2 2	67, 74, 83, 84	0
14	CN	60/61 (98%)	3.00	38 (63%) 0 0	69, 77, 84, 88	0
15	AO	88/89 (98%)	0.67	6 (6%) 17 20	56, 67, 80, 81	0
15	CO	88/89 (98%)	0.92	8 (9%) 9 11	59, 69, 80, 83	0
16	AP	82/88 (93%)	1.57	24 (29%) 0 0	57, 71, 80, 84	0
16	CP	82/88 (93%)	0.97	7 (8%) 10 12	58, 70, 80, 84	0
17	AQ	99/105 (94%)	0.81	11 (11%) 5 7	59, 71, 80, 84	0
17	CQ	99/105 (94%)	1.29	25 (25%) 0 0	61, 71, 81, 85	0
18	AR	68/88 (77%)	0.75	5 (7%) 14 18	59, 68, 81, 83	0
18	CR	68/88 (77%)	0.60	3 (4%) 34 41	61, 70, 80, 84	0
19	AS	83/93 (89%)	0.60	3 (3%) 42 49	71, 80, 86, 95	0
19	CS	83/93 (89%)	1.93	31 (37%) 0 0	74, 82, 89, 96	0
20	AT	96/106 (90%)	0.94	14 (14%) 2 3	57, 71, 81, 85	0
20	CT	96/106 (90%)	1.15	15 (15%) 2 2	58, 70, 82, 85	0
21	AU	23/27 (85%)	1.65	7 (30%) 0 0	67, 74, 77, 81	0
21	CU	23/27 (85%)	2.78	15 (65%) 0 0	71, 75, 80, 84	0
22	AV	13/24 (54%)	2.86	7 (53%) 0 0	58, 81, 96, 99	0
22	CV	12/24 (50%)	3.67	8 (66%) 0 0	63, 84, 93, 94	0
23	AW	66/76 (86%)	1.96	25 (37%) 0 0	68, 96, 103, 105	0
23	CW	64/76 (84%)	3.61	52 (81%) 0 0	73, 97, 103, 106	0
24	AX	72/77 (93%)	0.44	1 (1%) 75 81	39, 68, 87, 91	0
24	CX	72/77 (93%)	0.73	4 (5%) 24 29	53, 82, 93, 97	0
25	AY	67/76 (88%)	1.42	21 (31%) 0 0	44, 97, 102, 105	0
25	CY	66/76 (86%)	2.35	32 (48%) 0 0	47, 97, 102, 105	0
26	BA	2819/2915 (96%)	0.67	29 (1%) 82 86	26, 45, 89, 104	0
26	DA	2800/2915 (96%)	0.18	65 (2%) 60 67	30, 49, 90, 108	0
27	BB	120/121 (99%)	0.55	0 100 100	40, 64, 73, 86	0
27	DB	120/121 (99%)	0.20	5 (4%) 36 42	46, 69, 76, 90	0
28	BD	275/276 (99%)	0.81	7 (2%) 57 63	27, 43, 58, 82	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DD	275/276 (99%)	0.69	14 (5%) 28 33	29, 45, 61, 81	0
29	BE	204/206 (99%)	0.79	7 (3%) 45 52	25, 48, 66, 80	0
29	DE	204/206 (99%)	0.57	4 (1%) 65 72	29, 52, 67, 81	0
30	BF	203/210 (96%)	0.75	1 (0%) 91 94	26, 53, 76, 87	0
30	DF	203/210 (96%)	0.57	7 (3%) 45 52	30, 58, 77, 87	0
31	BG	181/182 (99%)	0.81	10 (5%) 25 30	51, 69, 81, 88	0
31	DG	181/182 (99%)	1.26	40 (22%) 0 0	56, 73, 82, 90	0
32	BH	174/180 (96%)	0.75	4 (2%) 60 67	51, 65, 75, 88	0
32	DH	174/180 (96%)	1.09	34 (19%) 1 1	55, 70, 78, 88	0
33	BI	146/148 (98%)	0.56	5 (3%) 45 52	50, 74, 82, 87	0
33	DI	146/148 (98%)	0.60	13 (8%) 9 11	52, 75, 82, 86	0
34	BN	140/140 (100%)	0.90	3 (2%) 63 70	32, 50, 67, 76	0
34	DN	140/140 (100%)	0.68	8 (5%) 23 28	36, 55, 70, 77	0
35	BO	122/122 (100%)	0.58	0 100 100	30, 43, 59, 70	0
35	DO	122/122 (100%)	0.75	3 (2%) 57 63	45, 59, 73, 78	0
36	BP	149/150 (99%)	0.82	3 (2%) 65 72	26, 55, 75, 83	0
36	DP	149/150 (99%)	0.95	22 (14%) 2 2	30, 59, 77, 85	0
37	BQ	141/141 (100%)	0.83	1 (0%) 87 90	36, 52, 67, 80	0
37	DQ	141/141 (100%)	1.25	26 (18%) 1 1	41, 57, 70, 82	0
38	BR	118/118 (100%)	0.68	0 100 100	25, 36, 54, 59	0
38	DR	118/118 (100%)	0.64	2 (1%) 70 76	41, 54, 65, 72	0
39	BS	110/112 (98%)	0.50	1 (0%) 84 88	38, 51, 65, 72	0
39	DS	110/112 (98%)	1.22	25 (22%) 0 0	63, 77, 84, 92	0
40	BT	131/146 (89%)	0.51	0 100 100	32, 47, 69, 82	0
40	DT	131/146 (89%)	0.66	4 (3%) 49 56	48, 63, 79, 85	0
41	BU	116/118 (98%)	0.80	1 (0%) 84 88	18, 33, 49, 59	0
41	DU	116/118 (98%)	0.82	10 (8%) 10 12	42, 61, 78, 84	0
42	BV	101/101 (100%)	0.55	0 100 100	21, 41, 58, 67	0
42	DV	101/101 (100%)	0.63	4 (3%) 38 45	41, 71, 83, 91	0
43	BW	112/113 (99%)	0.73	0 100 100	23, 34, 54, 79	0
43	DW	112/113 (99%)	0.69	5 (4%) 33 40	39, 50, 67, 83	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BX	95/96 (98%)	0.56	0 100 100	23, 38, 61, 84	0
44	DX	95/96 (98%)	0.97	9 (9%) 8 10	43, 60, 76, 79	0
45	BY	107/110 (97%)	0.51	1 (0%) 84 88	32, 50, 69, 83	0
45	DY	107/110 (97%)	1.19	18 (16%) 1 1	57, 71, 81, 88	0
46	BZ	171/206 (83%)	0.70	14 (8%) 11 14	39, 64, 91, 95	0
46	DZ	174/206 (84%)	1.53	46 (26%) 0 0	66, 84, 94, 101	0
47	B0	83/85 (97%)	0.88	6 (7%) 15 18	27, 39, 61, 73	0
47	D0	83/85 (97%)	1.49	21 (25%) 0 0	47, 66, 75, 82	0
48	B1	97/98 (98%)	0.80	7 (7%) 15 18	30, 48, 70, 76	0
48	D1	97/98 (98%)	0.95	13 (13%) 3 4	38, 58, 74, 83	0
49	B2	70/72 (97%)	0.57	0 100 100	34, 50, 64, 79	0
49	D2	70/72 (97%)	0.66	5 (7%) 16 19	56, 70, 80, 86	0
50	B3	59/60 (98%)	0.63	0 100 100	24, 37, 63, 71	0
50	D3	59/60 (98%)	0.96	7 (11%) 4 5	49, 64, 79, 85	0
51	B4	69/71 (97%)	0.48	5 (7%) 15 18	54, 73, 87, 92	0
51	D4	69/71 (97%)	1.13	12 (17%) 1 1	74, 88, 94, 99	0
52	B5	59/60 (98%)	0.63	1 (1%) 70 76	20, 33, 54, 67	0
52	D5	59/60 (98%)	0.55	2 (3%) 45 52	36, 51, 67, 73	0
53	B6	53/54 (98%)	0.60	1 (1%) 66 73	31, 44, 61, 68	0
53	D6	53/54 (98%)	1.10	8 (15%) 2 2	52, 63, 76, 79	0
54	B7	48/49 (97%)	1.03	3 (6%) 20 23	21, 30, 62, 76	0
54	D7	48/49 (97%)	1.31	8 (16%) 1 1	33, 42, 61, 70	0
55	B8	64/65 (98%)	0.74	2 (3%) 49 56	25, 36, 45, 60	0
55	D8	64/65 (98%)	1.51	18 (28%) 0 0	46, 58, 66, 72	0
56	B9	37/37 (100%)	1.07	2 (5%) 25 30	31, 49, 73, 74	0
56	D9	37/37 (100%)	1.27	5 (13%) 3 4	46, 57, 73, 76	0
All	All	20897/21748 (96%)	0.73	1673 (8%) 12 15	18, 64, 89, 109	0

All (1673) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	CM	124	PRO	12.7
2	CB	165	VAL	12.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
13	AM	124	PRO	11.3
23	CW	71	G	10.9
7	CG	83	ALA	10.6
13	CM	123	ALA	9.8
3	CC	155	GLY	9.1
7	CG	82	GLY	9.0
23	CW	70	G	8.9
23	CW	73	A	8.4
14	CN	25	VAL	8.4
23	AW	71	G	8.2
23	CW	72	C	8.2
9	CI	7	THR	8.1
3	CC	198	VAL	8.0
51	D4	49	PHE	8.0
23	CW	2	C	8.0
23	AW	70	G	8.0
46	DZ	114	GLY	8.0
13	AM	123	ALA	8.0
13	CM	90	LEU	7.8
13	CM	78	ILE	7.8
7	AG	82	GLY	7.8
9	CI	76	ALA	7.8
9	CI	109	VAL	7.8
23	CW	4	C	7.7
3	CC	8	ILE	7.6
22	CV	23	A	7.6
10	CJ	47	PHE	7.6
14	CN	34	TYR	7.4
13	CM	4	ILE	7.3
21	CU	14	TRP	7.2
14	CN	39	LEU	7.2
3	CC	189	ALA	7.1
19	CS	80	TYR	7.1
23	CW	3	C	7.1
46	DZ	155	LEU	7.1
9	CI	36	TYR	7.0
10	CJ	85	LEU	7.0
13	CM	122	LYS	7.0
22	CV	13	A	7.0
5	CE	12	LEU	7.0
25	CY	1	G	7.0
31	DG	28	VAL	6.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
46	DZ	120	ILE	6.8
13	CM	94	ARG	6.8
14	CN	61	TRP	6.7
45	DY	1	MET	6.7
26	DA	2155	G	6.7
19	CS	82	GLY	6.7
19	CS	79	THR	6.6
25	CY	36	A	6.6
1	CA	1030(B)	C	6.6
25	CY	34	G	6.5
23	CW	31	A	6.5
25	CY	18	G	6.5
2	CB	187	LEU	6.5
9	CI	61	ALA	6.4
22	AV	13	A	6.4
13	CM	120	LYS	6.4
13	CM	121	LYS	6.4
3	CC	124	ILE	6.4
3	CC	157	ILE	6.4
10	CJ	55	LYS	6.4
26	DA	229	A	6.3
9	CI	115	GLY	6.3
13	CM	102	ARG	6.3
39	DS	32	LEU	6.2
7	AG	83	ALA	6.2
9	CI	66	ARG	6.2
54	B7	46	VAL	6.2
31	DG	29	TRP	6.2
14	CN	37	PHE	6.1
26	DA	2132	U	6.1
13	CM	119	GLY	6.1
14	CN	29	ARG	6.0
44	DX	92	LEU	6.0
51	D4	57	GLU	6.0
2	CB	122	PHE	6.0
46	DZ	113	ALA	6.0
46	DZ	107	THR	5.9
3	CC	71	ALA	5.9
5	CE	22	GLY	5.9
14	AN	2	ALA	5.9
9	CI	14	VAL	5.9
9	CI	9	ARG	5.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
26	DA	2125	G	5.8
51	D4	52	THR	5.8
14	CN	44	LEU	5.7
26	DA	2112	G	5.7
3	CC	153	VAL	5.7
3	CC	190	ARG	5.7
21	CU	6	ARG	5.7
23	CW	69	G	5.6
14	CN	53	LEU	5.6
25	CY	35	A	5.6
26	DA	2154	G	5.6
2	CB	164	VAL	5.6
47	D0	45	PHE	5.6
2	CB	123	ALA	5.6
54	D7	46	VAL	5.6
3	CC	53	ALA	5.5
22	CV	24	A	5.5
13	CM	6	GLY	5.5
45	DY	106	LEU	5.5
2	CB	92	TYR	5.4
22	AV	24	A	5.4
42	DV	72	VAL	5.4
48	B1	98	LEU	5.4
1	CA	1030(A)	G	5.4
8	AH	3	THR	5.4
25	CY	56	C	5.4
25	CY	53	G	5.4
48	D1	2	SER	5.3
9	CI	123	PRO	5.3
21	CU	16	GLY	5.3
46	DZ	116	VAL	5.2
46	BZ	114	GLY	5.2
28	BD	276	LYS	5.2
5	CE	90	VAL	5.2
19	CS	41	VAL	5.2
7	CG	81	GLY	5.2
46	DZ	96	VAL	5.1
17	AQ	27	PHE	5.1
23	CW	38	A	5.1
3	CC	167	TRP	5.1
22	CV	22	U	5.1
23	CW	13	C	5.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
12	CL	64	TYR	5.0
1	CA	1532	U	5.0
25	AY	36	A	5.0
13	CM	87	TYR	5.0
25	CY	64	A	5.0
10	CJ	63	PHE	5.0
5	CE	94	ALA	5.0
45	DY	5	MET	5.0
1	AA	1532	U	5.0
7	AG	79	ARG	5.0
9	CI	15	ALA	4.9
2	CB	132	LYS	4.9
46	DZ	108	PRO	4.9
22	CV	21	C	4.9
2	CB	32	ILE	4.9
23	CW	75	C	4.8
13	AM	122	LYS	4.8
23	AW	4	C	4.8
3	CC	197	GLY	4.8
9	CI	67	GLY	4.8
47	D0	3	HIS	4.8
14	CN	2	ALA	4.8
1	CA	1035	A	4.7
17	CQ	54	GLY	4.7
7	CG	156	TRP	4.7
46	DZ	111	VAL	4.7
26	DA	2173	A	4.7
32	DH	105	LEU	4.7
2	CB	97	TRP	4.7
22	AV	14	A	4.7
26	DA	2133	G	4.7
46	DZ	156	LYS	4.7
2	AB	101	MET	4.7
31	DG	48	GLU	4.7
37	DQ	33	GLY	4.7
56	D9	37	GLY	4.7
2	CB	207	ALA	4.6
47	B0	7	LEU	4.6
16	AP	2	VAL	4.6
23	CW	5	G	4.6
46	DZ	171	ILE	4.6
13	CM	60	VAL	4.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
19	CS	52	TYR	4.6
23	CW	56	C	4.6
1	AA	1036	G	4.6
26	DA	2145	C	4.6
1	AA	1031	G	4.6
2	CB	201	ILE	4.6
25	AY	34	G	4.6
56	D9	16	VAL	4.6
19	CS	84	GLY	4.6
9	CI	110	GLU	4.6
26	BA	2140	C	4.5
1	AA	1257	U	4.5
9	AI	15	ALA	4.5
1	CA	1036	G	4.5
23	CW	24	G	4.5
21	AU	17	THR	4.5
23	AW	3	C	4.5
10	CJ	46	ARG	4.5
19	CS	71	LEU	4.5
19	CS	75	ALA	4.5
1	AA	1028	C	4.5
9	CI	125	TYR	4.5
46	DZ	143	GLY	4.5
9	AI	113	LYS	4.5
45	DY	45	VAL	4.5
9	CI	18	PHE	4.5
54	D7	48	LYS	4.5
9	CI	106	ALA	4.4
3	AC	204	LEU	4.4
3	CC	194	GLY	4.4
23	CW	40	C	4.4
31	DG	140	ILE	4.4
9	CI	49	PRO	4.4
9	CI	122	ALA	4.4
51	D4	54	GLY	4.4
14	CN	36	PHE	4.4
22	AV	12	A	4.4
10	CJ	74	ILE	4.4
26	DA	2802	G	4.4
3	CC	101	LEU	4.4
10	CJ	71	LEU	4.4
12	CL	18	VAL	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	CE	13	ILE	4.4
26	DA	896	A	4.4
23	CW	28	G	4.4
14	CN	4	LYS	4.3
1	CA	1030	C	4.3
9	AI	81	ILE	4.3
17	CQ	36	ILE	4.3
31	DG	19	LEU	4.3
10	CJ	44	VAL	4.3
4	AD	2	GLY	4.3
46	DZ	147	GLY	4.3
5	CE	109	ILE	4.3
9	AI	106	ALA	4.3
14	CN	10	ALA	4.3
3	CC	120	VAL	4.3
9	CI	124	GLN	4.3
20	CT	9	ASN	4.3
23	CW	14	A	4.3
23	AW	20	U	4.3
9	CI	79	LEU	4.3
23	CW	15	G	4.3
12	CL	32	PHE	4.3
8	CH	130	GLY	4.3
9	AI	19	LEU	4.3
19	CS	30	LEU	4.3
3	CC	129	ALA	4.3
25	CY	5	G	4.3
10	CJ	62	HIS	4.2
25	CY	2	C	4.2
21	CU	13	ILE	4.2
23	CW	10	G	4.2
14	CN	42	ILE	4.2
19	CS	49	ILE	4.2
5	CE	133	TYR	4.2
9	CI	10	ARG	4.2
3	AC	39	ILE	4.2
9	CI	85	LEU	4.2
44	DX	69	TYR	4.2
54	B7	47	ARG	4.2
15	CO	57	LEU	4.1
8	CH	93	VAL	4.1
26	DA	888	C	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
7	CG	154	TYR	4.1
9	CI	75	ASP	4.1
14	CN	38	GLY	4.1
9	CI	112	LYS	4.1
14	CN	50	LYS	4.1
10	CJ	54	PHE	4.1
22	AV	23	A	4.1
3	CC	4	LYS	4.1
26	BA	2132	U	4.1
3	CC	126	ARG	4.1
37	DQ	5	ARG	4.1
9	CI	116	LYS	4.1
26	DA	2156	G	4.1
16	AP	19	ILE	4.1
32	DH	6	ARG	4.1
1	CA	1220	G	4.0
25	CY	57	G	4.0
13	CM	101	GLN	4.0
9	CI	114	TYR	4.0
16	AP	38	TYR	4.0
23	CW	6	G	4.0
16	CP	51	VAL	4.0
10	AJ	98	ILE	4.0
53	D6	54	ILE	4.0
13	CM	88	ARG	4.0
46	DZ	149	SER	4.0
32	DH	107	VAL	4.0
54	D7	47	ARG	4.0
46	DZ	172	ALA	4.0
12	CL	90	VAL	4.0
23	CW	30	G	4.0
25	CY	6	G	4.0
2	CB	70	PHE	4.0
2	CB	71	VAL	4.0
10	CJ	49	VAL	4.0
10	CJ	72	VAL	4.0
53	D6	52	VAL	4.0
25	CY	61	C	4.0
20	CT	72	LEU	4.0
21	CU	2	GLY	4.0
23	AW	73	A	4.0
9	CI	4	TYR	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	CC	185	GLY	4.0
25	CY	62	C	3.9
26	BA	2145	C	3.9
7	CG	4	ARG	3.9
9	CI	127	LYS	3.9
3	CC	60	ALA	3.9
1	AA	1027	C	3.9
1	CA	1531	A	3.9
45	DY	55	TYR	3.9
46	BZ	106	GLY	3.9
53	D6	11	LEU	3.9
32	DH	72	ILE	3.9
28	BD	2	ALA	3.9
46	DZ	139	VAL	3.9
7	CG	22	LEU	3.9
23	AW	5	G	3.9
9	CI	69	GLY	3.9
14	CN	58	LYS	3.9
1	CA	1001	A	3.9
2	CB	101	MET	3.9
3	CC	145	GLY	3.9
14	CN	59	ALA	3.9
25	AY	24	G	3.9
23	CW	41	C	3.9
3	CC	184	TYR	3.9
46	DZ	125	LEU	3.9
14	CN	49	HIS	3.8
3	CC	160	ALA	3.8
2	CB	131	PRO	3.8
13	CM	97	PRO	3.8
41	DU	2	PRO	3.8
23	AW	69	G	3.8
26	DA	2153	G	3.8
47	D0	44	ARG	3.8
32	DH	113	VAL	3.8
23	CW	36	A	3.8
7	CG	79	ARG	3.8
54	B7	48	LYS	3.8
39	DS	56	LEU	3.8
45	DY	44	ILE	3.8
48	B1	2	SER	3.8
9	AI	109	VAL	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	CA	1034	G	3.8
3	AC	87	LEU	3.8
37	DQ	22	LYS	3.8
46	BZ	108	PRO	3.8
32	DH	106	THR	3.8
37	DQ	104	PHE	3.8
25	CY	19	G	3.8
21	CU	11	GLY	3.8
9	CI	19	LEU	3.8
46	BZ	141	VAL	3.8
4	CD	134	ASP	3.8
11	AK	25	TYR	3.8
16	AP	39	TYR	3.8
19	CS	66	MET	3.8
33	DI	38	LEU	3.8
51	D4	50	VAL	3.8
2	CB	228	GLY	3.7
23	CW	74	C	3.7
4	CD	47	ARG	3.7
21	CU	8	THR	3.7
37	DQ	65	PHE	3.7
2	AB	126	GLU	3.7
3	CC	57	ILE	3.7
31	DG	159	VAL	3.7
21	AU	2	GLY	3.7
26	DA	2170	A	3.7
46	DZ	115	GLY	3.7
19	CS	53	ASN	3.7
39	DS	11	LYS	3.7
3	CC	206	GLU	3.7
28	DD	37	LEU	3.7
3	AC	81	GLY	3.7
2	CB	152	PHE	3.7
3	CC	134	ILE	3.7
9	AI	47	LEU	3.7
23	CW	25	C	3.7
46	DZ	141	VAL	3.7
55	D8	26	LYS	3.7
10	CJ	48	THR	3.7
39	DS	3	ARG	3.7
9	CI	17	VAL	3.7
21	CU	17	THR	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
26	BA	1509	C	3.7
26	BA	2794	C	3.7
47	D0	69	PHE	3.7
22	AV	22	U	3.7
14	CN	55	GLY	3.7
8	CH	2	LEU	3.7
13	CM	82	MET	3.7
26	DA	1509	C	3.7
2	AB	133	LYS	3.6
26	DA	2793	G	3.6
10	AJ	18	ALA	3.6
10	CJ	50	ILE	3.6
46	BZ	120	ILE	3.6
51	D4	40	HIS	3.6
26	BA	2793	G	3.6
4	CD	146	ILE	3.6
12	CL	28	LYS	3.6
5	CE	81	GLU	3.6
17	CQ	84	LEU	3.6
47	D0	21	LEU	3.6
48	B1	97	LEU	3.6
46	DZ	170	THR	3.6
9	CI	80	GLY	3.6
1	CA	1202	G	3.6
14	CN	41	ARG	3.6
2	CB	29	ALA	3.6
8	CH	95	VAL	3.6
2	CB	163	PHE	3.6
9	CI	81	ILE	3.6
21	AU	15	ARG	3.6
26	BA	885	C	3.6
2	CB	33	TYR	3.6
20	CT	28	ALA	3.6
25	AY	47	U	3.6
26	DA	2113	U	3.6
9	CI	108	VAL	3.6
54	D7	1	MET	3.6
31	DG	41	GLN	3.6
21	CU	10	ARG	3.5
3	CC	6	HIS	3.5
39	DS	40	ILE	3.5
39	DS	54	LEU	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
39	DS	12	PHE	3.5
16	AP	68	ASP	3.5
22	CV	14	A	3.5
26	DA	2119	A	3.5
20	AT	67	ALA	3.5
1	AA	1034	G	3.5
1	CA	1002	G	3.5
1	CA	1224	G	3.5
7	AG	156	TRP	3.5
44	DX	68	ARG	3.5
3	CC	187	ALA	3.5
46	DZ	137	ILE	3.5
51	D4	51	ASP	3.5
7	CG	78	ARG	3.5
1	AA	1030(A)	G	3.5
23	CW	65	G	3.5
30	DF	208	GLY	3.5
26	BA	2146	C	3.5
26	DA	2146	C	3.5
31	DG	25	TYR	3.5
26	DA	2160	G	3.5
23	AW	14	A	3.4
3	CC	128	PHE	3.4
16	AP	60	LEU	3.4
19	CS	14	HIS	3.4
3	AC	206	GLU	3.4
2	CB	31	TYR	3.4
26	DA	2144	U	3.4
20	AT	74	LYS	3.4
23	AW	72	C	3.4
13	CM	105	THR	3.4
3	CC	154	SER	3.4
9	CI	30	GLY	3.4
17	AQ	35	VAL	3.4
21	CU	15	ARG	3.4
3	AC	8	ILE	3.4
3	AC	184	TYR	3.4
25	AY	1	G	3.4
25	CY	63	G	3.4
26	DA	2116	G	3.4
31	DG	11	TYR	3.4
9	CI	27	THR	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
19	CS	35	SER	3.4
41	DU	21	ALA	3.4
46	DZ	173	ALA	3.4
17	CQ	23	VAL	3.4
32	DH	123	PHE	3.4
36	DP	59	LEU	3.4
39	DS	7	TYR	3.4
37	DQ	28	ALA	3.4
39	DS	5	THR	3.4
13	CM	104	ARG	3.4
31	DG	149	VAL	3.4
8	CH	94	TYR	3.4
49	D2	60	LEU	3.4
2	CB	177	ALA	3.4
13	CM	118	ALA	3.4
44	DX	2	LYS	3.4
25	AY	35	A	3.4
1	CA	1001(A)	G	3.4
13	CM	7	VAL	3.4
31	DG	136	ARG	3.4
3	CC	204	LEU	3.4
9	CI	28	VAL	3.4
26	DA	2149	G	3.4
19	CS	81	ARG	3.4
4	AD	155	LEU	3.3
40	DT	75	ILE	3.3
51	B4	59	PHE	3.3
8	CH	124	ALA	3.3
9	CI	62	TYR	3.3
32	DH	102	ALA	3.3
1	AA	1030(B)	C	3.3
2	CB	37	ASN	3.3
25	CY	13	C	3.3
9	AI	126	SER	3.3
47	D0	37	LEU	3.3
1	CA	1150	U	3.3
9	CI	105	ASP	3.3
10	AJ	73	ASP	3.3
17	AQ	36	ILE	3.3
25	CY	47	U	3.3
28	DD	38	LYS	3.3
18	AR	78	LEU	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
20	AT	55	ILE	3.3
31	DG	35	GLU	3.3
31	DG	39	ILE	3.3
21	CU	5	ASP	3.3
23	AW	13	C	3.3
10	CJ	93	GLY	3.3
6	CF	55	ASP	3.3
1	AA	1030(C)	G	3.3
16	AP	59	TRP	3.3
26	BA	2131	G	3.3
2	AB	232	PRO	3.3
9	CI	102	LEU	3.3
47	D0	59	LEU	3.3
39	DS	35	ILE	3.3
26	DA	886	C	3.3
12	CL	13	LYS	3.3
44	DX	33	LYS	3.3
55	D8	35	GLN	3.3
26	DA	2123	G	3.2
9	AI	117	HIS	3.2
12	AL	29	GLY	3.2
23	CW	47	U	3.2
1	AA	1531	A	3.2
24	AX	67	C	3.2
25	AY	56	C	3.2
5	CE	105	VAL	3.2
12	CL	55	VAL	3.2
3	CC	171	GLY	3.2
4	CD	188	LEU	3.2
4	AD	5	ILE	3.2
5	AE	28	PHE	3.2
28	DD	2	ALA	3.2
20	CT	41	ILE	3.2
23	AW	6	G	3.2
25	AY	5	G	3.2
47	D0	4	LYS	3.2
46	DZ	118	GLN	3.2
32	DH	36	PRO	3.2
12	CL	27	LEU	3.2
1	AA	1002	G	3.2
9	CI	126	SER	3.2
9	AI	98	PRO	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
25	AY	13	C	3.2
2	CB	200	ILE	3.2
2	CB	48	MET	3.2
51	D4	55	ARG	3.2
17	AQ	28	PRO	3.2
26	DA	2138	C	3.2
31	DG	152	LEU	3.2
10	AJ	63	PHE	3.2
11	CK	126	ARG	3.2
42	DV	73	SER	3.2
36	DP	118	GLY	3.2
8	CH	112	LEU	3.2
16	AP	17	TYR	3.2
26	DA	2319	G	3.2
26	BA	2062	A	3.2
5	AE	118	ILE	3.2
46	DZ	146	ILE	3.2
14	CN	31	ARG	3.2
2	CB	115	LEU	3.2
3	CC	12	LEU	3.2
23	CW	27	G	3.1
26	DA	2131	G	3.1
2	CB	214	ILE	3.1
14	CN	7	ILE	3.1
19	CS	40	ILE	3.1
25	CY	21	A	3.1
9	CI	128	ARG	3.1
3	CC	87	LEU	3.1
10	CJ	65	LEU	3.1
36	DP	45	LEU	3.1
52	D5	58	LEU	3.1
3	CC	147	LYS	3.1
5	CE	11	ILE	3.1
10	CJ	13	HIS	3.1
23	AW	65	G	3.1
23	CW	23	A	3.1
25	AY	38	A	3.1
17	CQ	92	ARG	3.1
13	CM	64	TRP	3.1
16	CP	48	TRP	3.1
46	DZ	99	TYR	3.1
7	CG	84	ASN	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
23	AW	25	C	3.1
26	BA	2161	C	3.1
26	DA	2128	C	3.1
31	DG	2	PRO	3.1
26	DA	2115	G	3.1
31	DG	49	ASP	3.1
2	CB	34	ALA	3.1
3	CC	47	LEU	3.1
10	CJ	26	ALA	3.1
21	CU	24	ARG	3.1
3	CC	23	TYR	3.1
7	AG	154	TYR	3.1
3	AC	14	ILE	3.1
1	AA	1030(D)	A	3.1
25	CY	65	G	3.1
13	CM	99	ARG	3.1
2	CB	203	GLY	3.1
15	CO	60	VAL	3.1
31	DG	163	ALA	3.1
3	CC	65	ALA	3.1
22	CV	15	A	3.1
36	DP	32	THR	3.1
2	AB	165	VAL	3.1
14	CN	24	CYS	3.1
1	CA	1219	U	3.1
19	CS	32	LYS	3.1
20	CT	26	ASN	3.1
26	DA	2140	C	3.1
3	CC	121	ALA	3.1
3	CC	146	ALA	3.1
4	AD	135	LEU	3.1
13	AM	2	ALA	3.1
14	CN	47	LEU	3.1
17	CQ	73	VAL	3.1
25	CY	26	A	3.0
26	DA	652(B)	A	3.0
23	CW	34	G	3.0
26	DA	883	G	3.0
44	DX	1	MET	3.0
21	AU	18	TYR	3.0
3	CC	199	LYS	3.0
1	AA	163	C	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
7	CG	16	LEU	3.0
32	DH	52	VAL	3.0
23	CW	64	A	3.0
5	CE	30	ALA	3.0
13	CM	75	ALA	3.0
36	DP	57	THR	3.0
13	CM	74	VAL	3.0
32	DH	25	LYS	3.0
9	CI	12	GLU	3.0
27	DB	119	G	3.0
10	CJ	6	ILE	3.0
36	DP	75	ILE	3.0
47	D0	42	GLY	3.0
1	AA	1447	A	3.0
1	CA	1363(A)	A	3.0
23	CW	26	A	3.0
31	BG	146	TYR	3.0
40	DT	111	ARG	3.0
2	CB	118	LEU	3.0
5	CE	16	THR	3.0
10	AJ	40	LEU	3.0
51	D4	44	THR	3.0
1	AA	1026	G	3.0
26	DA	2164	C	3.0
5	AE	6	PHE	3.0
11	AK	29	ILE	3.0
25	CY	12	U	3.0
26	BA	271(K)	U	3.0
47	D0	74	ARG	3.0
12	CL	69	TYR	3.0
27	DB	59	A	3.0
19	CS	20	LEU	3.0
29	BE	195	LEU	3.0
32	DH	128	PRO	3.0
2	CB	197	VAL	3.0
13	CM	95	GLY	3.0
8	CH	9	MET	3.0
14	CN	27	CYS	3.0
26	BA	2143	C	3.0
26	DA	1026	U	3.0
7	AG	40	ALA	3.0
37	DQ	6	ARG	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
17	CQ	90	ILE	2.9
23	CW	19	G	2.9
25	AY	19	G	2.9
25	CY	22	G	2.9
4	CD	141	ARG	2.9
9	CI	103	THR	2.9
13	AM	97	PRO	2.9
32	BH	145	ALA	2.9
46	DZ	117	LEU	2.9
46	BZ	111	VAL	2.9
47	B0	3	HIS	2.9
9	CI	63	ILE	2.9
31	DG	88	ILE	2.9
14	CN	60	SER	2.9
32	DH	2	SER	2.9
9	AI	120	ARG	2.9
31	DG	51	ARG	2.9
25	CY	25	C	2.9
26	DA	2803	C	2.9
5	CE	123	LEU	2.9
46	DZ	5	LEU	2.9
14	CN	35	ARG	2.9
2	CB	211	ILE	2.9
25	CY	33	U	2.9
3	AC	168	ALA	2.9
23	AW	2	C	2.9
32	DH	103	LEU	2.9
39	DS	58	LEU	2.9
55	D8	61	LEU	2.9
9	CI	5	TYR	2.9
11	CK	25	TYR	2.9
9	AI	65	VAL	2.9
18	CR	87	ARG	2.9
44	DX	43	VAL	2.9
2	AB	200	ILE	2.9
36	DP	51	PHE	2.9
8	CH	131	GLY	2.9
17	CQ	98	LEU	2.9
39	BS	37	ALA	2.9
7	CG	32	ARG	2.9
31	DG	146	TYR	2.9
17	CQ	9	VAL	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
17	CQ	56	VAL	2.9
32	DH	115	VAL	2.9
27	DB	118	G	2.9
45	DY	63	LYS	2.9
14	CN	16	PHE	2.9
9	CI	42	ARG	2.9
20	AT	12	ALA	2.9
1	CA	1116	C	2.9
9	CI	65	VAL	2.9
9	CI	33	PHE	2.9
33	DI	35	LEU	2.9
39	DS	33	LYS	2.9
32	DH	157	TYR	2.9
26	DA	2174	C	2.8
2	AB	130	ARG	2.8
8	CH	92	ARG	2.8
19	CS	36	ARG	2.8
3	CC	5	ILE	2.8
47	D0	5	LYS	2.8
1	AA	1001(A)	G	2.8
45	DY	90	LEU	2.8
13	CM	77	ASN	2.8
4	AD	138	TYR	2.8
9	CI	107	ARG	2.8
36	DP	50	ARG	2.8
56	D9	3	VAL	2.8
26	DA	645	C	2.8
26	DA	885	C	2.8
26	DA	2139	C	2.8
41	DU	17	ILE	2.8
13	CM	72	ALA	2.8
14	CN	6	LEU	2.8
19	AS	71	LEU	2.8
47	D0	7	LEU	2.8
1	AA	162	A	2.8
3	CC	159	GLY	2.8
23	CW	29	G	2.8
25	AY	57	G	2.8
32	BH	2	SER	2.8
10	AJ	21	GLN	2.8
8	CH	134	ILE	2.8
24	CX	65	C	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
31	DG	157	ILE	2.8
45	DY	61	ILE	2.8
5	CE	21	ALA	2.8
13	CM	76	ALA	2.8
2	CB	133	LYS	2.8
4	AD	11	LEU	2.8
8	CH	119	LEU	2.8
10	AJ	90	LEU	2.8
4	AD	3	ARG	2.8
9	CI	83	ARG	2.8
39	DS	20	ARG	2.8
1	AA	1023	G	2.8
17	CQ	10	VAL	2.8
51	B4	50	VAL	2.8
8	AH	5	PRO	2.8
17	AQ	30	PRO	2.8
25	AY	12	U	2.8
46	DZ	121	HIS	2.8
2	AB	175	ARG	2.8
26	DA	2142	C	2.8
43	DW	82	LEU	2.8
1	AA	161	A	2.8
5	AE	55	VAL	2.8
39	DS	14	VAL	2.8
8	CH	65	TYR	2.8
1	CA	1030(C)	G	2.8
26	DA	2897	U	2.8
5	AE	108	ALA	2.8
2	AB	227	GLY	2.8
37	DQ	2	LEU	2.8
13	CM	117	VAL	2.8
25	AY	23	A	2.8
11	AK	75	TYR	2.8
14	CN	30	ALA	2.8
23	AW	15	G	2.8
17	AQ	99	SER	2.8
55	D8	25	MET	2.8
4	AD	180	GLY	2.7
4	CD	9	CYS	2.7
9	CI	88	TYR	2.7
9	CI	52	ALA	2.7
31	BG	93	THR	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	BH	4	ILE	2.7
8	CH	133	LEU	2.7
12	CL	60	LEU	2.7
34	DN	116	LEU	2.7
45	DY	31	LEU	2.7
1	CA	1115	C	2.7
49	D2	1	MET	2.7
2	CB	139	LYS	2.7
16	AP	21	VAL	2.7
37	DQ	18	LYS	2.7
45	DY	42	VAL	2.7
2	CB	162	ILE	2.7
3	CC	152	ILE	2.7
7	CG	152	ALA	2.7
13	AM	107	ALA	2.7
14	CN	40	CYS	2.7
20	CT	63	ILE	2.7
46	BZ	107	THR	2.7
48	D1	37	ILE	2.7
1	CA	983	A	2.7
23	CW	21	A	2.7
32	DH	71	LEU	2.7
5	CE	8	GLU	2.7
46	DZ	50	GLN	2.7
39	DS	57	LYS	2.7
1	CA	1033	G	2.7
23	CW	67	C	2.7
11	CK	114	VAL	2.7
2	CB	137	ARG	2.7
54	D7	23	ARG	2.7
7	CG	39	ALA	2.7
14	CN	46	GLU	2.7
8	CH	58	TYR	2.7
8	CH	111	ILE	2.7
13	CM	21	TYR	2.7
32	DH	7	LEU	2.7
32	DH	94	TYR	2.7
37	DQ	32	TYR	2.7
37	DQ	47	ILE	2.7
28	BD	38	LYS	2.7
19	CS	68	GLY	2.7
46	BZ	115	GLY	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
46	BZ	143	GLY	2.7
14	CN	26	ARG	2.7
46	DZ	119	GLU	2.7
26	DA	2124	G	2.7
19	CS	12	ASP	2.7
3	AC	193	TYR	2.7
3	CC	91	LEU	2.7
20	AT	43	LEU	2.7
34	DN	26	LEU	2.7
46	BZ	104	PHE	2.7
50	D3	53	LEU	2.7
23	CW	35	A	2.7
26	DA	2801(A)	A	2.7
28	DD	216	GLY	2.7
1	CA	1149	C	2.7
2	CB	136	VAL	2.7
10	CJ	58	ASP	2.7
26	DA	2896	C	2.7
12	CL	30	ALA	2.7
3	AC	94	LEU	2.7
4	CD	206	PHE	2.7
23	CW	52	G	2.7
46	DZ	57	ILE	2.7
46	DZ	144	LEU	2.7
19	CS	69	HIS	2.7
3	CC	158	GLY	2.7
7	AG	81	GLY	2.7
9	CI	72	GLY	2.7
16	AP	1	MET	2.7
1	CA	1286	A	2.7
1	CA	1354	C	2.7
10	CJ	59	SER	2.7
15	CO	4	THR	2.7
2	AB	214	ILE	2.7
4	AD	174	LEU	2.7
6	AF	79	LEU	2.7
18	AR	31	LEU	2.7
30	DF	32	LEU	2.7
31	BG	88	ILE	2.7
33	DI	30	LEU	2.7
55	D8	29	LYS	2.7
23	CW	57	G	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
26	DA	2147	G	2.7
37	DQ	1	MET	2.7
8	CH	135	CYS	2.6
30	BF	89	VAL	2.6
9	CI	93	ARG	2.6
2	CB	40	HIS	2.6
1	CA	1066	C	2.6
4	AD	110	PHE	2.6
5	CE	80	ILE	2.6
26	DA	2161	C	2.6
33	DI	12	LEU	2.6
9	AI	37	PHE	2.6
34	BN	71	ILE	2.6
1	CA	973	G	2.6
23	AW	44	G	2.6
8	CH	122	ARG	2.6
16	AP	28	ARG	2.6
28	BD	275	LYS	2.6
3	CC	173	VAL	2.6
32	DH	37	VAL	2.6
56	B9	7	VAL	2.6
56	B9	25	VAL	2.6
16	AP	7	ALA	2.6
5	AE	123	LEU	2.6
5	CE	99	GLY	2.6
19	CS	16	LEU	2.6
23	CW	66	U	2.6
45	DY	14	LEU	2.6
3	CC	186	PHE	2.6
17	CQ	100	LYS	2.6
31	DG	115	ARG	2.6
32	DH	38	SER	2.6
2	AB	97	TRP	2.6
33	BI	19	VAL	2.6
37	DQ	114	ALA	2.6
47	D0	2	ALA	2.6
48	D1	62	VAL	2.6
10	CJ	67	THR	2.6
19	CS	77	THR	2.6
47	D0	52	GLY	2.6
12	CL	70	ILE	2.6
4	CD	49	ARG	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	CA	1322	C	2.6
7	AG	85	TYR	2.6
32	DH	47	GLU	2.6
55	D8	38	GLY	2.6
14	CN	13	THR	2.6
48	B1	35	THR	2.6
1	AA	204	U	2.6
4	AD	50	ARG	2.6
10	CJ	41	PRO	2.6
36	DP	79	ARG	2.6
1	CA	1092	A	2.6
55	B8	65	GLU	2.6
2	CB	76	GLN	2.6
48	D1	38	SER	2.6
13	CM	65	LYS	2.6
3	AC	120	VAL	2.6
4	CD	122	ARG	2.6
5	CE	55	VAL	2.6
8	AH	93	VAL	2.6
20	CT	59	ALA	2.6
50	D3	21	ALA	2.6
53	D6	5	VAL	2.6
53	D6	14	THR	2.6
16	AP	6	LEU	2.6
23	CW	12	U	2.6
5	AE	129	ILE	2.6
48	B1	7	ILE	2.6
1	CA	1190	G	2.6
25	CY	15	G	2.6
1	CA	1357	A	2.6
22	AV	15	A	2.6
10	AJ	68	HIS	2.6
26	BA	2108	C	2.6
26	BA	2128	C	2.6
41	DU	47	TYR	2.6
5	CE	14	ARG	2.6
8	AH	4	ASP	2.6
9	AI	10	ARG	2.6
2	AB	123	ALA	2.6
5	AE	120	THR	2.6
33	DI	36	ALA	2.6
17	CQ	5	VAL	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
31	DG	70	VAL	2.6
18	AR	79	LEU	2.6
11	AK	42	TRP	2.6
55	D8	34	TRP	2.6
3	CC	81	GLY	2.6
9	CI	8	GLY	2.6
46	DZ	106	GLY	2.6
3	CC	122	GLU	2.6
5	CE	17	ALA	2.5
45	DY	91	GLU	2.6
8	CH	11	THR	2.5
41	DU	63	VAL	2.5
46	DZ	174	VAL	2.5
48	B1	70	VAL	2.5
28	DD	177	LEU	2.5
2	AB	135	GLN	2.5
2	AB	70	PHE	2.5
12	AL	7	ILE	2.5
12	CL	85	ILE	2.5
20	CT	55	ILE	2.5
31	DG	102	PHE	2.5
55	D8	41	ILE	2.5
5	AE	18	ARG	2.5
10	CJ	68	HIS	2.5
16	AP	29	ASP	2.5
19	CS	83	HIS	2.5
31	DG	86	MET	2.5
39	DS	34	HIS	2.5
3	AC	200	ALA	2.5
14	CN	11	LYS	2.5
25	AY	71	G	2.5
49	D2	8	LYS	2.5
23	AW	56	C	2.5
5	AE	119	LEU	2.5
18	CR	85	LEU	2.5
23	AW	50	U	2.5
32	DH	95	ARG	2.5
9	AI	77	ILE	2.5
11	CK	125	PHE	2.5
12	CL	88	GLY	2.5
32	DH	82	GLY	2.5
37	DQ	91	GLU	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	CC	200	ALA	2.5
9	CI	46	ALA	2.5
26	DA	2062	A	2.5
39	DS	92	TYR	2.5
5	CE	142	LEU	2.5
9	CI	26	VAL	2.5
31	DG	160	VAL	2.5
2	CB	66	GLY	2.5
3	CC	181	ASN	2.5
23	CW	45	U	2.5
3	CC	205	GLY	2.5
3	AC	128	PHE	2.5
8	AH	35	ILE	2.5
13	CM	92	HIS	2.5
28	DD	271	ILE	2.5
36	DP	76	LYS	2.5
2	CB	45	GLN	2.5
9	CI	121	ARG	2.5
14	AN	14	PRO	2.5
1	CA	1250	A	2.5
3	AC	32	LEU	2.5
3	CC	207	VAL	2.5
14	AN	15	LYS	2.5
17	CQ	22	LEU	2.5
26	DA	2114	A	2.5
34	DN	9	VAL	2.5
46	DZ	59	LEU	2.5
1	CA	1040	U	2.5
25	CY	66	U	2.5
4	AD	204	ILE	2.5
23	CW	22	G	2.5
37	DQ	60	ARG	2.5
12	CL	56	ALA	2.5
13	CM	10	PRO	2.5
21	AU	14	TRP	2.5
3	AC	207	VAL	2.5
3	CC	188	LEU	2.5
8	AH	2	LEU	2.5
9	CI	57	GLY	2.5
10	AJ	71	LEU	2.5
20	CT	20	LEU	2.5
32	DH	76	VAL	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
36	BP	37	GLY	2.5
36	DP	101	VAL	2.5
36	DP	125	VAL	2.5
48	D1	70	VAL	2.5
1	CA	969	A	2.5
1	CA	1041	A	2.5
27	DB	58	A	2.5
10	AJ	4	ILE	2.5
9	CI	20	ARG	2.5
10	CJ	51	ARG	2.5
25	AY	48	C	2.5
1	CA	1061	G	2.5
23	CW	18	G	2.5
3	AC	15	THR	2.5
5	AE	95	ALA	2.5
11	CK	68	ALA	2.5
20	AT	72	LEU	2.5
46	DZ	105	VAL	2.5
20	AT	18	GLN	2.5
26	BA	1026	U	2.5
4	AD	158	ILE	2.5
10	AJ	47	PHE	2.5
1	CA	962	C	2.5
1	CA	1039	C	2.5
11	CK	89	ALA	2.5
16	AP	41	PRO	2.5
3	CC	2	GLY	2.5
20	AT	75	ASN	2.5
3	AC	175	LEU	2.4
8	CH	104	ARG	2.4
13	CM	66	LEU	2.4
15	AO	34	LEU	2.4
2	CB	81	VAL	2.4
9	AI	127	LYS	2.4
37	DQ	97	VAL	2.4
53	D6	42	TRP	2.4
29	DE	77	ILE	2.4
54	D7	18	PHE	2.4
12	CL	48	PRO	2.4
23	CW	42	C	2.4
26	BA	888	C	2.4
7	CG	117	ALA	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
9	CI	43	ALA	2.4
14	AN	20	ALA	2.4
55	D8	7	HIS	2.4
1	CA	976	G	2.4
1	CA	1338	G	2.4
33	DI	9	LEU	2.4
3	CC	130	VAL	2.4
37	DQ	96	VAL	2.4
1	CA	961	U	2.4
3	AC	18	TRP	2.4
9	CI	77	ILE	2.4
5	AE	10	MET	2.4
1	CA	949	A	2.4
10	CJ	60	ARG	2.4
31	DG	17	PRO	2.4
50	D3	16	PRO	2.4
25	AY	3	C	2.4
54	D7	20	ALA	2.4
6	CF	21	LEU	2.4
10	AJ	49	VAL	2.4
16	AP	20	VAL	2.4
31	BG	149	VAL	2.4
33	DI	41	GLU	2.4
1	AA	1024	G	2.4
9	AI	114	TYR	2.4
25	AY	53	G	2.4
3	CC	22	TRP	2.4
47	D0	55	ARG	2.4
53	D6	20	ASN	2.4
3	CC	117	ALA	2.4
9	CI	117	HIS	2.4
11	AK	89	ALA	2.4
47	D0	43	THR	2.4
31	DG	164	GLU	2.4
6	AF	48	LEU	2.4
10	CJ	88	LEU	2.4
33	BI	6	LEU	2.4
3	AC	66	VAL	2.4
13	CM	79	LYS	2.4
15	AO	60	VAL	2.4
32	DH	35	VAL	2.4
37	DQ	63	LYS	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
6	CF	46	ARG	2.4
16	AP	25	ARG	2.4
32	DH	148	ILE	2.4
36	DP	91	PHE	2.4
39	DS	90	GLY	2.4
23	AW	34	G	2.4
55	D8	63	PRO	2.4
3	CC	69	HIS	2.4
5	CE	104	ALA	2.4
33	DI	46	ALA	2.4
36	DP	58	THR	2.4
1	CA	1225	A	2.4
37	DQ	37	LEU	2.4
10	CJ	66	ARG	2.4
21	AU	10	ARG	2.4
4	AD	170	VAL	2.4
16	CP	30	GLY	2.4
8	CH	83	ILE	2.4
15	CO	59	MET	2.4
39	DS	29	PHE	2.4
41	DU	40	PHE	2.4
48	D1	71	TYR	2.4
20	CT	44	ALA	2.4
39	DS	6	ALA	2.4
13	CM	103	THR	2.4
9	CI	71	SER	2.4
50	D3	26	LEU	2.4
8	CH	61	VAL	2.4
10	CJ	64	GLU	2.4
26	BA	2129	C	2.4
27	DB	90	A	2.4
28	DD	56	GLY	2.4
48	D1	30	VAL	2.4
23	CW	50	U	2.4
14	CN	14	PRO	2.4
16	AP	36	ILE	2.4
15	AO	69	TYR	2.4
35	DO	20	MET	2.4
36	DP	110	TYR	2.4
13	CM	42	ALA	2.4
36	DP	15	ARG	2.4
31	DG	161	THR	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	CC	111	LEU	2.4
8	AH	112	LEU	2.4
20	AT	24	LEU	2.4
29	DE	52	LEU	2.4
6	AF	92	LYS	2.3
4	AD	148	VAL	2.3
7	CG	105	VAL	2.3
17	AQ	11	VAL	2.3
34	BN	5	VAL	2.3
45	DY	51	VAL	2.3
23	AW	67	C	2.3
2	CB	41	ILE	2.3
5	AE	13	ILE	2.3
10	AJ	23	ILE	2.3
40	DT	110	ILE	2.3
3	AC	201	TYR	2.3
9	AI	59	PHE	2.3
50	D3	29	ARG	2.3
5	CE	20	GLN	2.3
37	DQ	121	ALA	2.3
47	B0	2	ALA	2.3
16	AP	44	THR	2.3
28	DD	259	THR	2.3
20	CT	24	LEU	2.3
8	AH	118	VAL	2.3
9	AI	108	VAL	2.3
33	DI	21	VAL	2.3
2	CB	232	PRO	2.3
20	AT	8	ARG	2.3
21	CU	22	ARG	2.3
23	AW	66	U	2.3
1	CA	1397	C	2.3
2	AB	208	ILE	2.3
8	AH	6	ILE	2.3
17	CQ	86	GLU	2.3
10	AJ	11	PHE	2.3
2	AB	148	TYR	2.3
8	AH	94	TYR	2.3
17	CQ	37	LYS	2.3
21	AU	21	TYR	2.3
31	DG	84	LYS	2.3
37	DQ	20	ALA	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
37	DQ	93	TYR	2.3
41	DU	48	ALA	2.3
12	AL	67	THR	2.3
41	DU	43	GLY	2.3
6	AF	61	LEU	2.3
8	AH	133	LEU	2.3
36	BP	105	LEU	2.3
16	AP	16	HIS	2.3
2	AB	71	VAL	2.3
2	AB	95	GLN	2.3
34	BN	46	VAL	2.3
1	CA	1257	U	2.3
46	DZ	62	PRO	2.3
28	DD	276	LYS	2.3
1	AA	1529	G	2.3
5	CE	118	ILE	2.3
14	AN	7	ILE	2.3
15	AO	87	ILE	2.3
26	DA	614(B)	G	2.3
17	CQ	44	ALA	2.3
37	DQ	36	ALA	2.3
8	CH	128	GLY	2.3
3	AC	188	LEU	2.3
7	CG	6	ARG	2.3
9	CI	111	ARG	2.3
13	CM	67	GLU	2.3
20	AT	13	LEU	2.3
32	DH	159	GLU	2.3
34	DN	69	GLN	2.3
46	DZ	140	ASP	2.3
46	DZ	148	ASP	2.3
4	AD	140	VAL	2.3
14	CN	18	VAL	2.3
28	DD	34	VAL	2.3
3	CC	142	MET	2.3
54	D7	22	MET	2.3
2	CB	127	ILE	2.3
19	AS	40	ILE	2.3
8	AH	31	PHE	2.3
9	CI	37	PHE	2.3
4	AD	167	GLY	2.3
4	AD	209	ARG	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
17	CQ	80	GLY	2.3
33	DI	100	ALA	2.3
13	CM	23	TYR	2.3
23	AW	10	G	2.3
26	BA	2805	G	2.3
39	DS	47	THR	2.3
2	AB	61	LEU	2.3
2	AB	187	LEU	2.3
9	CI	11	LYS	2.3
13	CM	13	LYS	2.3
3	CC	174	PRO	2.3
28	BD	142	VAL	2.3
37	BQ	97	VAL	2.3
2	CB	231	GLU	2.3
28	DD	252	TRP	2.3
3	AC	148	GLY	2.3
7	CG	5	ARG	2.3
17	AQ	90	ILE	2.3
39	DS	13	ARG	2.3
4	AD	147	ALA	2.3
36	DP	47	ASP	2.3
36	DP	87	ASP	2.3
26	DA	887	A	2.3
33	BI	68	LEU	2.3
1	CA	1305	G	2.3
26	DA	2127	G	2.3
48	D1	68	PRO	2.3
10	AJ	28	ARG	2.3
16	AP	42	ARG	2.3
47	D0	38	VAL	2.3
55	D8	14	VAL	2.3
35	DO	31	LYS	2.3
3	CC	80	GLY	2.3
3	CC	14	ILE	2.3
55	D8	58	ILE	2.3
2	CB	55	PHE	2.3
3	CC	196	LEU	2.3
43	DW	9	TYR	2.3
26	BA	2142	C	2.3
50	D3	23	LEU	2.3
55	D8	50	LEU	2.3
1	AA	927	G	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	CA	1156	G	2.2
3	AC	63	ASN	2.2
3	AC	64	VAL	2.2
4	AD	154	ASN	2.2
25	AY	22	G	2.2
26	BA	2792	G	2.2
2	AB	48	MET	2.2
2	AB	78	GLN	2.2
25	AY	20	U	2.2
2	AB	233	SER	2.2
9	CI	119	ALA	2.2
10	CJ	98	ILE	2.2
41	DU	46	ALA	2.2
55	D8	16	ILE	2.2
3	AC	91	LEU	2.2
4	CD	157	LEU	2.2
10	CJ	8	LEU	2.2
31	BG	152	LEU	2.2
31	DG	106	LEU	2.2
17	CQ	32	TYR	2.2
1	CA	1321	C	2.2
15	CO	55	GLY	2.2
47	D0	73	GLY	2.2
8	AH	95	VAL	2.2
12	AL	18	VAL	2.2
17	CQ	11	VAL	2.2
33	DI	37	VAL	2.2
45	BY	1	MET	2.2
24	CX	46	G	2.2
25	CY	29	G	2.2
25	CY	70	G	2.2
26	BA	2141	G	2.2
26	DA	2110	G	2.2
26	DA	2318	G	2.2
8	AH	134	ILE	2.2
20	CT	16	HIS	2.2
4	CD	135	LEU	2.2
8	AH	10	LEU	2.2
15	CO	34	LEU	2.2
48	D1	98	LEU	2.2
4	CD	207	TYR	2.2
8	CH	15	ASN	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
36	DP	68	GLN	2.2
1	CA	980	C	2.2
3	CC	183	ASP	2.2
48	D1	28	GLY	2.2
9	AI	110	GLU	2.2
23	CW	68	C	2.2
26	DA	2804	C	2.2
36	DP	95	VAL	2.2
1	CA	1348	U	2.2
23	AW	23	A	2.2
4	AD	122	ARG	2.2
8	AH	38	ILE	2.2
16	AP	69	THR	2.2
1	CA	1117	G	2.2
1	CA	1221	G	2.2
26	DA	2168	G	2.2
12	AL	27	LEU	2.2
31	BG	7	LEU	2.2
32	DH	171	LEU	2.2
19	CS	13	ASP	2.2
2	CB	75	LYS	2.2
33	BI	89	TYR	2.2
1	AA	1030	C	2.2
10	CJ	43	ARG	2.2
13	CM	17	VAL	2.2
46	BZ	116	VAL	2.2
46	DZ	161	VAL	2.2
48	D1	61	ARG	2.2
26	DA	614(A)	U	2.2
1	CA	1151	A	2.2
1	CA	1287	A	2.2
7	AG	7	ALA	2.2
4	AD	97	LEU	2.2
13	CM	106	ASN	2.2
13	CM	113	PRO	2.2
20	AT	69	GLY	2.2
32	DH	8	PRO	2.2
49	D2	24	LEU	2.2
55	D8	21	LYS	2.2
1	AA	1353	G	2.2
20	CT	86	ARG	2.2
46	DZ	4	ARG	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	CD	203	VAL	2.2
2	AB	207	ALA	2.2
12	CL	16	GLU	2.2
29	BE	28	ALA	2.2
39	DS	55	ALA	2.2
30	DF	186	ILE	2.2
31	DG	178	PHE	2.2
3	AC	185	GLY	2.2
7	AG	34	GLY	2.2
10	CJ	39	PRO	2.2
28	DD	155	LEU	2.2
32	DH	14	GLY	2.2
39	DS	26	LEU	2.2
44	DX	57	LEU	2.2
2	CB	30	ARG	2.2
14	AN	23	ARG	2.2
8	AH	58	TYR	2.2
13	CM	50	GLU	2.2
23	AW	1	G	2.2
26	DA	2792	G	2.2
4	AD	133	VAL	2.2
5	CE	10	MET	2.2
14	AN	18	VAL	2.2
14	CN	56	VAL	2.2
19	CS	44	MET	2.2
35	DO	57	VAL	2.2
37	DQ	35	VAL	2.2
52	D5	24	ALA	2.2
2	AB	222	ILE	2.2
3	AC	182	ILE	2.2
23	CW	61	C	2.2
25	CY	4	C	2.2
30	DF	77	ASP	2.2
3	CC	179	ARG	2.2
13	CM	100	GLY	2.2
14	AN	3	ARG	2.2
28	DD	210	GLY	2.2
31	BG	80	PHE	2.2
48	D1	22	GLY	2.2
51	B4	49	PHE	2.2
50	D3	12	PRO	2.2
55	D8	46	ARG	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
18	AR	66	LEU	2.2
31	DG	176	LEU	2.2
46	DZ	157	LEU	2.2
17	CQ	24	GLU	2.2
32	DH	13	LYS	2.1
1	AA	841	U	2.1
23	CW	44	G	2.1
23	CW	63	G	2.1
26	DA	2159	G	2.1
43	DW	85	VAL	2.1
3	AC	169	ALA	2.1
8	AH	16	ALA	2.1
3	CC	13	GLY	2.1
4	AD	132	ARG	2.1
45	DY	43	ASN	2.1
31	DG	44	GLY	2.1
51	D4	58	ARG	2.1
33	DI	88	ILE	2.1
1	CA	1325	C	2.1
7	CG	62	PHE	2.1
25	AY	62	C	2.1
43	DW	14	PRO	2.1
6	CF	45	LEU	2.1
9	AI	79	LEU	2.1
19	AS	15	LEU	2.1
29	BE	78	LEU	2.1
31	DG	107	LEU	2.1
49	D2	35	LEU	2.1
56	D9	11	CYS	2.1
17	CQ	42	TYR	2.1
17	CQ	95	TYR	2.1
47	D0	53	MET	2.1
1	CA	981	U	2.1
5	AE	21	ALA	2.1
5	AE	33	VAL	2.1
9	AI	14	VAL	2.1
10	AJ	44	VAL	2.1
34	DN	140	VAL	2.1
46	DZ	109	ALA	2.1
48	D1	51	VAL	2.1
11	AK	87	THR	2.1
3	AC	134	ILE	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	CC	72	LYS	2.1
12	CL	47	LYS	2.1
13	CM	111	LYS	2.1
17	AQ	37	LYS	2.1
19	CS	10	PHE	2.1
26	DA	652(U)	G	2.1
26	DA	2157	G	2.1
33	DI	79	ILE	2.1
2	AB	98	LEU	2.1
3	CC	43	LEU	2.1
8	AH	39	LEU	2.1
15	CO	66	LEU	2.1
47	B0	75	LEU	2.1
55	B8	60	LEU	2.1
46	BZ	52	SER	2.1
13	CM	80	ARG	2.1
24	CX	72	A	2.1
7	CG	109	ASN	2.1
3	CC	48	TYR	2.1
5	AE	113	ALA	2.1
5	CE	51	VAL	2.1
12	CL	123	LYS	2.1
13	AM	87	TYR	2.1
51	B4	4	GLY	2.1
19	CS	51	VAL	2.1
45	DY	65	ALA	2.1
11	CK	115	PRO	2.1
18	AR	52	PRO	2.1
36	DP	38	GLN	2.1
46	DZ	124	ILE	2.1
51	D4	42	PHE	2.1
8	AH	63	LEU	2.1
18	CR	66	LEU	2.1
34	DN	112	LEU	2.1
37	DQ	34	LEU	2.1
1	AA	1033	G	2.1
13	CM	110	ARG	2.1
43	DW	13	SER	2.1
3	CC	3	ASN	2.1
11	AK	117	ASN	2.1
38	DR	9	LYS	2.1
47	B0	5	LYS	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
26	BA	529	A	2.1
26	BA	2790	A	2.1
3	CC	193	TYR	2.1
10	AJ	20	ALA	2.1
20	CT	67	ALA	2.1
28	BD	193	VAL	2.1
29	BE	157	ALA	2.1
30	DF	89	VAL	2.1
39	DS	79	ALA	2.1
47	B0	51	VAL	2.1
53	D6	22	ALA	2.1
53	B6	23	THR	2.1
8	AH	100	ILE	2.1
10	AJ	96	ILE	2.1
2	CB	69	LEU	2.1
3	CC	33	LEU	2.1
16	CP	9	PHE	2.1
11	AK	81	ASP	2.1
17	AQ	98	LEU	2.1
17	CQ	6	LEU	2.1
31	BG	49	ASP	2.1
44	DX	9	LEU	2.1
47	D0	75	LEU	2.1
6	AF	54	LYS	2.1
13	AM	121	LYS	2.1
16	AP	27	LYS	2.1
34	DN	76	SER	2.1
45	DY	46	LYS	2.1
15	AO	55	GLY	2.1
25	CY	72	C	2.1
8	AH	53	VAL	2.1
9	CI	82	ALA	2.1
36	BP	12	ALA	2.1
26	DA	6	A	2.1
41	BU	8	VAL	2.1
51	D4	53	GLU	2.1
55	D8	22	VAL	2.1
4	AD	115	ARG	2.1
7	CG	76	ARG	2.1
13	CM	93	ARG	2.1
14	AN	21	TYR	2.1
20	CT	25	ARG	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	DH	51	ARG	2.1
46	DZ	79	ARG	2.1
8	AH	86	ILE	2.1
19	CS	6	LYS	2.1
4	AD	101	LEU	2.1
5	CE	119	LEU	2.1
15	AO	57	LEU	2.1
36	DP	3	LEU	2.1
45	DY	41	GLY	2.1
1	CA	1028	C	2.1
1	CA	951	G	2.1
1	CA	1186	G	2.1
2	AB	125	PRO	2.1
5	AE	88	LYS	2.1
8	CH	28	ALA	2.1
24	CX	4	G	2.1
29	BE	114	ALA	2.1
33	BI	36	ALA	2.1
47	D0	49	LYS	2.1
9	AI	17	VAL	2.1
16	CP	20	VAL	2.1
17	CQ	21	VAL	2.1
29	BE	12	THR	2.1
9	CI	54	ASP	2.1
21	CU	18	TYR	2.1
2	CB	113	HIS	2.1
5	CE	76	ILE	2.1
30	DF	78	ILE	2.1
3	AC	34	LEU	2.1
3	AC	52	LEU	2.1
13	AM	96	LEU	2.1
29	DE	51	PHE	2.1
41	DU	20	LEU	2.1
9	AI	8	GLY	2.1
10	CJ	61	GLU	2.1
12	CL	95	GLY	2.1
42	DV	101	GLY	2.1
7	CG	103	TRP	2.1
12	CL	15	ARG	2.1
16	CP	18	ARG	2.1
31	DG	33	ARG	2.1
37	DQ	103	MET	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
46	BZ	1	MET	2.0
7	CG	2	ALA	2.0
8	AH	89	PRO	2.0
31	DG	166	ASP	2.0
2	AB	15	VAL	2.0
26	BA	2506	U	2.0
29	DE	116	VAL	2.0
52	B5	60	VAL	2.0
1	CA	485	G	2.0
1	CA	1003	G	2.0
7	CG	120	ILE	2.0
11	CK	50	TYR	2.0
25	CY	52	G	2.0
26	BA	2154	G	2.0
31	DG	77	ILE	2.0
2	AB	118	LEU	2.0
19	CS	15	LEU	2.0
20	AT	62	LEU	2.0
31	BG	178	PHE	2.0
40	DT	114	LEU	2.0
10	CJ	10	GLY	2.0
55	D8	48	PHE	2.0
10	AJ	57	LYS	2.0
4	CD	115	ARG	2.0
4	CD	209	ARG	2.0
46	DZ	112	ARG	2.0
2	CB	202	PRO	2.0
28	DD	272	ALA	2.0
38	DR	35	THR	2.0
46	BZ	170	THR	2.0
1	CA	1218	C	2.0
3	CC	51	GLY	2.0
8	CH	45	ILE	2.0
15	CO	87	ILE	2.0
12	CL	19	ARG	2.0
12	CL	93	LEU	2.0
13	CM	9	ILE	2.0
56	D9	13	LYS	2.0
3	AC	179	ARG	2.0
4	AD	191	ARG	2.0
30	DF	140	LEU	2.0
31	BG	139	LEU	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	BH	3	ARG	2.0
1	CA	1024	G	2.0
26	BA	2133	G	2.0
26	BA	2162	G	2.0
26	DA	2148	G	2.0
26	BA	229	A	2.0
8	CH	138	TRP	2.0
16	AP	35	LYS	2.0
31	DG	110	ALA	2.0
32	DH	75	ALA	2.0
20	AT	71	THR	2.0
28	BD	50	THR	2.0
34	DN	8	GLN	2.0
51	B4	46	GLN	2.0
9	AI	26	VAL	2.0
23	CW	33	U	2.0
26	DA	2585	U	2.0
42	DV	79	VAL	2.0
5	CE	23	GLY	2.0
12	CL	14	GLY	2.0
21	CU	9	ARG	2.0
29	BE	106	GLY	2.0
6	CF	52	ILE	2.0
8	AH	109	ILE	2.0
9	CI	40	LEU	2.0
13	CM	48	LEU	2.0
31	DG	3	LEU	2.0
4	CD	93	PHE	2.0
17	AQ	95	TYR	2.0
22	CV	18	G	2.0
48	B1	69	LYS	2.0
2	AB	131	PRO	2.0
16	CP	41	PRO	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
25	7MG	CY	46	24/25	0.48	0.37	86,105,111,137	0
25	MIA	CY	37	22/30	0.61	0.38	72,95,113,138	0
25	5MU	CY	54	21/22	0.63	0.53	78,94,109,140	0
23	7MG	CW	46	24/25	0.66	0.27	79,96,109,133	0
25	PSU	CY	55	20/21	0.67	0.49	94,102,110,124	0
25	4SU	CY	8	20/21	0.68	0.22	93,103,113,128	0
23	4SU	CW	8	20/21	0.69	0.30	81,98,120,127	0
25	PSU	AY	55	20/21	0.70	0.29	93,101,108,122	0
23	7MG	AW	46	24/25	0.72	0.23	84,99,117,133	0
25	5MU	AY	54	21/22	0.73	0.26	80,96,105,131	0
25	7MG	AY	46	24/25	0.76	0.27	75,101,111,123	0
25	PSU	AY	39	20/21	0.76	0.30	78,90,117,123	0
25	PSU	CY	39	20/21	0.77	0.30	79,90,116,130	0
25	4SU	AY	8	20/21	0.78	0.16	82,96,103,118	0
23	PSU	CW	55	20/21	0.79	0.30	79,89,99,104	0
25	PSU	CY	32	20/21	0.79	0.21	80,92,101,107	0
25	MIA	AY	37	22/30	0.80	0.22	77,90,111,119	0
23	4SU	AW	8	20/21	0.81	0.20	86,95,112,128	0
25	PSU	AY	32	20/21	0.83	0.24	78,93,100,106	0
23	PSU	AW	55	20/21	0.84	0.27	77,90,98,104	0
23	MIA	CW	37	22/30	0.84	0.32	75,85,92,100	0
23	5MU	CW	54	21/22	0.84	0.24	74,88,99,101	0
23	PSU	CW	39	20/21	0.87	0.42	78,84,97,98	0
23	PSU	AW	32	20/21	0.88	0.25	77,83,92,98	0
23	PSU	CW	32	20/21	0.88	0.45	81,87,94,103	0
24	PSU	CX	55	20/21	0.89	0.15	70,80,91,96	0
23	31M	CW	76	41/42	0.89	0.41	50,63,73,88	20
23	5MU	AW	54	21/22	0.91	0.20	65,82,91,93	0
24	4SU	CX	8	20/21	0.91	0.17	77,87,95,97	0
24	5MU	CX	54	21/22	0.92	0.22	70,81,89,99	0
23	PSU	AW	39	20/21	0.93	0.23	73,82,95,97	0
23	MIA	AW	37	29/30	0.94	0.26	59,71,81,86	0
24	4SU	AX	8	20/21	0.94	0.18	54,66,82,89	0
23	31M	AW	76	41/42	0.94	0.33	37,54,66,83	9
24	5MC	AX	32	21/22	0.95	0.21	43,53,62,78	0
24	5MU	AX	54	21/22	0.95	0.20	49,68,79,84	0
24	PSU	AX	55	20/21	0.95	0.21	50,63,73,83	0
24	5MC	CX	32	21/22	0.96	0.21	63,76,86,88	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
57	MG	BA	3730	1/1	0.31	0.19	71,71,71,71	0
57	MG	BA	3427	1/1	0.41	0.20	61,61,61,61	0
57	MG	BA	3670	1/1	0.43	0.26	61,61,61,61	0
57	MG	DA	3448	1/1	0.43	0.20	70,70,70,70	0
57	MG	DA	3403	1/1	0.45	0.14	57,57,57,57	0
57	MG	BA	3721	1/1	0.46	0.32	82,82,82,82	0
57	MG	DA	3651	1/1	0.48	0.53	75,75,75,75	0
57	MG	DA	3530	1/1	0.51	0.13	74,74,74,74	0
57	MG	DA	3329	1/1	0.54	0.13	54,54,54,54	0
57	MG	AW	3004	1/1	0.57	0.14	49,49,49,49	0
57	MG	DA	3563	1/1	0.57	0.15	74,74,74,74	0
57	MG	CT	3001	1/1	0.58	0.12	56,56,56,56	0
57	MG	DR	5001	1/1	0.58	0.24	70,70,70,70	0
57	MG	BA	3636	1/1	0.58	0.14	64,64,64,64	0
57	MG	DA	3259	1/1	0.58	0.21	43,43,43,43	0
57	MG	BB	215	1/1	0.59	0.18	73,73,73,73	0
57	MG	DA	3673	1/1	0.60	0.14	69,69,69,69	0
57	MG	CA	3070	1/1	0.61	0.15	63,63,63,63	0
57	MG	DA	3320	1/1	0.61	0.15	55,55,55,55	0
57	MG	CA	3088	1/1	0.62	0.14	74,74,74,74	0
57	MG	BA	3616	1/1	0.62	0.21	65,65,65,65	0
57	MG	BA	3568	1/1	0.63	0.10	59,59,59,59	0
57	MG	AA	3004	1/1	0.63	0.15	67,67,67,67	0
57	MG	DA	3566	1/1	0.64	0.12	69,69,69,69	0
57	MG	DA	3213	1/1	0.64	0.32	63,63,63,63	0
57	MG	BA	3470	1/1	0.65	0.13	62,62,62,62	0
57	MG	D8	5001	1/1	0.65	0.23	66,66,66,66	0
57	MG	DA	3532	1/1	0.66	0.24	69,69,69,69	0
57	MG	CA	3051	1/1	0.66	0.19	81,81,81,81	0
57	MG	DA	3413	1/1	0.66	0.23	48,48,48,48	0
57	MG	DA	3518	1/1	0.66	0.24	54,54,54,54	0
57	MG	AA	3153	1/1	0.66	0.18	74,74,74,74	0
57	MG	DA	3256	1/1	0.67	0.19	62,62,62,62	0
57	MG	CX	3002	1/1	0.67	0.14	70,70,70,70	0
57	MG	AX	3014	1/1	0.67	0.19	72,72,72,72	0
57	MG	DA	3244	1/1	0.69	0.11	71,71,71,71	0
57	MG	DA	3076	1/1	0.69	0.14	58,58,58,58	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	DB	3011	1/1	0.69	0.14	72,72,72,72	0
57	MG	BA	3678	1/1	0.70	0.08	65,65,65,65	0
57	MG	DA	3125	1/1	0.71	0.26	70,70,70,70	0
57	MG	DA	3633	1/1	0.71	0.12	58,58,58,58	0
57	MG	CA	3018	1/1	0.72	0.16	69,69,69,69	0
57	MG	BA	3070	1/1	0.72	0.37	59,59,59,59	0
57	MG	BA	3003	1/1	0.72	0.19	60,60,60,60	0
57	MG	DA	3316	1/1	0.72	0.11	45,45,45,45	0
57	MG	BA	3053	1/1	0.72	0.21	54,54,54,54	0
57	MG	AA	3103	1/1	0.73	0.24	73,73,73,73	0
57	MG	DA	3546	1/1	0.73	0.11	71,71,71,71	0
57	MG	BA	3257	1/1	0.73	0.23	53,53,53,53	0
57	MG	BA	3540	1/1	0.73	0.23	37,37,37,37	0
57	MG	DA	3060	1/1	0.74	0.15	64,64,64,64	0
57	MG	DA	3616	1/1	0.74	0.11	71,71,71,71	0
57	MG	DD	303	1/1	0.74	0.62	87,87,87,87	0
57	MG	AA	3169	1/1	0.74	0.13	62,62,62,62	0
57	MG	BA	3300	1/1	0.74	0.25	57,57,57,57	0
57	MG	AA	3206	1/1	0.74	0.19	64,64,64,64	0
57	MG	BA	3401	1/1	0.75	0.16	35,35,35,35	0
57	MG	BB	209	1/1	0.75	0.32	65,65,65,65	0
57	MG	B4	502	1/1	0.75	0.14	71,71,71,71	0
57	MG	BA	3641	1/1	0.75	0.21	68,68,68,68	0
57	MG	DA	3608	1/1	0.75	0.13	68,68,68,68	0
57	MG	BA	3503	1/1	0.75	0.12	49,49,49,49	0
57	MG	BA	3538	1/1	0.75	0.15	40,40,40,40	0
57	MG	BA	3704	1/1	0.76	0.14	77,77,77,77	0
57	MG	DA	3252	1/1	0.76	0.08	37,37,37,37	0
57	MG	BA	3602	1/1	0.76	0.16	53,53,53,53	0
57	MG	BF	308	1/1	0.76	0.20	46,46,46,46	0
57	MG	DB	3008	1/1	0.76	0.20	67,67,67,67	0
57	MG	DA	3531	1/1	0.76	0.18	61,61,61,61	0
57	MG	DA	3635	1/1	0.76	0.11	38,38,38,38	0
57	MG	BA	3362	1/1	0.76	0.20	41,41,41,41	0
57	MG	AA	3013	1/1	0.76	0.17	69,69,69,69	0
57	MG	BA	3353	1/1	0.76	0.12	50,50,50,50	0
57	MG	BA	3095	1/1	0.76	0.24	51,51,51,51	0
57	MG	BA	3225	1/1	0.76	0.16	61,61,61,61	0
57	MG	BF	304	1/1	0.76	0.18	45,45,45,45	0
57	MG	DA	3642	1/1	0.76	0.28	54,54,54,54	0
57	MG	DA	3620	1/1	0.76	0.12	68,68,68,68	0
57	MG	CJ	5001	1/1	0.76	0.08	73,73,73,73	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	BA	3560	1/1	0.77	0.14	56,56,56,56	0
57	MG	DA	3262	1/1	0.77	0.10	65,65,65,65	0
57	MG	BA	3615	1/1	0.77	0.21	68,68,68,68	0
57	MG	BB	214	1/1	0.77	0.18	49,49,49,49	0
57	MG	BA	3733	1/1	0.77	0.11	58,58,58,58	0
57	MG	DA	3383	1/1	0.77	0.21	54,54,54,54	0
57	MG	DA	3205	1/1	0.77	0.10	56,56,56,56	0
57	MG	DA	3234	1/1	0.77	0.21	63,63,63,63	0
57	MG	AA	3084	1/1	0.78	0.24	51,51,51,51	0
57	MG	BA	3421	1/1	0.78	0.17	32,32,32,32	0
57	MG	DA	3585	1/1	0.78	0.12	43,43,43,43	0
57	MG	BA	3716	1/1	0.78	0.12	65,65,65,65	0
57	MG	BA	3771	1/1	0.78	0.29	50,50,50,50	0
57	MG	DA	3610	1/1	0.78	0.22	64,64,64,64	0
57	MG	DA	3218	1/1	0.78	0.13	59,59,59,59	0
57	MG	DA	3554	1/1	0.78	0.10	62,62,62,62	0
57	MG	CA	3017	1/1	0.78	0.19	53,53,53,53	0
57	MG	BA	3638	1/1	0.79	0.14	63,63,63,63	0
57	MG	CA	3013	1/1	0.79	0.13	69,69,69,69	0
57	MG	DA	3212	1/1	0.79	0.15	45,45,45,45	0
57	MG	BA	3724	1/1	0.79	0.18	62,62,62,62	0
57	MG	AE	202	1/1	0.79	0.12	80,80,80,80	0
57	MG	CA	3024	1/1	0.79	0.10	74,74,74,74	0
57	MG	DA	3335	1/1	0.79	0.16	47,47,47,47	0
59	ZN	D4	501	1/1	0.79	0.07	144,144,144,144	0
57	MG	DA	3607	1/1	0.79	0.14	65,65,65,65	0
57	MG	BA	3114	1/1	0.79	0.18	53,53,53,53	0
57	MG	DP	201	1/1	0.79	0.29	70,70,70,70	0
57	MG	DA	3417	1/1	0.79	0.11	52,52,52,52	0
57	MG	BA	3757	1/1	0.80	0.20	76,76,76,76	0
57	MG	CA	3064	1/1	0.80	0.17	60,60,60,60	0
57	MG	BA	3052	1/1	0.80	0.16	56,56,56,56	0
57	MG	AA	3069	1/1	0.80	0.19	68,68,68,68	0
57	MG	DA	3222	1/1	0.80	0.14	57,57,57,57	0
57	MG	BA	3020	1/1	0.80	0.22	53,53,53,53	0
57	MG	DA	3078	1/1	0.80	0.19	57,57,57,57	0
57	MG	BA	3781	1/1	0.80	0.20	41,41,41,41	0
57	MG	AA	3160	1/1	0.80	0.21	59,59,59,59	0
57	MG	CA	3166	1/1	0.80	0.14	66,66,66,66	0
57	MG	BA	3728	1/1	0.80	0.33	48,48,48,48	0
57	MG	DA	3340	1/1	0.80	0.18	58,58,58,58	0
57	MG	DA	3025	1/1	0.80	0.16	54,54,54,54	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	AX	3011	1/1	0.80	0.20	78,78,78,78	0
57	MG	CA	3152	1/1	0.80	0.20	76,76,76,76	0
57	MG	DG	3001	1/1	0.81	0.09	55,55,55,55	0
57	MG	AA	3183	1/1	0.81	0.15	65,65,65,65	0
57	MG	DA	3082	1/1	0.81	0.14	47,47,47,47	0
57	MG	BB	218	1/1	0.81	0.22	77,77,77,77	0
57	MG	AA	3138	1/1	0.81	0.18	71,71,71,71	0
57	MG	DA	3321	1/1	0.81	0.08	48,48,48,48	0
57	MG	BA	3316	1/1	0.81	0.12	66,66,66,66	0
57	MG	DA	3118	1/1	0.81	0.15	77,77,77,77	0
57	MG	BA	3066	1/1	0.81	0.19	49,49,49,49	0
57	MG	DA	3451	1/1	0.81	0.16	55,55,55,55	0
57	MG	AA	3170	1/1	0.81	0.13	75,75,75,75	0
57	MG	CX	3003	1/1	0.81	0.22	54,54,54,54	0
57	MG	DA	3669	1/1	0.81	0.25	55,55,55,55	0
57	MG	AA	3091	1/1	0.81	0.14	60,60,60,60	0
57	MG	BA	3172	1/1	0.81	0.19	46,46,46,46	0
57	MG	BA	3463	1/1	0.81	0.20	48,48,48,48	0
57	MG	DA	3402	1/1	0.81	0.10	66,66,66,66	0
57	MG	BA	3693	1/1	0.81	0.19	56,56,56,56	0
57	MG	CA	3146	1/1	0.81	0.19	66,66,66,66	0
57	MG	AW	3001	1/1	0.81	0.11	60,60,60,60	0
57	MG	DA	3408	1/1	0.81	0.08	58,58,58,58	0
57	MG	BA	3715	1/1	0.81	0.14	63,63,63,63	0
57	MG	DA	3589	1/1	0.81	0.07	68,68,68,68	0
57	MG	DA	3630	1/1	0.82	0.19	61,61,61,61	0
57	MG	BA	3342	1/1	0.82	0.10	46,46,46,46	0
57	MG	DA	3553	1/1	0.82	0.10	49,49,49,49	0
57	MG	BA	3707	1/1	0.82	0.24	44,44,44,44	0
57	MG	DA	3513	1/1	0.82	0.16	52,52,52,52	0
57	MG	CA	3107	1/1	0.82	0.20	80,80,80,80	0
57	MG	BA	3695	1/1	0.82	0.18	67,67,67,67	0
57	MG	DA	3333	1/1	0.82	0.13	41,41,41,41	0
57	MG	DA	3487	1/1	0.82	0.21	62,62,62,62	0
57	MG	BA	3709	1/1	0.82	0.20	62,62,62,62	0
57	MG	DA	3394	1/1	0.82	0.18	65,65,65,65	0
57	MG	DA	3406	1/1	0.82	0.11	51,51,51,51	0
57	MG	DA	3342	1/1	0.82	0.11	42,42,42,42	0
57	MG	BA	3761	1/1	0.82	0.16	59,59,59,59	0
57	MG	BA	3242	1/1	0.82	0.21	55,55,55,55	0
57	MG	DA	3582	1/1	0.82	0.07	56,56,56,56	0
57	MG	DA	3276	1/1	0.82	0.12	49,49,49,49	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	CA	3109	1/1	0.82	0.13	67,67,67,67	0
57	MG	BA	3317	1/1	0.82	0.18	53,53,53,53	0
57	MG	BA	3473	1/1	0.82	0.19	56,56,56,56	0
57	MG	DA	3308	1/1	0.82	0.15	61,61,61,61	0
57	MG	DA	3628	1/1	0.82	0.24	76,76,76,76	0
57	MG	BA	3273	1/1	0.82	0.22	54,54,54,54	0
57	MG	BA	3335	1/1	0.82	0.23	52,52,52,52	0
57	MG	BA	3760	1/1	0.82	0.19	44,44,44,44	0
57	MG	CA	3149	1/1	0.82	0.14	52,52,52,52	0
57	MG	BA	3418	1/1	0.82	0.17	30,30,30,30	0
57	MG	BA	3587	1/1	0.83	0.17	36,36,36,36	0
57	MG	BA	3788	1/1	0.83	0.15	51,51,51,51	0
57	MG	BA	3372	1/1	0.83	0.16	28,28,28,28	0
57	MG	AA	3002	1/1	0.83	0.15	71,71,71,71	0
57	MG	AA	3023	1/1	0.83	0.13	74,74,74,74	0
57	MG	BA	3154	1/1	0.83	0.23	47,47,47,47	0
57	MG	CA	3058	1/1	0.83	0.13	68,68,68,68	0
57	MG	CA	3009	1/1	0.83	0.11	64,64,64,64	0
57	MG	B5	101	1/1	0.83	0.24	51,51,51,51	0
57	MG	BA	3759	1/1	0.83	0.18	33,33,33,33	0
57	MG	AA	3189	1/1	0.83	0.12	65,65,65,65	0
57	MG	DA	3268	1/1	0.83	0.17	51,51,51,51	0
57	MG	DA	3385	1/1	0.83	0.11	52,52,52,52	0
57	MG	AA	3020	1/1	0.83	0.13	76,76,76,76	0
57	MG	AA	3008	1/1	0.83	0.27	73,73,73,73	0
57	MG	DA	3075	1/1	0.83	0.29	59,59,59,59	0
57	MG	DA	3544	1/1	0.83	0.12	65,65,65,65	0
57	MG	AA	3127	1/1	0.83	0.16	65,65,65,65	0
57	MG	CA	3087	1/1	0.83	0.19	67,67,67,67	0
57	MG	DA	3446	1/1	0.83	0.11	45,45,45,45	0
57	MG	BA	3769	1/1	0.83	0.18	52,52,52,52	0
57	MG	DA	3422	1/1	0.83	0.08	46,46,46,46	0
57	MG	BA	3669	1/1	0.83	0.09	62,62,62,62	0
57	MG	BA	3434	1/1	0.83	0.13	55,55,55,55	0
57	MG	AA	3017	1/1	0.83	0.18	71,71,71,71	0
57	MG	BA	3802	1/1	0.83	0.47	54,54,54,54	0
57	MG	AA	3139	1/1	0.83	0.14	59,59,59,59	0
57	MG	BA	3594	1/1	0.83	0.12	40,40,40,40	0
57	MG	BA	3446	1/1	0.83	0.17	40,40,40,40	0
57	MG	AA	3005	1/1	0.84	0.14	62,62,62,62	0
57	MG	DA	3421	1/1	0.84	0.13	50,50,50,50	0
57	MG	BA	3438	1/1	0.84	0.14	60,60,60,60	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	DA	3646	1/1	0.84	0.14	59,59,59,59	0
57	MG	CA	3066	1/1	0.84	0.14	66,66,66,66	0
57	MG	DA	3044	1/1	0.84	0.10	62,62,62,62	0
57	MG	AA	3025	1/1	0.84	0.24	62,62,62,62	0
57	MG	DA	3431	1/1	0.84	0.23	50,50,50,50	0
57	MG	BA	3512	1/1	0.84	0.18	52,52,52,52	0
57	MG	DA	3450	1/1	0.84	0.10	40,40,40,40	0
57	MG	DA	3414	1/1	0.84	0.13	43,43,43,43	0
57	MG	DA	3071	1/1	0.84	0.13	59,59,59,59	0
57	MG	BA	3179	1/1	0.84	0.17	50,50,50,50	0
57	MG	BA	3480	1/1	0.84	0.20	35,35,35,35	0
57	MG	DA	3247	1/1	0.84	0.09	45,45,45,45	0
57	MG	DA	3147	1/1	0.84	0.15	56,56,56,56	0
57	MG	BA	3391	1/1	0.84	0.24	63,63,63,63	0
57	MG	BA	3764	1/1	0.84	0.17	51,51,51,51	0
57	MG	DA	3088	1/1	0.84	0.18	47,47,47,47	0
57	MG	DA	3430	1/1	0.84	0.11	37,37,37,37	0
57	MG	DA	3122	1/1	0.84	0.11	49,49,49,49	0
57	MG	CV	101	1/1	0.84	0.13	72,72,72,72	0
57	MG	CA	3098	1/1	0.84	0.09	65,65,65,65	0
57	MG	DA	3476	1/1	0.84	0.14	62,62,62,62	0
57	MG	CA	3021	1/1	0.84	0.14	61,61,61,61	0
57	MG	BA	3018	1/1	0.84	0.20	56,56,56,56	0
57	MG	BA	3794	1/1	0.84	0.26	51,51,51,51	0
57	MG	BA	3404	1/1	0.84	0.13	59,59,59,59	0
57	MG	BA	3253	1/1	0.84	0.23	55,55,55,55	0
57	MG	DA	3468	1/1	0.84	0.27	66,66,66,66	0
57	MG	DA	3497	1/1	0.84	0.11	55,55,55,55	0
57	MG	BA	3129	1/1	0.84	0.28	58,58,58,58	0
57	MG	CA	3140	1/1	0.84	0.15	67,67,67,67	0
57	MG	CA	3116	1/1	0.84	0.22	68,68,68,68	0
57	MG	BA	3546	1/1	0.85	0.19	40,40,40,40	0
57	MG	BA	3754	1/1	0.85	0.18	48,48,48,48	0
57	MG	CA	3052	1/1	0.85	0.21	72,72,72,72	0
57	MG	DA	3362	1/1	0.85	0.21	44,44,44,44	0
57	MG	AA	3079	1/1	0.85	0.13	68,68,68,68	0
57	MG	D0	101	1/1	0.85	0.08	71,71,71,71	0
57	MG	BA	3755	1/1	0.85	0.15	55,55,55,55	0
57	MG	DA	3425	1/1	0.85	0.12	61,61,61,61	0
57	MG	BA	3432	1/1	0.85	0.14	58,58,58,58	0
57	MG	BA	3231	1/1	0.85	0.32	63,63,63,63	0
57	MG	AA	3034	1/1	0.85	0.11	47,47,47,47	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	BA	3293	1/1	0.85	0.26	50,50,50,50	0
57	MG	BA	3296	1/1	0.85	0.18	53,53,53,53	0
57	MG	AA	3166	1/1	0.85	0.14	69,69,69,69	0
57	MG	BA	3443	1/1	0.85	0.23	37,37,37,37	0
57	MG	CA	3141	1/1	0.85	0.04	92,92,92,92	0
57	MG	AA	3196	1/1	0.85	0.21	74,74,74,74	0
57	MG	DU	3002	1/1	0.85	0.40	55,55,55,55	0
57	MG	DA	3661	1/1	0.85	0.16	62,62,62,62	0
57	MG	AA	3073	1/1	0.85	0.10	56,56,56,56	0
57	MG	BA	3453	1/1	0.85	0.32	45,45,45,45	0
57	MG	AA	3041	1/1	0.85	0.21	46,46,46,46	0
57	MG	BA	3301	1/1	0.85	0.13	60,60,60,60	0
57	MG	BA	3718	1/1	0.85	0.11	71,71,71,71	0
57	MG	AA	3184	1/1	0.85	0.12	60,60,60,60	0
57	MG	DA	3498	1/1	0.85	0.08	51,51,51,51	0
57	MG	BA	3456	1/1	0.85	0.18	49,49,49,49	0
57	MG	BA	3506	1/1	0.85	0.10	58,58,58,58	0
57	MG	AA	3001	1/1	0.85	0.14	61,61,61,61	0
57	MG	BB	220	1/1	0.85	0.13	57,57,57,57	0
57	MG	DA	3069	1/1	0.85	0.23	57,57,57,57	0
57	MG	AA	3033	1/1	0.85	0.14	59,59,59,59	0
57	MG	DA	3571	1/1	0.85	0.12	56,56,56,56	0
57	MG	B2	3001	1/1	0.85	0.21	56,56,56,56	0
57	MG	DA	3410	1/1	0.85	0.13	53,53,53,53	0
57	MG	DA	3139	1/1	0.85	0.17	53,53,53,53	0
57	MG	DA	3657	1/1	0.85	0.10	63,63,63,63	0
57	MG	CA	3016	1/1	0.85	0.11	57,57,57,57	0
57	MG	CA	3158	1/1	0.85	0.13	67,67,67,67	0
57	MG	DA	3178	1/1	0.85	0.22	50,50,50,50	0
57	MG	DA	3415	1/1	0.85	0.11	68,68,68,68	0
57	MG	BA	3681	1/1	0.85	0.08	66,66,66,66	0
57	MG	BA	3305	1/1	0.85	0.09	62,62,62,62	0
57	MG	DE	303	1/1	0.85	0.12	54,54,54,54	0
57	MG	DA	3180	1/1	0.85	0.20	42,42,42,42	0
57	MG	AA	3047	1/1	0.85	0.17	63,63,63,63	0
57	MG	BA	3530	1/1	0.86	0.22	49,49,49,49	0
57	MG	DA	3495	1/1	0.86	0.11	47,47,47,47	0
57	MG	BA	3284	1/1	0.86	0.27	43,43,43,43	0
57	MG	DA	3462	1/1	0.86	0.20	42,42,42,42	0
57	MG	AA	3177	1/1	0.86	0.08	66,66,66,66	0
57	MG	DA	3658	1/1	0.86	0.12	62,62,62,62	0
57	MG	BA	3426	1/1	0.86	0.20	37,37,37,37	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	BA	3308	1/1	0.86	0.19	43,43,43,43	0
57	MG	DA	3641	1/1	0.86	0.20	69,69,69,69	0
57	MG	DA	3360	1/1	0.86	0.16	46,46,46,46	0
57	MG	BB	202	1/1	0.86	0.28	59,59,59,59	0
57	MG	CA	3073	1/1	0.86	0.14	57,57,57,57	0
57	MG	DA	3592	1/1	0.86	0.07	51,51,51,51	0
57	MG	CA	3033	1/1	0.86	0.19	71,71,71,71	0
57	MG	BA	3598	1/1	0.86	0.14	63,63,63,63	0
57	MG	BA	3680	1/1	0.86	0.11	68,68,68,68	0
57	MG	DA	3309	1/1	0.86	0.09	51,51,51,51	0
57	MG	DA	3440	1/1	0.86	0.09	61,61,61,61	0
57	MG	BA	3213	1/1	0.86	0.26	40,40,40,40	0
57	MG	CA	3097	1/1	0.86	0.15	69,69,69,69	0
57	MG	DA	3484	1/1	0.86	0.12	62,62,62,62	0
57	MG	DA	3523	1/1	0.86	0.10	59,59,59,59	0
57	MG	BA	3165	1/1	0.86	0.17	45,45,45,45	0
57	MG	DA	3667	1/1	0.86	0.12	50,50,50,50	0
57	MG	CE	3001	1/1	0.86	0.10	79,79,79,79	0
57	MG	AA	3214	1/1	0.86	0.17	73,73,73,73	0
57	MG	AA	3192	1/1	0.86	0.14	71,71,71,71	0
57	MG	BE	305	1/1	0.86	0.17	43,43,43,43	0
57	MG	DA	3528	1/1	0.86	0.15	62,62,62,62	0
57	MG	DA	3138	1/1	0.86	0.13	55,55,55,55	0
57	MG	DB	3012	1/1	0.86	0.33	61,61,61,61	0
57	MG	BA	3447	1/1	0.86	0.10	72,72,72,72	0
57	MG	DA	3185	1/1	0.86	0.11	68,68,68,68	0
57	MG	BA	3601	1/1	0.86	0.12	55,55,55,55	0
57	MG	AA	3054	1/1	0.86	0.13	53,53,53,53	0
57	MG	BA	3180	1/1	0.86	0.17	47,47,47,47	0
57	MG	DA	3035	1/1	0.86	0.20	52,52,52,52	0
57	MG	BA	3274	1/1	0.86	0.14	49,49,49,49	0
57	MG	DA	3312	1/1	0.86	0.10	54,54,54,54	0
57	MG	CA	3115	1/1	0.86	0.09	63,63,63,63	0
57	MG	AA	3065	1/1	0.86	0.20	63,63,63,63	0
57	MG	DA	3654	1/1	0.86	0.12	56,56,56,56	0
57	MG	DA	3062	1/1	0.86	0.20	63,63,63,63	0
57	MG	DA	3577	1/1	0.86	0.14	58,58,58,58	0
57	MG	BA	3486	1/1	0.86	0.13	57,57,57,57	0
57	MG	DA	3575	1/1	0.87	0.14	64,64,64,64	0
57	MG	BA	3419	1/1	0.87	0.23	37,37,37,37	0
57	MG	DA	3437	1/1	0.87	0.16	52,52,52,52	0
57	MG	DA	3676	1/1	0.87	0.33	67,67,67,67	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	BA	3513	1/1	0.87	0.15	59,59,59,59	0
57	MG	CA	3027	1/1	0.87	0.20	64,64,64,64	0
57	MG	BA	3732	1/1	0.87	0.26	51,51,51,51	0
57	MG	DA	3148	1/1	0.87	0.12	54,54,54,54	0
57	MG	DA	3356	1/1	0.87	0.10	36,36,36,36	0
57	MG	BA	3147	1/1	0.87	0.16	45,45,45,45	0
57	MG	AA	3089	1/1	0.87	0.15	60,60,60,60	0
57	MG	BA	3658	1/1	0.87	0.26	61,61,61,61	0
57	MG	BA	3742	1/1	0.87	0.24	65,65,65,65	0
57	MG	DA	3110	1/1	0.87	0.31	58,58,58,58	0
57	MG	DF	3001	1/1	0.87	0.20	44,44,44,44	0
57	MG	DA	3242	1/1	0.87	0.11	52,52,52,52	0
57	MG	DA	3659	1/1	0.87	0.14	48,48,48,48	0
57	MG	DA	3632	1/1	0.87	0.15	36,36,36,36	0
57	MG	DA	3400	1/1	0.87	0.12	54,54,54,54	0
57	MG	DA	3140	1/1	0.87	0.15	58,58,58,58	0
57	MG	BX	3002	1/1	0.87	0.19	46,46,46,46	0
57	MG	AA	3031	1/1	0.87	0.23	70,70,70,70	0
57	MG	BA	3548	1/1	0.87	0.17	40,40,40,40	0
57	MG	BA	3637	1/1	0.87	0.11	39,39,39,39	0
57	MG	DA	3007	1/1	0.87	0.14	50,50,50,50	0
57	MG	BA	3584	1/1	0.87	0.20	63,63,63,63	0
57	MG	DA	3217	1/1	0.87	0.14	38,38,38,38	0
57	MG	CA	3138	1/1	0.87	0.19	80,80,80,80	0
57	MG	DA	3240	1/1	0.87	0.09	48,48,48,48	0
57	MG	AA	3038	1/1	0.87	0.33	68,68,68,68	0
57	MG	AA	3124	1/1	0.87	0.09	47,47,47,47	0
57	MG	BA	3258	1/1	0.87	0.13	44,44,44,44	0
57	MG	AA	3197	1/1	0.87	0.26	70,70,70,70	0
57	MG	BA	3780	1/1	0.87	0.11	62,62,62,62	0
57	MG	CA	3124	1/1	0.87	0.12	59,59,59,59	0
57	MG	DQ	3004	1/1	0.87	0.28	54,54,54,54	0
57	MG	DA	3521	1/1	0.87	0.13	58,58,58,58	0
57	MG	DA	3339	1/1	0.87	0.15	61,61,61,61	0
57	MG	BA	3583	1/1	0.87	0.21	45,45,45,45	0
57	MG	BA	3001	1/1	0.87	0.14	53,53,53,53	0
57	MG	BA	3386	1/1	0.87	0.16	53,53,53,53	0
57	MG	BA	3206	1/1	0.87	0.23	49,49,49,49	0
57	MG	BA	3071	1/1	0.87	0.35	59,59,59,59	0
57	MG	DA	3061	1/1	0.87	0.13	48,48,48,48	0
57	MG	BA	3074	1/1	0.87	0.21	46,46,46,46	0
57	MG	DA	3283	1/1	0.87	0.11	51,51,51,51	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	AA	3045	1/1	0.87	0.12	58,58,58,58	0
57	MG	BA	3684	1/1	0.87	0.12	68,68,68,68	0
57	MG	CA	3168	1/1	0.87	0.11	56,56,56,56	0
57	MG	BA	3318	1/1	0.87	0.12	41,41,41,41	0
57	MG	CA	3090	1/1	0.87	0.10	67,67,67,67	0
57	MG	BA	3545	1/1	0.87	0.14	65,65,65,65	0
57	MG	DA	3002	1/1	0.87	0.10	48,48,48,48	0
57	MG	BB	211	1/1	0.87	0.10	51,51,51,51	0
57	MG	AA	3121	1/1	0.87	0.12	70,70,70,70	0
57	MG	AA	3190	1/1	0.87	0.10	58,58,58,58	0
57	MG	AA	3049	1/1	0.87	0.21	64,64,64,64	0
57	MG	DA	3361	1/1	0.87	0.12	44,44,44,44	0
57	MG	DA	3558	1/1	0.87	0.17	61,61,61,61	0
57	MG	BA	3128	1/1	0.87	0.14	69,69,69,69	0
57	MG	AA	3051	1/1	0.87	0.23	73,73,73,73	0
57	MG	BA	3710	1/1	0.88	0.17	57,57,57,57	0
57	MG	DA	3606	1/1	0.88	0.10	71,71,71,71	0
57	MG	BA	3267	1/1	0.88	0.19	65,65,65,65	0
57	MG	BA	3033	1/1	0.88	0.29	53,53,53,53	0
57	MG	AA	3019	1/1	0.88	0.11	66,66,66,66	0
57	MG	DA	3527	1/1	0.88	0.12	60,60,60,60	0
57	MG	DA	3567	1/1	0.88	0.27	62,62,62,62	0
57	MG	B7	105	1/1	0.88	0.16	56,56,56,56	0
57	MG	BA	3030	1/1	0.88	0.18	46,46,46,46	0
57	MG	BA	3740	1/1	0.88	0.16	28,28,28,28	0
57	MG	BA	3526	1/1	0.88	0.17	44,44,44,44	0
57	MG	BA	3619	1/1	0.88	0.20	58,58,58,58	0
57	MG	BA	3673	1/1	0.88	0.17	55,55,55,55	0
57	MG	DA	3208	1/1	0.88	0.36	58,58,58,58	0
57	MG	BA	3624	1/1	0.88	0.10	68,68,68,68	0
57	MG	BA	3430	1/1	0.88	0.16	37,37,37,37	0
57	MG	DA	3380	1/1	0.88	0.07	55,55,55,55	0
57	MG	BA	3578	1/1	0.88	0.09	46,46,46,46	0
57	MG	CA	3157	1/1	0.88	0.11	58,58,58,58	0
57	MG	DA	3288	1/1	0.88	0.14	52,52,52,52	0
57	MG	DA	3591	1/1	0.88	0.17	55,55,55,55	0
57	MG	AA	3026	1/1	0.88	0.13	70,70,70,70	0
57	MG	DA	3334	1/1	0.88	0.15	52,52,52,52	0
57	MG	DA	3323	1/1	0.88	0.11	50,50,50,50	0
57	MG	AA	3107	1/1	0.88	0.18	64,64,64,64	0
57	MG	DA	3609	1/1	0.88	0.10	46,46,46,46	0
57	MG	BA	3057	1/1	0.88	0.20	34,34,34,34	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	CA	3003	1/1	0.88	0.12	57,57,57,57	0
57	MG	BA	3162	1/1	0.88	0.15	38,38,38,38	0
57	MG	BA	3297	1/1	0.88	0.14	43,43,43,43	0
57	MG	BA	3002	1/1	0.88	0.10	50,50,50,50	0
57	MG	DA	3274	1/1	0.88	0.15	58,58,58,58	0
57	MG	AA	3072	1/1	0.88	0.12	66,66,66,66	0
57	MG	DA	3388	1/1	0.88	0.15	53,53,53,53	0
57	MG	BA	3566	1/1	0.88	0.21	67,67,67,67	0
57	MG	DA	3056	1/1	0.88	0.09	51,51,51,51	0
57	MG	DB	3003	1/1	0.88	0.12	57,57,57,57	0
57	MG	BA	3266	1/1	0.88	0.19	39,39,39,39	0
57	MG	BA	3006	1/1	0.88	0.19	48,48,48,48	0
57	MG	BA	3514	1/1	0.88	0.23	48,48,48,48	0
57	MG	DA	3590	1/1	0.88	0.10	51,51,51,51	0
57	MG	BA	3442	1/1	0.88	0.17	44,44,44,44	0
57	MG	DA	3603	1/1	0.88	0.06	41,41,41,41	0
57	MG	BA	3333	1/1	0.88	0.20	38,38,38,38	0
57	MG	BA	3072	1/1	0.88	0.14	47,47,47,47	0
57	MG	DA	3093	1/1	0.88	0.09	62,62,62,62	0
57	MG	DA	3636	1/1	0.88	0.32	63,63,63,63	0
57	MG	BA	3532	1/1	0.88	0.15	52,52,52,52	0
57	MG	DA	3469	1/1	0.88	0.28	44,44,44,44	0
57	MG	BA	3471	1/1	0.88	0.27	53,53,53,53	0
57	MG	AA	3046	1/1	0.88	0.22	55,55,55,55	0
57	MG	AX	3002	1/1	0.88	0.17	58,58,58,58	0
57	MG	BA	3679	1/1	0.88	0.12	62,62,62,62	0
57	MG	AA	3145	1/1	0.88	0.12	66,66,66,66	0
57	MG	BA	3502	1/1	0.88	0.12	56,56,56,56	0
57	MG	DA	3618	1/1	0.88	0.12	53,53,53,53	0
57	MG	BA	3409	1/1	0.88	0.16	30,30,30,30	0
57	MG	AX	3010	1/1	0.88	0.21	59,59,59,59	0
57	MG	CA	3163	1/1	0.88	0.09	63,63,63,63	0
57	MG	DA	3614	1/1	0.88	0.07	65,65,65,65	0
57	MG	AA	3200	1/1	0.88	0.08	73,73,73,73	0
57	MG	AA	3128	1/1	0.88	0.08	57,57,57,57	0
57	MG	CA	3039	1/1	0.88	0.11	68,68,68,68	0
57	MG	DA	3216	1/1	0.88	0.22	56,56,56,56	0
57	MG	DA	3572	1/1	0.88	0.06	62,62,62,62	0
57	MG	DA	3526	1/1	0.88	0.11	48,48,48,48	0
57	MG	BA	3117	1/1	0.88	0.20	59,59,59,59	0
57	MG	DA	3092	1/1	0.88	0.18	45,45,45,45	0
57	MG	DA	3367	1/1	0.88	0.14	61,61,61,61	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	BA	3275	1/1	0.88	0.17	58,58,58,58	0
57	MG	AA	3094	1/1	0.88	0.17	59,59,59,59	0
57	MG	BA	3185	1/1	0.88	0.19	57,57,57,57	0
57	MG	BA	3212	1/1	0.88	0.24	54,54,54,54	0
57	MG	BA	3337	1/1	0.88	0.17	58,58,58,58	0
57	MG	DB	3002	1/1	0.88	0.17	65,65,65,65	0
57	MG	BA	3122	1/1	0.88	0.15	41,41,41,41	0
57	MG	DA	3332	1/1	0.89	0.11	53,53,53,53	0
57	MG	BA	3397	1/1	0.89	0.15	30,30,30,30	0
57	MG	CA	3020	1/1	0.89	0.11	56,56,56,56	0
57	MG	CA	3159	1/1	0.89	0.18	70,70,70,70	0
57	MG	DA	3371	1/1	0.89	0.13	58,58,58,58	0
57	MG	DA	3355	1/1	0.89	0.12	58,58,58,58	0
57	MG	CA	3076	1/1	0.89	0.14	57,57,57,57	0
57	MG	DA	3638	1/1	0.89	0.10	51,51,51,51	0
57	MG	DX	101	1/1	0.89	0.12	51,51,51,51	0
57	MG	CA	3156	1/1	0.89	0.10	73,73,73,73	0
57	MG	DA	3248	1/1	0.89	0.12	56,56,56,56	0
57	MG	CA	3062	1/1	0.89	0.17	64,64,64,64	0
57	MG	CA	3022	1/1	0.89	0.20	78,78,78,78	0
57	MG	BA	3008	1/1	0.89	0.17	47,47,47,47	0
57	MG	CA	3128	1/1	0.89	0.15	65,65,65,65	0
57	MG	DA	3275	1/1	0.89	0.17	42,42,42,42	0
57	MG	BV	203	1/1	0.89	0.19	38,38,38,38	0
57	MG	CA	3041	1/1	0.89	0.13	59,59,59,59	0
57	MG	BA	3402	1/1	0.89	0.14	40,40,40,40	0
57	MG	AA	3176	1/1	0.89	0.10	67,67,67,67	0
57	MG	BA	3023	1/1	0.89	0.22	36,36,36,36	0
57	MG	BA	3596	1/1	0.89	0.10	64,64,64,64	0
57	MG	BA	3499	1/1	0.89	0.10	58,58,58,58	0
57	MG	DA	3311	1/1	0.89	0.17	54,54,54,54	0
57	MG	DA	3420	1/1	0.89	0.24	60,60,60,60	0
57	MG	BQ	3005	1/1	0.89	0.13	49,49,49,49	0
57	MG	DA	3444	1/1	0.89	0.06	44,44,44,44	0
57	MG	DA	3481	1/1	0.89	0.41	55,55,55,55	0
57	MG	BA	3314	1/1	0.89	0.13	58,58,58,58	0
57	MG	AM	201	1/1	0.89	0.16	51,51,51,51	0
57	MG	AA	3064	1/1	0.89	0.24	60,60,60,60	0
57	MG	DA	3151	1/1	0.89	0.09	55,55,55,55	0
57	MG	AA	3108	1/1	0.89	0.28	67,67,67,67	0
57	MG	DA	3564	1/1	0.89	0.16	61,61,61,61	0
57	MG	DA	3593	1/1	0.89	0.11	40,40,40,40	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	DA	3124	1/1	0.89	0.15	57,57,57,57	0
57	MG	DA	3106	1/1	0.89	0.13	52,52,52,52	0
57	MG	DA	3470	1/1	0.89	0.19	45,45,45,45	0
57	MG	BA	3106	1/1	0.89	0.22	42,42,42,42	0
57	MG	BA	3324	1/1	0.89	0.17	45,45,45,45	0
57	MG	DA	3206	1/1	0.89	0.13	50,50,50,50	0
57	MG	DA	3492	1/1	0.89	0.12	55,55,55,55	0
57	MG	DA	3223	1/1	0.89	0.15	50,50,50,50	0
57	MG	BA	3810	1/1	0.89	0.18	41,41,41,41	0
57	MG	BA	3745	1/1	0.89	0.08	75,75,75,75	0
57	MG	BA	3573	1/1	0.89	0.16	51,51,51,51	0
57	MG	DA	3095	1/1	0.89	0.15	58,58,58,58	0
57	MG	BA	3444	1/1	0.89	0.21	29,29,29,29	0
57	MG	BA	3092	1/1	0.89	0.16	37,37,37,37	0
57	MG	DA	3077	1/1	0.89	0.23	61,61,61,61	0
57	MG	BA	3590	1/1	0.89	0.16	50,50,50,50	0
57	MG	CA	3061	1/1	0.89	0.28	66,66,66,66	0
57	MG	AA	3210	1/1	0.89	0.27	59,59,59,59	0
57	MG	DA	3313	1/1	0.89	0.16	47,47,47,47	0
57	MG	BA	3131	1/1	0.89	0.11	58,58,58,58	0
57	MG	DA	3090	1/1	0.89	0.10	52,52,52,52	0
57	MG	DA	3098	1/1	0.89	0.17	53,53,53,53	0
57	MG	BA	3361	1/1	0.89	0.13	49,49,49,49	0
57	MG	AA	3102	1/1	0.89	0.25	59,59,59,59	0
57	MG	DA	3626	1/1	0.89	0.07	67,67,67,67	0
57	MG	BA	3298	1/1	0.89	0.16	51,51,51,51	0
57	MG	BA	3749	1/1	0.89	0.12	56,56,56,56	0
57	MG	BA	3125	1/1	0.89	0.17	47,47,47,47	0
57	MG	BA	3790	1/1	0.89	0.18	34,34,34,34	0
57	MG	BA	3032	1/1	0.89	0.20	47,47,47,47	0
57	MG	BU	201	1/1	0.89	0.15	43,43,43,43	0
57	MG	BA	3431	1/1	0.89	0.17	59,59,59,59	0
57	MG	AA	3093	1/1	0.89	0.12	66,66,66,66	0
57	MG	BA	3703	1/1	0.89	0.10	64,64,64,64	0
57	MG	BA	3622	1/1	0.89	0.19	48,48,48,48	0
57	MG	BA	3058	1/1	0.89	0.15	49,49,49,49	0
57	MG	DA	3066	1/1	0.89	0.10	42,42,42,42	0
57	MG	CA	3044	1/1	0.89	0.23	62,62,62,62	0
57	MG	DA	3605	1/1	0.89	0.12	58,58,58,58	0
57	MG	CA	3036	1/1	0.89	0.14	66,66,66,66	0
57	MG	BA	3640	1/1	0.89	0.17	53,53,53,53	0
57	MG	BA	3741	1/1	0.89	0.74	64,64,64,64	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	CA	3081	1/1	0.89	0.09	46,46,46,46	0
57	MG	BA	3618	1/1	0.89	0.14	65,65,65,65	0
57	MG	AA	3209	1/1	0.89	0.08	59,59,59,59	0
57	MG	BZ	3001	1/1	0.89	0.29	55,55,55,55	0
57	MG	BA	3315	1/1	0.89	0.19	31,31,31,31	0
57	MG	BA	3445	1/1	0.89	0.30	63,63,63,63	0
57	MG	BA	3793	1/1	0.89	0.13	40,40,40,40	0
57	MG	BA	3109	1/1	0.89	0.18	51,51,51,51	0
57	MG	DA	3621	1/1	0.89	0.08	44,44,44,44	0
57	MG	BE	301	1/1	0.89	0.14	35,35,35,35	0
57	MG	BA	3697	1/1	0.89	0.17	61,61,61,61	0
57	MG	CA	3004	1/1	0.89	0.25	66,66,66,66	0
57	MG	BA	3399	1/1	0.89	0.20	45,45,45,45	0
57	MG	AA	3042	1/1	0.89	0.09	57,57,57,57	0
57	MG	DP	202	1/1	0.89	0.11	53,53,53,53	0
57	MG	BA	3192	1/1	0.90	0.28	46,46,46,46	0
57	MG	DA	3141	1/1	0.90	0.27	61,61,61,61	0
57	MG	CA	3054	1/1	0.90	0.30	69,69,69,69	0
57	MG	DA	3214	1/1	0.90	0.24	59,59,59,59	0
57	MG	DA	3126	1/1	0.90	0.08	55,55,55,55	0
57	MG	AA	3142	1/1	0.90	0.11	41,41,41,41	0
59	ZN	DY	501	1/1	0.90	0.15	96,96,96,96	0
57	MG	BA	3047	1/1	0.90	0.22	60,60,60,60	0
57	MG	BA	3312	1/1	0.90	0.18	32,32,32,32	0
57	MG	DA	3666	1/1	0.90	0.14	35,35,35,35	0
57	MG	DA	3465	1/1	0.90	0.12	46,46,46,46	0
57	MG	BA	3465	1/1	0.90	0.18	43,43,43,43	0
57	MG	BA	3276	1/1	0.90	0.31	54,54,54,54	0
57	MG	BA	3411	1/1	0.90	0.19	33,33,33,33	0
57	MG	BA	3811	1/1	0.90	0.14	65,65,65,65	0
57	MG	DA	3132	1/1	0.90	0.23	52,52,52,52	0
57	MG	DA	3070	1/1	0.90	0.13	58,58,58,58	0
57	MG	BA	3581	1/1	0.90	0.19	30,30,30,30	0
57	MG	AA	3100	1/1	0.90	0.12	65,65,65,65	0
57	MG	BA	3634	1/1	0.90	0.14	62,62,62,62	0
57	MG	BA	3623	1/1	0.90	0.26	55,55,55,55	0
57	MG	AA	3135	1/1	0.90	0.24	65,65,65,65	0
57	MG	CA	3038	1/1	0.90	0.14	58,58,58,58	0
57	MG	DA	3280	1/1	0.90	0.16	33,33,33,33	0
57	MG	DA	3301	1/1	0.90	0.19	52,52,52,52	0
57	MG	BA	3394	1/1	0.90	0.18	40,40,40,40	0
57	MG	BA	3541	1/1	0.90	0.16	38,38,38,38	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	AA	3036	1/1	0.90	0.17	61,61,61,61	0
57	MG	BA	3648	1/1	0.90	0.11	65,65,65,65	0
57	MG	DA	3033	1/1	0.90	0.10	42,42,42,42	0
57	MG	DA	3378	1/1	0.90	0.13	57,57,57,57	0
57	MG	AA	3058	1/1	0.90	0.28	59,59,59,59	0
57	MG	CA	3130	1/1	0.90	0.09	57,57,57,57	0
57	MG	DB	3001	1/1	0.90	0.17	64,64,64,64	0
57	MG	BA	3700	1/1	0.90	0.16	61,61,61,61	0
57	MG	CA	3002	1/1	0.90	0.12	63,63,63,63	0
57	MG	DA	3452	1/1	0.90	0.16	51,51,51,51	0
57	MG	DA	3209	1/1	0.90	0.24	53,53,53,53	0
57	MG	DA	3677	1/1	0.90	0.47	52,52,52,52	0
57	MG	BA	3686	1/1	0.90	0.25	60,60,60,60	0
57	MG	BA	3177	1/1	0.90	0.19	46,46,46,46	0
57	MG	AX	3016	1/1	0.90	0.10	56,56,56,56	0
57	MG	AA	3204	1/1	0.90	0.13	53,53,53,53	0
57	MG	CA	3006	1/1	0.90	0.14	64,64,64,64	0
57	MG	AA	3194	1/1	0.90	0.11	56,56,56,56	0
57	MG	BA	3429	1/1	0.90	0.10	65,65,65,65	0
57	MG	DA	3401	1/1	0.90	0.10	38,38,38,38	0
57	MG	DA	3499	1/1	0.90	0.10	53,53,53,53	0
57	MG	DA	3502	1/1	0.90	0.10	55,55,55,55	0
57	MG	DA	3615	1/1	0.90	0.09	65,65,65,65	0
57	MG	DB	3004	1/1	0.90	0.15	55,55,55,55	0
57	MG	BA	3612	1/1	0.90	0.14	21,21,21,21	0
57	MG	AA	3185	1/1	0.90	0.12	82,82,82,82	0
57	MG	BN	3004	1/1	0.90	0.12	60,60,60,60	0
57	MG	DA	3556	1/1	0.90	0.11	67,67,67,67	0
57	MG	BA	3104	1/1	0.90	0.13	42,42,42,42	0
57	MG	BA	3461	1/1	0.90	0.10	62,62,62,62	0
57	MG	BA	3664	1/1	0.90	0.16	55,55,55,55	0
57	MG	CA	3057	1/1	0.90	0.18	76,76,76,76	0
57	MG	DA	3337	1/1	0.90	0.13	41,41,41,41	0
57	MG	DA	3424	1/1	0.90	0.09	61,61,61,61	0
57	MG	BA	3702	1/1	0.90	0.27	51,51,51,51	0
57	MG	DA	3119	1/1	0.90	0.22	39,39,39,39	0
57	MG	BA	3666	1/1	0.90	0.19	50,50,50,50	0
57	MG	AA	3146	1/1	0.90	0.13	66,66,66,66	0
57	MG	BA	3199	1/1	0.90	0.15	46,46,46,46	0
57	MG	DA	3547	1/1	0.90	0.14	54,54,54,54	0
57	MG	AA	3143	1/1	0.90	0.08	60,60,60,60	0
57	MG	DA	3103	1/1	0.90	0.10	58,58,58,58	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	BA	3550	1/1	0.90	0.19	36,36,36,36	0
57	MG	BA	3195	1/1	0.90	0.11	46,46,46,46	0
57	MG	DA	3270	1/1	0.90	0.10	46,46,46,46	0
57	MG	DA	3524	1/1	0.90	0.17	61,61,61,61	0
57	MG	DA	3314	1/1	0.90	0.12	43,43,43,43	0
57	MG	AA	3187	1/1	0.90	0.13	62,62,62,62	0
57	MG	DA	3463	1/1	0.90	0.14	55,55,55,55	0
57	MG	DA	3215	1/1	0.90	0.13	59,59,59,59	0
57	MG	DA	3271	1/1	0.90	0.15	48,48,48,48	0
57	MG	DA	3245	1/1	0.90	0.12	54,54,54,54	0
57	MG	BD	309	1/1	0.90	0.32	57,57,57,57	0
57	MG	BA	3659	1/1	0.90	0.19	61,61,61,61	0
57	MG	AA	3117	1/1	0.90	0.12	79,79,79,79	0
57	MG	DA	3328	1/1	0.90	0.08	47,47,47,47	0
57	MG	AA	3059	1/1	0.90	0.12	78,78,78,78	0
57	MG	DA	3221	1/1	0.90	0.27	52,52,52,52	0
57	MG	CA	3026	1/1	0.90	0.20	63,63,63,63	0
57	MG	DA	3018	1/1	0.90	0.20	62,62,62,62	0
57	MG	AA	3211	1/1	0.90	0.12	47,47,47,47	0
57	MG	DA	3146	1/1	0.90	0.10	55,55,55,55	0
57	MG	BA	3599	1/1	0.90	0.21	43,43,43,43	0
57	MG	BA	3485	1/1	0.90	0.09	42,42,42,42	0
57	MG	DA	3129	1/1	0.90	0.12	46,46,46,46	0
57	MG	BB	210	1/1	0.90	0.07	61,61,61,61	0
57	MG	BA	3351	1/1	0.90	0.17	30,30,30,30	0
57	MG	DA	3133	1/1	0.90	0.22	50,50,50,50	0
57	MG	DA	3051	1/1	0.90	0.11	48,48,48,48	0
57	MG	BA	3501	1/1	0.90	0.23	71,71,71,71	0
57	MG	AA	3057	1/1	0.90	0.22	64,64,64,64	0
57	MG	BA	3478	1/1	0.91	0.19	58,58,58,58	0
57	MG	BA	3304	1/1	0.91	0.15	67,67,67,67	0
57	MG	AX	3007	1/1	0.91	0.10	67,67,67,67	0
57	MG	BA	3285	1/1	0.91	0.27	50,50,50,50	0
57	MG	BA	3073	1/1	0.91	0.22	61,61,61,61	0
57	MG	DA	3120	1/1	0.91	0.13	49,49,49,49	0
57	MG	DA	3134	1/1	0.91	0.21	41,41,41,41	0
57	MG	BA	3746	1/1	0.91	0.11	51,51,51,51	0
57	MG	BA	3396	1/1	0.91	0.15	50,50,50,50	0
57	MG	BA	3061	1/1	0.91	0.23	29,29,29,29	0
57	MG	BA	3226	1/1	0.91	0.27	47,47,47,47	0
57	MG	BA	3508	1/1	0.91	0.20	51,51,51,51	0
57	MG	BA	3150	1/1	0.91	0.17	55,55,55,55	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	BA	3366	1/1	0.91	0.12	57,57,57,57	0
57	MG	DA	3239	1/1	0.91	0.24	56,56,56,56	0
57	MG	B7	104	1/1	0.91	0.27	48,48,48,48	0
57	MG	DA	3622	1/1	0.91	0.21	61,61,61,61	0
57	MG	DA	3279	1/1	0.91	0.12	56,56,56,56	0
57	MG	B1	101	1/1	0.91	0.50	51,51,51,51	0
57	MG	DA	3236	1/1	0.91	0.26	47,47,47,47	0
57	MG	CA	3046	1/1	0.91	0.09	69,69,69,69	0
57	MG	CA	3012	1/1	0.91	0.21	60,60,60,60	0
57	MG	AA	3066	1/1	0.91	0.31	60,60,60,60	0
57	MG	BA	3668	1/1	0.91	0.17	53,53,53,53	0
57	MG	BA	3321	1/1	0.91	0.24	55,55,55,55	0
57	MG	DA	3405	1/1	0.91	0.16	46,46,46,46	0
57	MG	DA	3085	1/1	0.91	0.08	53,53,53,53	0
57	MG	BA	3621	1/1	0.91	0.17	53,53,53,53	0
57	MG	BO	202	1/1	0.91	0.09	65,65,65,65	0
57	MG	AA	3131	1/1	0.91	0.15	71,71,71,71	0
57	MG	CA	3075	1/1	0.91	0.18	59,59,59,59	0
57	MG	CW	3001	1/1	0.91	0.22	67,67,67,67	0
57	MG	BA	3507	1/1	0.91	0.20	49,49,49,49	0
57	MG	AA	3198	1/1	0.91	0.13	61,61,61,61	0
57	MG	CA	3153	1/1	0.91	0.16	70,70,70,70	0
57	MG	DA	3049	1/1	0.91	0.27	52,52,52,52	0
57	MG	DD	309	1/1	0.91	0.20	59,59,59,59	0
57	MG	AA	3080	1/1	0.91	0.21	58,58,58,58	0
57	MG	BA	3121	1/1	0.91	0.21	64,64,64,64	0
57	MG	BA	3606	1/1	0.91	0.14	61,61,61,61	0
57	MG	BD	302	1/1	0.91	0.27	50,50,50,50	0
57	MG	BA	3575	1/1	0.91	0.12	48,48,48,48	0
57	MG	BA	3005	1/1	0.91	0.16	30,30,30,30	0
57	MG	DA	3550	1/1	0.91	0.13	57,57,57,57	0
57	MG	BA	3561	1/1	0.91	0.12	45,45,45,45	0
57	MG	DA	3170	1/1	0.91	0.12	53,53,53,53	0
57	MG	AN	502	1/1	0.91	0.29	63,63,63,63	0
57	MG	BA	3303	1/1	0.91	0.17	36,36,36,36	0
57	MG	DA	3317	1/1	0.91	0.12	44,44,44,44	0
57	MG	DA	3130	1/1	0.91	0.18	52,52,52,52	0
57	MG	DA	3165	1/1	0.91	0.24	57,57,57,57	0
57	MG	BO	201	1/1	0.91	0.19	50,50,50,50	0
57	MG	BA	3007	1/1	0.91	0.19	55,55,55,55	0
57	MG	AA	3133	1/1	0.91	0.16	56,56,56,56	0
57	MG	CA	3100	1/1	0.91	0.09	52,52,52,52	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	BN	3002	1/1	0.91	0.16	39,39,39,39	0
57	MG	DA	3243	1/1	0.91	0.12	55,55,55,55	0
57	MG	CA	3118	1/1	0.91	0.19	68,68,68,68	0
57	MG	DA	3038	1/1	0.91	0.16	47,47,47,47	0
57	MG	DA	3004	1/1	0.91	0.17	40,40,40,40	0
57	MG	BA	3750	1/1	0.91	0.17	27,27,27,27	0
57	MG	DA	3588	1/1	0.91	0.30	65,65,65,65	0
57	MG	DA	3643	1/1	0.91	0.13	61,61,61,61	0
57	MG	AA	3188	1/1	0.91	0.08	69,69,69,69	0
57	MG	BA	3229	1/1	0.91	0.22	54,54,54,54	0
57	MG	BA	3143	1/1	0.91	0.26	45,45,45,45	0
57	MG	BA	3654	1/1	0.91	0.20	57,57,57,57	0
57	MG	BA	3495	1/1	0.91	0.13	37,37,37,37	0
57	MG	CA	3028	1/1	0.91	0.13	41,41,41,41	0
57	MG	BA	3423	1/1	0.91	0.18	44,44,44,44	0
57	MG	DA	3407	1/1	0.91	0.04	66,66,66,66	0
57	MG	BA	3024	1/1	0.91	0.19	49,49,49,49	0
57	MG	CA	3129	1/1	0.91	0.09	43,43,43,43	0
57	MG	BA	3562	1/1	0.91	0.14	37,37,37,37	0
57	MG	DA	3604	1/1	0.91	0.18	59,59,59,59	0
57	MG	DA	3429	1/1	0.91	0.14	41,41,41,41	0
57	MG	BA	3019	1/1	0.91	0.15	42,42,42,42	0
57	MG	BA	3466	1/1	0.91	0.17	49,49,49,49	0
57	MG	BB	206	1/1	0.91	0.30	47,47,47,47	0
57	MG	DA	3011	1/1	0.91	0.08	48,48,48,48	0
57	MG	BA	3210	1/1	0.91	0.33	49,49,49,49	0
57	MG	BA	3126	1/1	0.91	0.16	54,54,54,54	0
57	MG	BA	3650	1/1	0.91	0.12	52,52,52,52	0
57	MG	DA	3494	1/1	0.91	0.12	47,47,47,47	0
57	MG	BA	3400	1/1	0.91	0.21	33,33,33,33	0
57	MG	CA	3055	1/1	0.91	0.09	69,69,69,69	0
57	MG	CA	3160	1/1	0.91	0.17	62,62,62,62	0
57	MG	BA	3227	1/1	0.91	0.24	57,57,57,57	0
57	MG	AA	3028	1/1	0.91	0.22	76,76,76,76	0
57	MG	BA	3631	1/1	0.91	0.18	42,42,42,42	0
57	MG	AA	3063	1/1	0.91	0.10	35,35,35,35	0
57	MG	BA	3405	1/1	0.91	0.19	63,63,63,63	0
57	MG	BA	3269	1/1	0.91	0.16	53,53,53,53	0
57	MG	DA	3653	1/1	0.91	0.14	52,52,52,52	0
57	MG	DA	3097	1/1	0.91	0.21	33,33,33,33	0
57	MG	BA	3252	1/1	0.91	0.41	60,60,60,60	0
57	MG	BA	3120	1/1	0.91	0.21	55,55,55,55	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	BA	3683	1/1	0.91	0.15	73,73,73,73	0
57	MG	CA	3011	1/1	0.91	0.23	61,61,61,61	0
57	MG	CA	3111	1/1	0.91	0.16	64,64,64,64	0
57	MG	BA	3433	1/1	0.91	0.20	32,32,32,32	0
57	MG	CA	3144	1/1	0.91	0.19	71,71,71,71	0
57	MG	AA	3021	1/1	0.91	0.14	63,63,63,63	0
57	MG	AA	3003	1/1	0.91	0.30	72,72,72,72	0
57	MG	DA	3538	1/1	0.91	0.11	58,58,58,58	0
57	MG	AA	3162	1/1	0.91	0.07	66,66,66,66	0
57	MG	AA	3030	1/1	0.91	0.18	60,60,60,60	0
57	MG	CA	3091	1/1	0.91	0.12	55,55,55,55	0
57	MG	AX	3003	1/1	0.91	0.13	71,71,71,71	0
57	MG	DA	3116	1/1	0.91	0.48	52,52,52,52	0
57	MG	BA	3413	1/1	0.91	0.13	47,47,47,47	0
57	MG	CA	3150	1/1	0.91	0.21	56,56,56,56	0
57	MG	CA	3007	1/1	0.91	0.13	57,57,57,57	0
57	MG	BA	3164	1/1	0.91	0.21	48,48,48,48	0
57	MG	BA	3255	1/1	0.91	0.15	47,47,47,47	0
57	MG	BX	3003	1/1	0.92	0.17	35,35,35,35	0
57	MG	DA	3050	1/1	0.92	0.17	59,59,59,59	0
57	MG	AA	3119	1/1	0.92	0.12	51,51,51,51	0
57	MG	BA	3290	1/1	0.92	0.28	40,40,40,40	0
57	MG	AA	3061	1/1	0.92	0.34	55,55,55,55	0
57	MG	BA	3385	1/1	0.92	0.16	59,59,59,59	0
57	MG	D3	3001	1/1	0.92	0.20	57,57,57,57	0
57	MG	BA	3767	1/1	0.92	0.12	73,73,73,73	0
57	MG	DA	3398	1/1	0.92	0.14	45,45,45,45	0
57	MG	DA	3083	1/1	0.92	0.18	40,40,40,40	0
57	MG	BA	3779	1/1	0.92	0.29	66,66,66,66	0
57	MG	AA	3097	1/1	0.92	0.34	56,56,56,56	0
57	MG	BA	3407	1/1	0.92	0.15	47,47,47,47	0
57	MG	DA	3586	1/1	0.92	0.16	60,60,60,60	0
57	MG	DA	3137	1/1	0.92	0.23	54,54,54,54	0
57	MG	BA	3388	1/1	0.92	0.19	48,48,48,48	0
57	MG	BX	3001	1/1	0.92	0.82	48,48,48,48	0
57	MG	DA	3135	1/1	0.92	0.12	38,38,38,38	0
57	MG	BA	3412	1/1	0.92	0.23	40,40,40,40	0
57	MG	BA	3043	1/1	0.92	0.15	48,48,48,48	0
57	MG	BA	3734	1/1	0.92	0.16	52,52,52,52	0
57	MG	CA	3074	1/1	0.92	0.23	64,64,64,64	0
57	MG	DA	3668	1/1	0.92	0.39	60,60,60,60	0
57	MG	BA	3477	1/1	0.92	0.18	61,61,61,61	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	DA	3576	1/1	0.92	0.09	53,53,53,53	0
57	MG	BA	3240	1/1	0.92	0.40	47,47,47,47	0
57	MG	BA	3292	1/1	0.92	0.15	48,48,48,48	0
57	MG	B6	102	1/1	0.92	0.11	68,68,68,68	0
57	MG	CA	3059	1/1	0.92	0.25	72,72,72,72	0
57	MG	AA	3171	1/1	0.92	0.10	51,51,51,51	0
57	MG	DA	3128	1/1	0.92	0.15	58,58,58,58	0
57	MG	DA	3219	1/1	0.92	0.17	53,53,53,53	0
57	MG	DA	3100	1/1	0.92	0.16	43,43,43,43	0
57	MG	DA	3001	1/1	0.92	0.17	60,60,60,60	0
57	MG	DV	3003	1/1	0.92	0.10	65,65,65,65	0
57	MG	BA	3100	1/1	0.92	0.17	39,39,39,39	0
57	MG	BA	3310	1/1	0.92	0.24	58,58,58,58	0
57	MG	BA	3207	1/1	0.92	0.24	54,54,54,54	0
57	MG	BA	3651	1/1	0.92	0.19	45,45,45,45	0
57	MG	DA	3423	1/1	0.92	0.12	49,49,49,49	0
57	MG	BA	3671	1/1	0.92	0.16	63,63,63,63	0
57	MG	BA	3812	1/1	0.92	0.28	47,47,47,47	0
57	MG	DA	3263	1/1	0.92	0.13	41,41,41,41	0
57	MG	BA	3346	1/1	0.92	0.10	27,27,27,27	0
57	MG	BA	3271	1/1	0.92	0.17	58,58,58,58	0
57	MG	BA	3554	1/1	0.92	0.13	51,51,51,51	0
57	MG	BA	3628	1/1	0.92	0.25	49,49,49,49	0
57	MG	DA	3543	1/1	0.92	0.08	53,53,53,53	0
57	MG	BA	3136	1/1	0.92	0.14	30,30,30,30	0
57	MG	DA	3456	1/1	0.92	0.07	50,50,50,50	0
57	MG	DA	3473	1/1	0.92	0.12	50,50,50,50	0
57	MG	AA	3109	1/1	0.92	0.14	62,62,62,62	0
57	MG	BA	3717	1/1	0.92	0.16	50,50,50,50	0
57	MG	AX	3008	1/1	0.92	0.19	70,70,70,70	0
57	MG	BF	302	1/1	0.92	0.18	46,46,46,46	0
57	MG	BA	3714	1/1	0.92	0.11	57,57,57,57	0
57	MG	CA	3120	1/1	0.92	0.18	64,64,64,64	0
57	MG	BA	3022	1/1	0.92	0.19	60,60,60,60	0
57	MG	BY	502	1/1	0.92	0.25	40,40,40,40	0
57	MG	AA	3022	1/1	0.92	0.10	71,71,71,71	0
57	MG	AX	3009	1/1	0.92	0.18	64,64,64,64	0
57	MG	BA	3542	1/1	0.92	0.18	45,45,45,45	0
57	MG	DA	3325	1/1	0.92	0.12	35,35,35,35	0
57	MG	BA	3652	1/1	0.92	0.15	67,67,67,67	0
57	MG	AA	3037	1/1	0.92	0.22	55,55,55,55	0
57	MG	BA	3357	1/1	0.92	0.23	25,25,25,25	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	BA	3369	1/1	0.92	0.15	44,44,44,44	0
57	MG	BA	3347	1/1	0.92	0.15	44,44,44,44	0
57	MG	BA	3799	1/1	0.92	0.06	49,49,49,49	0
57	MG	DA	3112	1/1	0.92	0.16	59,59,59,59	0
57	MG	BA	3708	1/1	0.92	0.21	50,50,50,50	0
57	MG	DA	3382	1/1	0.92	0.07	48,48,48,48	0
57	MG	BA	3424	1/1	0.92	0.25	39,39,39,39	0
57	MG	AA	3122	1/1	0.92	0.11	56,56,56,56	0
57	MG	DA	3354	1/1	0.92	0.19	44,44,44,44	0
57	MG	BA	3459	1/1	0.92	0.19	48,48,48,48	0
57	MG	BA	3098	1/1	0.92	0.23	40,40,40,40	0
57	MG	DA	3063	1/1	0.92	0.22	54,54,54,54	0
57	MG	BA	3134	1/1	0.92	0.17	48,48,48,48	0
57	MG	AA	3115	1/1	0.92	0.09	79,79,79,79	0
57	MG	DA	3250	1/1	0.92	0.18	69,69,69,69	0
57	MG	BA	3101	1/1	0.92	0.19	53,53,53,53	0
57	MG	BA	3307	1/1	0.92	0.17	29,29,29,29	0
57	MG	BG	202	1/1	0.92	0.21	41,41,41,41	0
57	MG	DA	3478	1/1	0.92	0.12	59,59,59,59	0
57	MG	BA	3493	1/1	0.92	0.16	58,58,58,58	0
57	MG	DA	3153	1/1	0.92	0.19	47,47,47,47	0
57	MG	BA	3203	1/1	0.92	0.24	40,40,40,40	0
57	MG	CA	3008	1/1	0.92	0.27	51,51,51,51	0
57	MG	BE	307	1/1	0.92	0.15	62,62,62,62	0
57	MG	BA	3016	1/1	0.92	0.13	38,38,38,38	0
57	MG	BA	3017	1/1	0.92	0.25	48,48,48,48	0
57	MG	DA	3173	1/1	0.92	0.12	53,53,53,53	0
57	MG	DA	3047	1/1	0.92	0.15	49,49,49,49	0
57	MG	BA	3151	1/1	0.92	0.26	52,52,52,52	0
57	MG	BA	3051	1/1	0.92	0.19	43,43,43,43	0
57	MG	DA	3079	1/1	0.92	0.17	55,55,55,55	0
57	MG	DA	3409	1/1	0.92	0.15	57,57,57,57	0
57	MG	BA	3675	1/1	0.92	0.19	67,67,67,67	0
57	MG	AA	3161	1/1	0.92	0.23	65,65,65,65	0
57	MG	DA	3505	1/1	0.92	0.08	56,56,56,56	0
57	MG	DD	304	1/1	0.92	0.38	52,52,52,52	0
57	MG	DA	3164	1/1	0.92	0.12	51,51,51,51	0
57	MG	AA	3163	1/1	0.92	0.18	56,56,56,56	0
57	MG	BA	3239	1/1	0.92	0.34	48,48,48,48	0
57	MG	BA	3182	1/1	0.92	0.14	55,55,55,55	0
57	MG	DA	3391	1/1	0.92	0.09	45,45,45,45	0
57	MG	BA	3127	1/1	0.92	0.29	57,57,57,57	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	DA	3091	1/1	0.92	0.10	48,48,48,48	0
57	MG	DA	3503	1/1	0.92	0.14	52,52,52,52	0
57	MG	BA	3099	1/1	0.92	0.22	41,41,41,41	0
57	MG	DA	3392	1/1	0.92	0.19	70,70,70,70	0
57	MG	DA	3595	1/1	0.92	0.17	59,59,59,59	0
57	MG	AA	3202	1/1	0.92	0.14	57,57,57,57	0
57	MG	DA	3267	1/1	0.92	0.16	49,49,49,49	0
57	MG	BA	3535	1/1	0.92	0.19	31,31,31,31	0
57	MG	CA	3135	1/1	0.92	0.15	63,63,63,63	0
57	MG	DA	3273	1/1	0.92	0.11	47,47,47,47	0
57	MG	BA	3138	1/1	0.92	0.34	42,42,42,42	0
57	MG	DA	3327	1/1	0.92	0.12	57,57,57,57	0
57	MG	DA	3194	1/1	0.92	0.10	56,56,56,56	0
57	MG	DA	3162	1/1	0.92	0.36	50,50,50,50	0
57	MG	BA	3145	1/1	0.92	0.10	44,44,44,44	0
57	MG	BA	3662	1/1	0.92	0.10	61,61,61,61	0
57	MG	BA	3387	1/1	0.92	0.15	54,54,54,54	0
57	MG	AA	3191	1/1	0.92	0.21	47,47,47,47	0
57	MG	DA	3251	1/1	0.92	0.17	62,62,62,62	0
57	MG	BA	3403	1/1	0.92	0.08	54,54,54,54	0
57	MG	B0	102	1/1	0.92	0.22	48,48,48,48	0
57	MG	DA	3637	1/1	0.92	0.59	58,58,58,58	0
57	MG	BA	3322	1/1	0.92	0.17	52,52,52,52	0
57	MG	CA	3095	1/1	0.92	0.14	64,64,64,64	0
57	MG	CA	3112	1/1	0.92	0.15	69,69,69,69	0
57	MG	AA	3201	1/1	0.92	0.13	52,52,52,52	0
57	MG	AY	3003	1/1	0.92	0.30	53,53,53,53	0
57	MG	BA	3797	1/1	0.92	0.17	53,53,53,53	0
57	MG	DA	3048	1/1	0.92	0.06	53,53,53,53	0
57	MG	BB	219	1/1	0.92	0.11	67,67,67,67	0
57	MG	CA	3014	1/1	0.92	0.21	58,58,58,58	0
57	MG	BA	3722	1/1	0.92	0.19	47,47,47,47	0
57	MG	AA	3070	1/1	0.92	0.18	52,52,52,52	0
57	MG	BA	3515	1/1	0.92	0.12	53,53,53,53	0
57	MG	BA	3455	1/1	0.92	0.16	64,64,64,64	0
57	MG	DA	3227	1/1	0.93	0.28	41,41,41,41	0
57	MG	BA	3173	1/1	0.93	0.15	48,48,48,48	0
57	MG	BE	308	1/1	0.93	0.17	40,40,40,40	0
57	MG	AA	3101	1/1	0.93	0.16	43,43,43,43	0
57	MG	BA	3320	1/1	0.93	0.22	48,48,48,48	0
57	MG	CA	3102	1/1	0.93	0.08	68,68,68,68	0
57	MG	AA	3027	1/1	0.93	0.15	50,50,50,50	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	BB	201	1/1	0.93	0.17	55,55,55,55	0
57	MG	DW	3003	1/1	0.93	0.09	72,72,72,72	0
57	MG	BA	3014	1/1	0.93	0.29	42,42,42,42	0
57	MG	AA	3130	1/1	0.93	0.08	56,56,56,56	0
57	MG	BA	3713	1/1	0.93	0.18	33,33,33,33	0
57	MG	BA	3118	1/1	0.93	0.17	48,48,48,48	0
57	MG	BA	3706	1/1	0.93	0.11	53,53,53,53	0
57	MG	BA	3021	1/1	0.93	0.19	49,49,49,49	0
57	MG	DA	3536	1/1	0.93	0.11	48,48,48,48	0
57	MG	DA	3009	1/1	0.93	0.15	48,48,48,48	0
57	MG	CA	3170	1/1	0.93	0.18	58,58,58,58	0
57	MG	BA	3291	1/1	0.93	0.21	33,33,33,33	0
57	MG	DA	3652	1/1	0.93	0.39	67,67,67,67	0
57	MG	BA	3119	1/1	0.93	0.13	45,45,45,45	0
57	MG	BA	3580	1/1	0.93	0.13	55,55,55,55	0
57	MG	BA	3078	1/1	0.93	0.24	51,51,51,51	0
57	MG	DA	3013	1/1	0.93	0.09	40,40,40,40	0
57	MG	BA	3537	1/1	0.93	0.16	45,45,45,45	0
57	MG	DA	3074	1/1	0.93	0.13	37,37,37,37	0
57	MG	DA	3246	1/1	0.93	0.14	43,43,43,43	0
57	MG	CA	3142	1/1	0.93	0.13	69,69,69,69	0
57	MG	CA	3086	1/1	0.93	0.13	64,64,64,64	0
57	MG	DA	3482	1/1	0.93	0.10	50,50,50,50	0
57	MG	BA	3149	1/1	0.93	0.18	40,40,40,40	0
57	MG	AA	3060	1/1	0.93	0.27	46,46,46,46	0
57	MG	AA	3012	1/1	0.93	0.16	46,46,46,46	0
57	MG	DA	3540	1/1	0.93	0.17	42,42,42,42	0
57	MG	AA	3155	1/1	0.93	0.24	48,48,48,48	0
57	MG	DA	3545	1/1	0.93	0.13	35,35,35,35	0
57	MG	AA	3141	1/1	0.93	0.23	61,61,61,61	0
57	MG	BA	3302	1/1	0.93	0.12	69,69,69,69	0
57	MG	AA	3095	1/1	0.93	0.29	60,60,60,60	0
57	MG	AA	3178	1/1	0.93	0.15	59,59,59,59	0
57	MG	DA	3358	1/1	0.93	0.14	45,45,45,45	0
57	MG	DA	3211	1/1	0.93	0.14	48,48,48,48	0
57	MG	AA	3136	1/1	0.93	0.10	70,70,70,70	0
57	MG	BP	202	1/1	0.93	0.21	36,36,36,36	0
57	MG	DV	3001	1/1	0.93	0.23	70,70,70,70	0
57	MG	BA	3075	1/1	0.93	0.24	45,45,45,45	0
57	MG	DA	3551	1/1	0.93	0.08	55,55,55,55	0
57	MG	BA	3800	1/1	0.93	0.23	38,38,38,38	0
57	MG	AA	3193	1/1	0.93	0.08	72,72,72,72	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	DA	3163	1/1	0.93	0.15	49,49,49,49	0
57	MG	BA	3161	1/1	0.93	0.17	52,52,52,52	0
57	MG	BA	3464	1/1	0.93	0.14	45,45,45,45	0
57	MG	DA	3064	1/1	0.93	0.20	49,49,49,49	0
57	MG	BA	3604	1/1	0.93	0.15	36,36,36,36	0
57	MG	DA	3549	1/1	0.93	0.10	57,57,57,57	0
57	MG	DA	3029	1/1	0.93	0.35	49,49,49,49	0
57	MG	BA	3639	1/1	0.93	0.46	48,48,48,48	0
57	MG	DA	3045	1/1	0.93	0.29	51,51,51,51	0
57	MG	BA	3576	1/1	0.93	0.07	57,57,57,57	0
57	MG	BU	202	1/1	0.93	0.29	40,40,40,40	0
57	MG	BA	3505	1/1	0.93	0.12	55,55,55,55	0
57	MG	AE	201	1/1	0.93	0.15	59,59,59,59	0
57	MG	DA	3578	1/1	0.93	0.18	59,59,59,59	0
57	MG	DA	3149	1/1	0.93	0.06	56,56,56,56	0
57	MG	BA	3201	1/1	0.93	0.20	62,62,62,62	0
57	MG	DA	3397	1/1	0.93	0.09	57,57,57,57	0
57	MG	CA	3060	1/1	0.93	0.08	65,65,65,65	0
57	MG	AA	3181	1/1	0.93	0.16	51,51,51,51	0
57	MG	DA	3514	1/1	0.93	0.13	42,42,42,42	0
57	MG	BA	3328	1/1	0.93	0.27	40,40,40,40	0
57	MG	BA	3250	1/1	0.93	0.68	42,42,42,42	0
57	MG	DA	3670	1/1	0.93	0.42	60,60,60,60	0
57	MG	BA	3533	1/1	0.93	0.10	59,59,59,59	0
57	MG	DA	3351	1/1	0.93	0.12	48,48,48,48	0
57	MG	DA	3650	1/1	0.93	0.12	67,67,67,67	0
57	MG	BA	3690	1/1	0.93	0.18	58,58,58,58	0
57	MG	DA	3006	1/1	0.93	0.10	38,38,38,38	0
57	MG	BA	3277	1/1	0.93	0.65	47,47,47,47	0
57	MG	DA	3291	1/1	0.93	0.20	44,44,44,44	0
57	MG	BV	204	1/1	0.93	0.21	49,49,49,49	0
57	MG	DA	3131	1/1	0.93	0.21	46,46,46,46	0
57	MG	BA	3055	1/1	0.93	0.21	45,45,45,45	0
57	MG	DA	3041	1/1	0.93	0.09	38,38,38,38	0
57	MG	AA	3007	1/1	0.93	0.13	57,57,57,57	0
57	MG	BA	3295	1/1	0.93	0.19	38,38,38,38	0
57	MG	DA	3381	1/1	0.93	0.17	56,56,56,56	0
57	MG	DA	3065	1/1	0.93	0.18	43,43,43,43	0
57	MG	DA	3432	1/1	0.93	0.12	37,37,37,37	0
57	MG	BA	3642	1/1	0.93	0.12	48,48,48,48	0
57	MG	BA	3406	1/1	0.93	0.10	50,50,50,50	0
57	MG	DA	3672	1/1	0.93	0.16	71,71,71,71	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	AA	3055	1/1	0.93	0.21	57,57,57,57	0
57	MG	DA	3426	1/1	0.93	0.22	49,49,49,49	0
57	MG	CA	3117	1/1	0.93	0.10	71,71,71,71	0
57	MG	AA	3029	1/1	0.93	0.22	53,53,53,53	0
57	MG	DA	3617	1/1	0.93	0.07	56,56,56,56	0
57	MG	BA	3519	1/1	0.93	0.08	55,55,55,55	0
57	MG	BA	3228	1/1	0.93	0.25	59,59,59,59	0
57	MG	AA	3149	1/1	0.93	0.10	46,46,46,46	0
57	MG	AA	3076	1/1	0.93	0.26	77,77,77,77	0
57	MG	AA	3088	1/1	0.93	0.27	65,65,65,65	0
57	MG	BA	3646	1/1	0.93	0.17	42,42,42,42	0
57	MG	BA	3807	1/1	0.93	0.17	47,47,47,47	0
57	MG	BN	3006	1/1	0.93	0.20	49,49,49,49	0
57	MG	CA	3165	1/1	0.93	0.11	45,45,45,45	0
57	MG	DA	3017	1/1	0.93	0.06	55,55,55,55	0
57	MG	DB	3005	1/1	0.93	0.08	59,59,59,59	0
57	MG	BA	3079	1/1	0.93	0.19	39,39,39,39	0
57	MG	DA	3108	1/1	0.93	0.07	52,52,52,52	0
57	MG	BA	3355	1/1	0.93	0.17	61,61,61,61	0
57	MG	AA	3085	1/1	0.93	0.18	48,48,48,48	0
57	MG	BA	3585	1/1	0.93	0.09	46,46,46,46	0
57	MG	AA	3071	1/1	0.93	0.22	53,53,53,53	0
57	MG	AA	3067	1/1	0.93	0.26	57,57,57,57	0
57	MG	BA	3765	1/1	0.93	0.22	48,48,48,48	0
57	MG	DA	3127	1/1	0.93	0.15	35,35,35,35	0
57	MG	BA	3200	1/1	0.93	0.15	67,67,67,67	0
57	MG	BA	3341	1/1	0.93	0.12	51,51,51,51	0
57	MG	DA	3438	1/1	0.93	0.20	47,47,47,47	0
57	MG	CA	3164	1/1	0.93	0.16	60,60,60,60	0
57	MG	BA	3282	1/1	0.93	0.16	39,39,39,39	0
57	MG	DA	3255	1/1	0.93	0.09	51,51,51,51	0
57	MG	CA	3078	1/1	0.93	0.14	44,44,44,44	0
57	MG	BA	3190	1/1	0.93	0.20	52,52,52,52	0
57	MG	AA	3096	1/1	0.93	0.22	63,63,63,63	0
57	MG	BA	3773	1/1	0.93	0.25	52,52,52,52	0
57	MG	DA	3625	1/1	0.93	0.07	69,69,69,69	0
57	MG	BA	3035	1/1	0.93	0.26	39,39,39,39	0
57	MG	DA	3447	1/1	0.93	0.15	58,58,58,58	0
57	MG	BA	3688	1/1	0.93	0.16	46,46,46,46	0
57	MG	DA	3675	1/1	0.93	0.13	52,52,52,52	0
57	MG	DA	3201	1/1	0.93	0.14	61,61,61,61	0
57	MG	DA	3284	1/1	0.93	0.12	47,47,47,47	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	DA	3517	1/1	0.93	0.05	51,51,51,51	0
57	MG	BA	3261	1/1	0.93	0.11	61,61,61,61	0
57	MG	DA	3631	1/1	0.93	0.12	57,57,57,57	0
57	MG	BA	3524	1/1	0.93	0.13	42,42,42,42	0
57	MG	BA	3223	1/1	0.93	0.13	41,41,41,41	0
57	MG	BA	3077	1/1	0.93	0.17	49,49,49,49	0
57	MG	DA	3237	1/1	0.93	0.14	56,56,56,56	0
57	MG	B7	102	1/1	0.93	0.16	47,47,47,47	0
57	MG	DA	3036	1/1	0.93	0.14	48,48,48,48	0
57	MG	B9	502	1/1	0.93	0.19	48,48,48,48	0
57	MG	BA	3186	1/1	0.93	0.45	45,45,45,45	0
57	MG	DA	3121	1/1	0.93	0.07	44,44,44,44	0
57	MG	AA	3078	1/1	0.93	0.27	66,66,66,66	0
57	MG	CA	3040	1/1	0.93	0.11	51,51,51,51	0
57	MG	AA	3140	1/1	0.93	0.15	53,53,53,53	0
57	MG	BA	3768	1/1	0.93	0.12	47,47,47,47	0
57	MG	BA	3656	1/1	0.93	0.27	53,53,53,53	0
57	MG	DA	3627	1/1	0.93	0.17	63,63,63,63	0
57	MG	BA	3555	1/1	0.93	0.14	29,29,29,29	0
57	MG	AN	503	1/1	0.93	0.15	54,54,54,54	0
57	MG	BA	3457	1/1	0.93	0.19	32,32,32,32	0
57	MG	AA	3056	1/1	0.93	0.13	61,61,61,61	0
57	MG	BA	3319	1/1	0.93	0.19	46,46,46,46	0
57	MG	BA	3595	1/1	0.93	0.09	51,51,51,51	0
57	MG	CA	3082	1/1	0.93	0.15	79,79,79,79	0
57	MG	BA	3265	1/1	0.93	0.21	54,54,54,54	0
57	MG	BA	3758	1/1	0.93	0.11	45,45,45,45	0
57	MG	CA	3114	1/1	0.93	0.04	57,57,57,57	0
57	MG	BA	3531	1/1	0.93	0.21	26,26,26,26	0
57	MG	DA	3152	1/1	0.93	0.20	51,51,51,51	0
57	MG	BA	3439	1/1	0.93	0.13	33,33,33,33	0
57	MG	DA	3557	1/1	0.93	0.15	51,51,51,51	0
57	MG	DA	3107	1/1	0.93	0.13	51,51,51,51	0
57	MG	AA	3152	1/1	0.93	0.10	62,62,62,62	0
57	MG	DA	3032	1/1	0.93	0.15	48,48,48,48	0
57	MG	DA	3396	1/1	0.93	0.10	40,40,40,40	0
57	MG	AE	203	1/1	0.93	0.18	63,63,63,63	0
57	MG	DA	3612	1/1	0.94	0.09	62,62,62,62	0
57	MG	CA	3145	1/1	0.94	0.14	66,66,66,66	0
57	MG	CA	3083	1/1	0.94	0.10	79,79,79,79	0
57	MG	BA	3520	1/1	0.94	0.16	61,61,61,61	0
57	MG	BA	3504	1/1	0.94	0.13	56,56,56,56	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	BA	3096	1/1	0.94	0.23	54,54,54,54	0
57	MG	BA	3511	1/1	0.94	0.14	30,30,30,30	0
57	MG	BA	3738	1/1	0.94	0.15	43,43,43,43	0
57	MG	BA	3220	1/1	0.94	0.22	29,29,29,29	0
57	MG	BE	303	1/1	0.94	0.20	51,51,51,51	0
57	MG	BA	3183	1/1	0.94	0.18	42,42,42,42	0
57	MG	BA	3329	1/1	0.94	0.19	60,60,60,60	0
57	MG	BA	3655	1/1	0.94	0.14	50,50,50,50	0
57	MG	DA	3067	1/1	0.94	0.26	57,57,57,57	0
57	MG	BA	3065	1/1	0.94	0.19	60,60,60,60	0
57	MG	DA	3533	1/1	0.94	0.11	43,43,43,43	0
57	MG	DA	3114	1/1	0.94	0.15	55,55,55,55	0
57	MG	BA	3785	1/1	0.94	0.23	59,59,59,59	0
57	MG	DA	3104	1/1	0.94	0.29	53,53,53,53	0
57	MG	BA	3805	1/1	0.94	0.12	44,44,44,44	0
57	MG	BA	3064	1/1	0.94	0.13	43,43,43,43	0
57	MG	AY	3002	1/1	0.94	0.24	56,56,56,56	0
57	MG	BA	3536	1/1	0.94	0.27	49,49,49,49	0
57	MG	BA	3155	1/1	0.94	0.27	44,44,44,44	0
57	MG	BA	3009	1/1	0.94	0.17	28,28,28,28	0
57	MG	CA	3037	1/1	0.94	0.14	73,73,73,73	0
57	MG	DA	3249	1/1	0.94	0.14	45,45,45,45	0
57	MG	DA	3331	1/1	0.94	0.17	37,37,37,37	0
57	MG	BA	3543	1/1	0.94	0.23	37,37,37,37	0
57	MG	AA	3104	1/1	0.94	0.28	59,59,59,59	0
57	MG	BA	3633	1/1	0.94	0.12	49,49,49,49	0
57	MG	BA	3747	1/1	0.94	0.20	52,52,52,52	0
57	MG	CA	3079	1/1	0.94	0.21	66,66,66,66	0
57	MG	BA	3448	1/1	0.94	0.24	32,32,32,32	0
57	MG	BA	3236	1/1	0.94	0.20	49,49,49,49	0
57	MG	DA	3024	1/1	0.94	0.21	59,59,59,59	0
57	MG	AA	3111	1/1	0.94	0.09	79,79,79,79	0
57	MG	CA	3025	1/1	0.94	0.14	51,51,51,51	0
57	MG	CA	3094	1/1	0.94	0.11	70,70,70,70	0
57	MG	AW	3003	1/1	0.94	0.13	72,72,72,72	0
57	MG	BA	3170	1/1	0.94	0.16	38,38,38,38	0
57	MG	DA	3516	1/1	0.94	0.07	67,67,67,67	0
57	MG	DA	3154	1/1	0.94	0.17	48,48,48,48	0
57	MG	DA	3054	1/1	0.94	0.23	48,48,48,48	0
57	MG	BA	3809	1/1	0.94	0.13	63,63,63,63	0
57	MG	CA	3126	1/1	0.94	0.11	67,67,67,67	0
57	MG	DA	3336	1/1	0.94	0.19	40,40,40,40	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	CA	3010	1/1	0.94	0.17	56,56,56,56	0
57	MG	AA	3083	1/1	0.94	0.31	57,57,57,57	0
57	MG	BA	3306	1/1	0.94	0.17	37,37,37,37	0
57	MG	DA	3324	1/1	0.94	0.11	33,33,33,33	0
57	MG	BA	3663	1/1	0.94	0.19	41,41,41,41	0
57	MG	CA	3068	1/1	0.94	0.15	48,48,48,48	0
57	MG	BA	3243	1/1	0.94	0.17	53,53,53,53	0
57	MG	BA	3649	1/1	0.94	0.11	40,40,40,40	0
57	MG	DA	3434	1/1	0.94	0.11	39,39,39,39	0
57	MG	BA	3389	1/1	0.94	0.13	55,55,55,55	0
57	MG	BA	3157	1/1	0.94	0.24	45,45,45,45	0
57	MG	DA	3230	1/1	0.94	0.22	73,73,73,73	0
57	MG	DA	3656	1/1	0.94	0.13	58,58,58,58	0
57	MG	DA	3260	1/1	0.94	0.09	55,55,55,55	0
57	MG	DA	3623	1/1	0.94	0.09	66,66,66,66	0
57	MG	DA	3511	1/1	0.94	0.16	49,49,49,49	0
57	MG	BA	3365	1/1	0.94	0.13	62,62,62,62	0
57	MG	AA	3132	1/1	0.94	0.19	55,55,55,55	0
57	MG	DA	3411	1/1	0.94	0.22	53,53,53,53	0
57	MG	AA	3175	1/1	0.94	0.18	63,63,63,63	0
57	MG	BA	3523	1/1	0.94	0.11	48,48,48,48	0
57	MG	DA	3573	1/1	0.94	0.12	43,43,43,43	0
57	MG	DA	3660	1/1	0.94	0.09	61,61,61,61	0
57	MG	AA	3009	1/1	0.94	0.18	57,57,57,57	0
57	MG	BA	3217	1/1	0.94	0.16	37,37,37,37	0
57	MG	DA	3202	1/1	0.94	0.11	57,57,57,57	0
57	MG	AA	3016	1/1	0.94	0.09	63,63,63,63	0
57	MG	BA	3610	1/1	0.94	0.09	61,61,61,61	0
57	MG	AA	3075	1/1	0.94	0.11	49,49,49,49	0
57	MG	BA	3279	1/1	0.94	0.24	43,43,43,43	0
57	MG	AA	3014	1/1	0.94	0.21	32,32,32,32	0
57	MG	DA	3264	1/1	0.94	0.13	40,40,40,40	0
57	MG	DA	3254	1/1	0.94	0.07	52,52,52,52	0
57	MG	BA	3219	1/1	0.94	0.17	36,36,36,36	0
57	MG	BA	3522	1/1	0.94	0.09	52,52,52,52	0
57	MG	BA	3176	1/1	0.94	0.17	45,45,45,45	0
57	MG	BA	3323	1/1	0.94	0.20	30,30,30,30	0
57	MG	DA	3624	1/1	0.94	0.19	56,56,56,56	0
57	MG	BU	205	1/1	0.94	0.24	47,47,47,47	0
57	MG	BA	3340	1/1	0.94	0.14	39,39,39,39	0
57	MG	DD	306	1/1	0.94	0.28	39,39,39,39	0
57	MG	AA	3032	1/1	0.94	0.19	67,67,67,67	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	CA	3108	1/1	0.94	0.31	68,68,68,68	0
57	MG	DA	3235	1/1	0.94	0.20	45,45,45,45	0
57	MG	DA	3587	1/1	0.94	0.12	56,56,56,56	0
57	MG	BA	3509	1/1	0.94	0.21	31,31,31,31	0
57	MG	BA	3415	1/1	0.94	0.16	28,28,28,28	0
57	MG	DD	302	1/1	0.94	0.15	42,42,42,42	0
57	MG	BA	3054	1/1	0.94	0.28	36,36,36,36	0
57	MG	DA	3053	1/1	0.94	0.10	47,47,47,47	0
57	MG	AA	3159	1/1	0.94	0.12	66,66,66,66	0
57	MG	DA	3043	1/1	0.94	0.15	38,38,38,38	0
57	MG	DA	3490	1/1	0.94	0.13	47,47,47,47	0
57	MG	BA	3084	1/1	0.94	0.22	38,38,38,38	0
57	MG	BA	3268	1/1	0.94	0.22	55,55,55,55	0
60	K	AX	3001	1/1	0.94	0.12	65,65,65,65	0
57	MG	AA	3068	1/1	0.94	0.14	69,69,69,69	0
57	MG	BA	3743	1/1	0.94	0.17	44,44,44,44	0
57	MG	CA	3161	1/1	0.94	0.09	56,56,56,56	0
57	MG	DA	3039	1/1	0.94	0.10	43,43,43,43	0
57	MG	BA	3350	1/1	0.94	0.20	28,28,28,28	0
57	MG	DA	3203	1/1	0.94	0.57	50,50,50,50	0
57	MG	BA	3166	1/1	0.94	0.14	38,38,38,38	0
57	MG	BA	3377	1/1	0.94	0.14	44,44,44,44	0
57	MG	DA	3172	1/1	0.94	0.09	62,62,62,62	0
57	MG	DA	3158	1/1	0.94	0.16	60,60,60,60	0
57	MG	DA	3300	1/1	0.94	0.20	45,45,45,45	0
57	MG	BA	3685	1/1	0.94	0.19	53,53,53,53	0
57	MG	CA	3030	1/1	0.94	0.22	57,57,57,57	0
57	MG	CA	3096	1/1	0.94	0.10	44,44,44,44	0
57	MG	BA	3672	1/1	0.94	0.20	43,43,43,43	0
57	MG	DQ	3003	1/1	0.94	0.15	51,51,51,51	0
57	MG	BA	3682	1/1	0.94	0.19	53,53,53,53	0
57	MG	DB	3009	1/1	0.94	0.18	59,59,59,59	0
57	MG	DA	3594	1/1	0.94	0.31	54,54,54,54	0
57	MG	BA	3452	1/1	0.94	0.16	55,55,55,55	0
57	MG	BA	3777	1/1	0.94	0.17	40,40,40,40	0
57	MG	DA	3302	1/1	0.94	0.28	70,70,70,70	0
57	MG	BA	3063	1/1	0.94	0.15	59,59,59,59	0
57	MG	CA	3053	1/1	0.94	0.15	41,41,41,41	0
57	MG	BA	3436	1/1	0.94	0.14	40,40,40,40	0
57	MG	BA	3294	1/1	0.94	0.23	61,61,61,61	0
57	MG	BA	3417	1/1	0.94	0.24	38,38,38,38	0
57	MG	DA	3229	1/1	0.94	0.22	50,50,50,50	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	AA	3052	1/1	0.94	0.29	65,65,65,65	0
57	MG	CA	3139	1/1	0.94	0.14	62,62,62,62	0
57	MG	DA	3238	1/1	0.94	0.27	44,44,44,44	0
57	MG	BU	208	1/1	0.94	0.21	40,40,40,40	0
57	MG	DA	3232	1/1	0.94	0.13	62,62,62,62	0
57	MG	DA	3102	1/1	0.94	0.19	40,40,40,40	0
57	MG	BA	3748	1/1	0.94	0.15	29,29,29,29	0
57	MG	BA	3204	1/1	0.94	0.23	36,36,36,36	0
57	MG	CA	3077	1/1	0.94	0.08	66,66,66,66	0
57	MG	AA	3199	1/1	0.94	0.15	73,73,73,73	0
57	MG	AA	3123	1/1	0.94	0.26	51,51,51,51	0
57	MG	AA	3098	1/1	0.94	0.18	55,55,55,55	0
57	MG	BA	3739	1/1	0.94	0.22	40,40,40,40	0
57	MG	BA	3189	1/1	0.94	0.19	39,39,39,39	0
57	MG	BA	3344	1/1	0.94	0.12	66,66,66,66	0
57	MG	BA	3237	1/1	0.94	0.15	45,45,45,45	0
57	MG	CA	3110	1/1	0.94	0.09	65,65,65,65	0
57	MG	DA	3479	1/1	0.94	0.17	43,43,43,43	0
57	MG	CA	3125	1/1	0.94	0.08	63,63,63,63	0
57	MG	BA	3564	1/1	0.94	0.16	44,44,44,44	0
57	MG	CA	3035	1/1	0.94	0.09	59,59,59,59	0
57	MG	DA	3379	1/1	0.94	0.14	63,63,63,63	0
57	MG	DA	3188	1/1	0.94	0.19	48,48,48,48	0
57	MG	AA	3174	1/1	0.94	0.10	50,50,50,50	0
57	MG	BA	3352	1/1	0.94	0.22	53,53,53,53	0
57	MG	BR	201	1/1	0.94	0.26	57,57,57,57	0
57	MG	DA	3662	1/1	0.94	0.13	62,62,62,62	0
57	MG	AX	3004	1/1	0.94	0.15	64,64,64,64	0
57	MG	BA	3376	1/1	0.94	0.16	48,48,48,48	0
57	MG	DA	3179	1/1	0.94	0.12	52,52,52,52	0
57	MG	DA	3584	1/1	0.94	0.18	53,53,53,53	0
57	MG	CA	3119	1/1	0.94	0.16	64,64,64,64	0
57	MG	BQ	3003	1/1	0.94	0.27	49,49,49,49	0
57	MG	DA	3458	1/1	0.94	0.05	52,52,52,52	0
57	MG	DA	3427	1/1	0.94	0.14	45,45,45,45	0
57	MG	CA	3122	1/1	0.94	0.21	64,64,64,64	0
57	MG	DA	3634	1/1	0.94	0.14	60,60,60,60	0
57	MG	DB	3013	1/1	0.94	0.17	64,64,64,64	0
57	MG	BA	3196	1/1	0.94	0.25	38,38,38,38	0
57	MG	DA	3200	1/1	0.94	0.09	66,66,66,66	0
57	MG	DA	3472	1/1	0.94	0.16	44,44,44,44	0
57	MG	BA	3801	1/1	0.94	0.31	50,50,50,50	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	DA	3428	1/1	0.94	0.18	37,37,37,37	0
57	MG	DA	3419	1/1	0.94	0.11	32,32,32,32	0
57	MG	BA	3559	1/1	0.94	0.08	47,47,47,47	0
57	MG	DA	3368	1/1	0.94	0.24	50,50,50,50	0
57	MG	CF	3001	1/1	0.94	0.12	46,46,46,46	0
57	MG	DA	3655	1/1	0.94	0.11	64,64,64,64	0
57	MG	BA	3770	1/1	0.94	0.16	45,45,45,45	0
57	MG	DA	3195	1/1	0.94	0.09	43,43,43,43	0
57	MG	AA	3172	1/1	0.94	0.10	72,72,72,72	0
57	MG	BA	3516	1/1	0.94	0.19	52,52,52,52	0
57	MG	BA	3289	1/1	0.94	0.21	56,56,56,56	0
57	MG	BA	3803	1/1	0.94	0.23	44,44,44,44	0
57	MG	DA	3037	1/1	0.94	0.16	43,43,43,43	0
57	MG	DA	3210	1/1	0.94	0.17	53,53,53,53	0
57	MG	DA	3486	1/1	0.95	0.09	47,47,47,47	0
57	MG	DA	3196	1/1	0.95	0.22	49,49,49,49	0
57	MG	BA	3246	1/1	0.95	0.35	39,39,39,39	0
57	MG	DA	3507	1/1	0.95	0.14	43,43,43,43	0
57	MG	BA	3600	1/1	0.95	0.31	44,44,44,44	0
57	MG	AA	3050	1/1	0.95	0.15	33,33,33,33	0
57	MG	DA	3372	1/1	0.95	0.08	56,56,56,56	0
57	MG	DA	3287	1/1	0.95	0.10	41,41,41,41	0
57	MG	BQ	3001	1/1	0.95	0.22	45,45,45,45	0
57	MG	DA	3303	1/1	0.95	0.09	48,48,48,48	0
57	MG	DA	3113	1/1	0.95	0.19	60,60,60,60	0
57	MG	AA	3213	1/1	0.95	0.23	54,54,54,54	0
57	MG	AA	3116	1/1	0.95	0.11	55,55,55,55	0
57	MG	BA	3440	1/1	0.95	0.12	42,42,42,42	0
57	MG	DA	3073	1/1	0.95	0.09	42,42,42,42	0
57	MG	DA	3015	1/1	0.95	0.20	52,52,52,52	0
57	MG	AW	3002	1/1	0.95	0.22	53,53,53,53	0
57	MG	DA	3477	1/1	0.95	0.09	43,43,43,43	0
57	MG	CK	3001	1/1	0.95	0.17	45,45,45,45	0
57	MG	DA	3087	1/1	0.95	0.18	58,58,58,58	0
57	MG	BA	3015	1/1	0.95	0.16	32,32,32,32	0
57	MG	BA	3496	1/1	0.95	0.17	41,41,41,41	0
57	MG	DA	3389	1/1	0.95	0.14	46,46,46,46	0
57	MG	DA	3167	1/1	0.95	0.13	41,41,41,41	0
57	MG	CA	3063	1/1	0.95	0.23	58,58,58,58	0
57	MG	DA	3488	1/1	0.95	0.07	41,41,41,41	0
57	MG	DA	3290	1/1	0.95	0.15	59,59,59,59	0
57	MG	BA	3723	1/1	0.95	0.07	47,47,47,47	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	BA	3539	1/1	0.95	0.20	52,52,52,52	0
57	MG	DA	3377	1/1	0.95	0.10	38,38,38,38	0
57	MG	BA	3087	1/1	0.95	0.24	42,42,42,42	0
57	MG	BD	301	1/1	0.95	0.23	40,40,40,40	0
57	MG	BA	3171	1/1	0.95	0.25	31,31,31,31	0
57	MG	DA	3439	1/1	0.95	0.23	42,42,42,42	0
57	MG	CA	3106	1/1	0.95	0.07	56,56,56,56	0
57	MG	BA	3026	1/1	0.95	0.15	41,41,41,41	0
57	MG	DA	3467	1/1	0.95	0.25	40,40,40,40	0
57	MG	BA	3194	1/1	0.95	0.18	47,47,47,47	0
57	MG	BA	3062	1/1	0.95	0.27	42,42,42,42	0
57	MG	DO	5001	1/1	0.95	0.13	59,59,59,59	0
57	MG	AX	3015	1/1	0.95	0.21	42,42,42,42	0
57	MG	DA	3598	1/1	0.95	0.08	61,61,61,61	0
57	MG	BA	3081	1/1	0.95	0.21	46,46,46,46	0
57	MG	DA	3226	1/1	0.95	0.38	45,45,45,45	0
57	MG	DA	3318	1/1	0.95	0.14	40,40,40,40	0
57	MG	DA	3600	1/1	0.95	0.35	70,70,70,70	0
57	MG	CA	3080	1/1	0.95	0.09	49,49,49,49	0
57	MG	BA	3798	1/1	0.95	0.20	28,28,28,28	0
57	MG	CA	3113	1/1	0.95	0.11	67,67,67,67	0
57	MG	DA	3475	1/1	0.95	0.16	51,51,51,51	0
57	MG	DA	3030	1/1	0.95	0.14	39,39,39,39	0
57	MG	CA	3136	1/1	0.95	0.14	72,72,72,72	0
57	MG	AA	3039	1/1	0.95	0.15	56,56,56,56	0
57	MG	DA	3023	1/1	0.95	0.30	40,40,40,40	0
57	MG	CA	3032	1/1	0.95	0.24	62,62,62,62	0
57	MG	DA	3501	1/1	0.95	0.15	37,37,37,37	0
57	MG	BA	3027	1/1	0.95	0.11	26,26,26,26	0
57	MG	AA	3150	1/1	0.95	0.20	57,57,57,57	0
57	MG	BA	3354	1/1	0.95	0.10	48,48,48,48	0
57	MG	BA	3552	1/1	0.95	0.26	29,29,29,29	0
57	MG	BD	304	1/1	0.95	0.22	32,32,32,32	0
57	MG	BA	3712	1/1	0.95	0.18	53,53,53,53	0
57	MG	BA	3325	1/1	0.95	0.15	48,48,48,48	0
57	MG	DA	3583	1/1	0.95	0.15	51,51,51,51	0
57	MG	BA	3667	1/1	0.95	0.15	61,61,61,61	0
57	MG	AA	3195	1/1	0.95	0.12	57,57,57,57	0
57	MG	B3	3001	1/1	0.95	0.12	34,34,34,34	0
57	MG	CX	3004	1/1	0.95	0.18	63,63,63,63	0
57	MG	BA	3205	1/1	0.95	0.27	50,50,50,50	0
57	MG	AY	3001	1/1	0.95	0.39	65,65,65,65	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	DA	3207	1/1	0.95	0.30	63,63,63,63	0
57	MG	BA	3395	1/1	0.95	0.17	38,38,38,38	0
57	MG	BA	3359	1/1	0.95	0.30	62,62,62,62	0
57	MG	DA	3224	1/1	0.95	0.17	49,49,49,49	0
57	MG	BA	3557	1/1	0.95	0.16	33,33,33,33	0
57	MG	BA	3383	1/1	0.95	0.12	53,53,53,53	0
57	MG	CA	3127	1/1	0.95	0.18	62,62,62,62	0
57	MG	BA	3215	1/1	0.95	0.27	36,36,36,36	0
57	MG	DA	3117	1/1	0.95	0.20	52,52,52,52	0
57	MG	BA	3031	1/1	0.95	0.19	52,52,52,52	0
57	MG	AA	3205	1/1	0.95	0.22	51,51,51,51	0
57	MG	DA	3645	1/1	0.95	0.07	45,45,45,45	0
57	MG	BA	3209	1/1	0.95	0.24	54,54,54,54	0
57	MG	DA	3272	1/1	0.95	0.10	41,41,41,41	0
57	MG	BA	3579	1/1	0.95	0.17	49,49,49,49	0
57	MG	BA	3617	1/1	0.95	0.16	51,51,51,51	0
57	MG	AA	3156	1/1	0.95	0.26	63,63,63,63	0
57	MG	BA	3783	1/1	0.95	0.12	56,56,56,56	0
57	MG	AA	3118	1/1	0.95	0.17	47,47,47,47	0
57	MG	AA	3106	1/1	0.95	0.10	57,57,57,57	0
57	MG	BA	3056	1/1	0.95	0.21	40,40,40,40	0
57	MG	BA	3381	1/1	0.95	0.16	46,46,46,46	0
57	MG	BA	3527	1/1	0.95	0.16	54,54,54,54	0
57	MG	DA	3519	1/1	0.95	0.18	63,63,63,63	0
57	MG	DA	3343	1/1	0.95	0.16	50,50,50,50	0
57	MG	DA	3136	1/1	0.95	0.14	52,52,52,52	0
57	MG	DA	3304	1/1	0.95	0.06	48,48,48,48	0
57	MG	DA	3522	1/1	0.95	0.12	71,71,71,71	0
57	MG	BA	3808	1/1	0.95	0.16	42,42,42,42	0
57	MG	BA	3130	1/1	0.95	0.08	44,44,44,44	0
57	MG	BU	207	1/1	0.95	0.17	38,38,38,38	0
57	MG	BA	3796	1/1	0.95	0.25	45,45,45,45	0
57	MG	DA	3186	1/1	0.95	0.15	54,54,54,54	0
57	MG	DA	3541	1/1	0.95	0.14	44,44,44,44	0
57	MG	BA	3687	1/1	0.95	0.21	22,22,22,22	0
57	MG	DA	3570	1/1	0.95	0.13	31,31,31,31	0
57	MG	DQ	3002	1/1	0.95	0.10	51,51,51,51	0
57	MG	BA	3123	1/1	0.95	0.22	32,32,32,32	0
57	MG	BA	3632	1/1	0.95	0.07	50,50,50,50	0
57	MG	BA	3577	1/1	0.95	0.19	51,51,51,51	0
57	MG	BA	3090	1/1	0.95	0.31	53,53,53,53	0
57	MG	DA	3474	1/1	0.95	0.14	51,51,51,51	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	BA	3635	1/1	0.95	0.13	58,58,58,58	0
57	MG	BQ	3004	1/1	0.95	0.27	42,42,42,42	0
57	MG	DA	3602	1/1	0.95	0.10	65,65,65,65	0
57	MG	DA	3483	1/1	0.95	0.32	55,55,55,55	0
57	MG	BA	3156	1/1	0.95	0.29	41,41,41,41	0
57	MG	DA	3539	1/1	0.95	0.12	53,53,53,53	0
57	MG	DA	3181	1/1	0.95	0.13	50,50,50,50	0
57	MG	DA	3277	1/1	0.95	0.11	55,55,55,55	0
57	MG	CA	3019	1/1	0.95	0.10	65,65,65,65	0
57	MG	AA	3035	1/1	0.95	0.21	56,56,56,56	0
57	MG	DA	3496	1/1	0.95	0.07	53,53,53,53	0
57	MG	BA	3775	1/1	0.95	0.16	33,33,33,33	0
57	MG	BA	3484	1/1	0.95	0.13	54,54,54,54	0
57	MG	CA	3015	1/1	0.95	0.22	56,56,56,56	0
57	MG	CA	3104	1/1	0.95	0.12	68,68,68,68	0
57	MG	CA	3029	1/1	0.95	0.17	63,63,63,63	0
57	MG	BA	3398	1/1	0.95	0.21	32,32,32,32	0
57	MG	AA	3015	1/1	0.95	0.15	65,65,65,65	0
57	MG	DA	3611	1/1	0.95	0.14	48,48,48,48	0
57	MG	BA	3110	1/1	0.95	0.17	41,41,41,41	0
57	MG	BA	3482	1/1	0.95	0.15	51,51,51,51	0
57	MG	BA	3178	1/1	0.95	0.13	46,46,46,46	0
57	MG	DA	3548	1/1	0.95	0.06	60,60,60,60	0
57	MG	DA	3386	1/1	0.95	0.11	35,35,35,35	0
57	MG	DA	3418	1/1	0.95	0.11	52,52,52,52	0
57	MG	DA	3295	1/1	0.95	0.21	44,44,44,44	0
57	MG	DA	3225	1/1	0.95	0.07	49,49,49,49	0
57	MG	BA	3249	1/1	0.95	0.13	49,49,49,49	0
57	MG	BA	3661	1/1	0.95	0.09	44,44,44,44	0
57	MG	AA	3129	1/1	0.95	0.11	47,47,47,47	0
57	MG	CA	3169	1/1	0.95	0.24	51,51,51,51	0
57	MG	AA	3165	1/1	0.95	0.20	54,54,54,54	0
57	MG	BA	3592	1/1	0.95	0.20	28,28,28,28	0
57	MG	BA	3567	1/1	0.95	0.15	34,34,34,34	0
57	MG	CA	3092	1/1	0.95	0.10	50,50,50,50	0
57	MG	DA	3174	1/1	0.95	0.13	44,44,44,44	0
57	MG	BA	3133	1/1	0.95	0.19	45,45,45,45	0
57	MG	DA	3485	1/1	0.95	0.12	52,52,52,52	0
57	MG	CA	3042	1/1	0.95	0.11	59,59,59,59	0
57	MG	BA	3146	1/1	0.95	0.17	40,40,40,40	0
57	MG	DA	3565	1/1	0.95	0.08	59,59,59,59	0
57	MG	BA	3795	1/1	0.95	0.15	35,35,35,35	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	BA	3288	1/1	0.95	0.20	56,56,56,56	0
57	MG	AA	3010	1/1	0.95	0.17	52,52,52,52	0
57	MG	DA	3581	1/1	0.95	0.22	57,57,57,57	0
57	MG	CA	3031	1/1	0.95	0.10	68,68,68,68	0
57	MG	BA	3348	1/1	0.95	0.18	36,36,36,36	0
57	MG	DA	3375	1/1	0.95	0.16	39,39,39,39	0
57	MG	BA	3620	1/1	0.95	0.15	40,40,40,40	0
57	MG	AA	3081	1/1	0.95	0.11	48,48,48,48	0
57	MG	BA	3608	1/1	0.95	0.31	62,62,62,62	0
57	MG	AA	3157	1/1	0.95	0.17	45,45,45,45	0
57	MG	AA	3179	1/1	0.95	0.13	69,69,69,69	0
57	MG	BA	3175	1/1	0.95	0.20	20,20,20,20	0
57	MG	BA	3283	1/1	0.95	0.20	35,35,35,35	0
57	MG	DA	3183	1/1	0.95	0.15	38,38,38,38	0
57	MG	CA	3154	1/1	0.95	0.17	56,56,56,56	0
57	MG	DB	3006	1/1	0.95	0.14	57,57,57,57	0
57	MG	DA	3376	1/1	0.95	0.16	61,61,61,61	0
57	MG	BA	3570	1/1	0.95	0.16	42,42,42,42	0
57	MG	CA	3101	1/1	0.95	0.11	49,49,49,49	0
57	MG	AA	3167	1/1	0.95	0.10	57,57,57,57	0
59	ZN	B4	501	1/1	0.95	0.15	89,89,89,89	0
57	MG	BA	3626	1/1	0.95	0.25	44,44,44,44	0
57	MG	CA	3121	1/1	0.95	0.14	63,63,63,63	0
57	MG	DE	304	1/1	0.95	0.15	43,43,43,43	0
57	MG	BA	3571	1/1	0.95	0.18	58,58,58,58	0
57	MG	CA	3151	1/1	0.95	0.27	59,59,59,59	0
57	MG	DA	3441	1/1	0.95	0.11	45,45,45,45	0
57	MG	BA	3510	1/1	0.95	0.17	46,46,46,46	0
57	MG	DA	3674	1/1	0.95	0.15	37,37,37,37	0
57	MG	CD	301	1/1	0.95	0.19	56,56,56,56	0
57	MG	BA	3551	1/1	0.95	0.19	36,36,36,36	0
57	MG	AA	3134	1/1	0.95	0.14	66,66,66,66	0
57	MG	BA	3593	1/1	0.95	0.22	38,38,38,38	0
57	MG	BA	3163	1/1	0.95	0.14	55,55,55,55	0
57	MG	DA	3640	1/1	0.95	0.19	43,43,43,43	0
57	MG	BP	201	1/1	0.95	0.28	41,41,41,41	0
57	MG	CA	3132	1/1	0.95	0.13	66,66,66,66	0
57	MG	BU	204	1/1	0.95	0.16	35,35,35,35	0
57	MG	DA	3510	1/1	0.95	0.25	49,49,49,49	0
57	MG	DA	3649	1/1	0.95	0.05	58,58,58,58	0
57	MG	BA	3218	1/1	0.95	0.20	47,47,47,47	0
57	MG	BP	205	1/1	0.95	0.18	65,65,65,65	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	BA	3782	1/1	0.95	0.16	65,65,65,65	0
57	MG	DA	3568	1/1	0.95	0.08	52,52,52,52	0
57	MG	DA	3080	1/1	0.95	0.10	55,55,55,55	0
57	MG	AF	3001	1/1	0.95	0.26	44,44,44,44	0
57	MG	BA	3262	1/1	0.95	0.14	41,41,41,41	0
57	MG	BA	3751	1/1	0.95	0.17	26,26,26,26	0
57	MG	DA	3286	1/1	0.95	0.14	42,42,42,42	0
57	MG	DA	3562	1/1	0.95	0.12	64,64,64,64	0
57	MG	CA	3001	1/1	0.95	0.10	75,75,75,75	0
57	MG	BA	3500	1/1	0.95	0.14	56,56,56,56	0
57	MG	DA	3364	1/1	0.95	0.07	40,40,40,40	0
57	MG	AA	3144	1/1	0.95	0.14	46,46,46,46	0
57	MG	DY	502	1/1	0.95	0.13	50,50,50,50	0
57	MG	BA	3373	1/1	0.95	0.17	48,48,48,48	0
57	MG	DA	3433	1/1	0.95	0.18	46,46,46,46	0
57	MG	BA	3451	1/1	0.95	0.16	31,31,31,31	0
57	MG	DA	3348	1/1	0.95	0.10	34,34,34,34	0
57	MG	BE	306	1/1	0.95	0.20	26,26,26,26	0
57	MG	DA	3629	1/1	0.95	0.27	62,62,62,62	0
57	MG	DA	3359	1/1	0.95	0.13	47,47,47,47	0
57	MG	BA	3068	1/1	0.95	0.18	43,43,43,43	0
57	MG	BA	3647	1/1	0.95	0.09	56,56,56,56	0
57	MG	BW	201	1/1	0.95	0.31	44,44,44,44	0
57	MG	BA	3517	1/1	0.96	0.14	45,45,45,45	0
57	MG	BD	308	1/1	0.96	0.23	46,46,46,46	0
57	MG	BA	3586	1/1	0.96	0.09	53,53,53,53	0
57	MG	AX	3012	1/1	0.96	0.17	59,59,59,59	0
57	MG	DA	3457	1/1	0.96	0.07	54,54,54,54	0
57	MG	DA	3068	1/1	0.96	0.10	58,58,58,58	0
57	MG	BA	3720	1/1	0.96	0.14	65,65,65,65	0
57	MG	AA	3114	1/1	0.96	0.17	59,59,59,59	0
57	MG	DA	3515	1/1	0.96	0.15	45,45,45,45	0
57	MG	BA	3729	1/1	0.96	0.19	47,47,47,47	0
57	MG	DA	3639	1/1	0.96	0.48	59,59,59,59	0
57	MG	DA	3199	1/1	0.96	0.11	47,47,47,47	0
57	MG	BA	3614	1/1	0.96	0.11	63,63,63,63	0
57	MG	BA	3645	1/1	0.96	0.20	33,33,33,33	0
57	MG	BA	3211	1/1	0.96	0.15	55,55,55,55	0
57	MG	DA	3145	1/1	0.96	0.17	43,43,43,43	0
57	MG	DA	3298	1/1	0.96	0.16	59,59,59,59	0
57	MG	DA	3123	1/1	0.96	0.20	56,56,56,56	0
57	MG	AX	3013	1/1	0.96	0.13	58,58,58,58	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	AA	3044	1/1	0.96	0.25	60,60,60,60	0
57	MG	DA	3293	1/1	0.96	0.14	54,54,54,54	0
57	MG	AA	3006	1/1	0.96	0.12	52,52,52,52	0
57	MG	AA	3110	1/1	0.96	0.13	48,48,48,48	0
57	MG	DA	3353	1/1	0.96	0.16	42,42,42,42	0
57	MG	BA	3627	1/1	0.96	0.17	56,56,56,56	0
57	MG	DA	3504	1/1	0.96	0.07	47,47,47,47	0
57	MG	BQ	3002	1/1	0.96	0.23	43,43,43,43	0
57	MG	CA	3143	1/1	0.96	0.10	64,64,64,64	0
57	MG	BA	3382	1/1	0.96	0.09	63,63,63,63	0
57	MG	DA	3150	1/1	0.96	0.08	56,56,56,56	0
57	MG	DA	3559	1/1	0.96	0.12	43,43,43,43	0
57	MG	DA	3461	1/1	0.96	0.11	62,62,62,62	0
57	MG	DA	3443	1/1	0.96	0.10	54,54,54,54	0
57	MG	BA	3525	1/1	0.96	0.17	34,34,34,34	0
57	MG	BA	3264	1/1	0.96	0.22	58,58,58,58	0
57	MG	DA	3233	1/1	0.96	0.19	53,53,53,53	0
57	MG	BA	3256	1/1	0.96	0.15	40,40,40,40	0
57	MG	BA	3108	1/1	0.96	0.32	44,44,44,44	0
57	MG	DA	3489	1/1	0.96	0.13	51,51,51,51	0
57	MG	BA	3591	1/1	0.96	0.17	35,35,35,35	0
57	MG	BW	204	1/1	0.96	0.22	42,42,42,42	0
57	MG	BB	205	1/1	0.96	0.20	60,60,60,60	0
57	MG	BB	216	1/1	0.96	0.23	51,51,51,51	0
57	MG	BA	3224	1/1	0.96	0.22	65,65,65,65	0
57	MG	DA	3319	1/1	0.96	0.12	41,41,41,41	0
57	MG	BA	3238	1/1	0.96	0.24	62,62,62,62	0
57	MG	DA	3387	1/1	0.96	0.10	42,42,42,42	0
57	MG	DA	3159	1/1	0.96	0.15	58,58,58,58	0
57	MG	BA	3529	1/1	0.96	0.20	56,56,56,56	0
57	MG	DA	3160	1/1	0.96	0.10	56,56,56,56	0
57	MG	BA	3088	1/1	0.96	0.35	48,48,48,48	0
57	MG	DA	3366	1/1	0.96	0.14	42,42,42,42	0
57	MG	CA	3067	1/1	0.96	0.31	61,61,61,61	0
57	MG	BP	204	1/1	0.96	0.06	46,46,46,46	0
57	MG	DA	3081	1/1	0.96	0.28	55,55,55,55	0
57	MG	BA	3437	1/1	0.96	0.14	36,36,36,36	0
57	MG	BE	304	1/1	0.96	0.19	42,42,42,42	0
57	MG	BA	3589	1/1	0.96	0.21	27,27,27,27	0
57	MG	DA	3055	1/1	0.96	0.17	49,49,49,49	0
57	MG	DA	3520	1/1	0.96	0.11	57,57,57,57	0
57	MG	DA	3537	1/1	0.96	0.08	44,44,44,44	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	CA	3023	1/1	0.96	0.14	44,44,44,44	0
57	MG	BA	3692	1/1	0.96	0.15	40,40,40,40	0
57	MG	CA	3093	1/1	0.96	0.10	55,55,55,55	0
57	MG	DA	3350	1/1	0.96	0.12	51,51,51,51	0
57	MG	B3	3002	1/1	0.96	0.12	66,66,66,66	0
57	MG	DA	3241	1/1	0.96	0.13	45,45,45,45	0
57	MG	BA	3629	1/1	0.96	0.16	43,43,43,43	0
57	MG	BA	3528	1/1	0.96	0.18	56,56,56,56	0
57	MG	DA	3014	1/1	0.96	0.21	46,46,46,46	0
57	MG	BA	3272	1/1	0.96	0.61	48,48,48,48	0
57	MG	BA	3727	1/1	0.96	0.13	51,51,51,51	0
57	MG	BA	3494	1/1	0.96	0.09	49,49,49,49	0
57	MG	DA	3176	1/1	0.96	0.19	41,41,41,41	0
57	MG	DW	3002	1/1	0.96	0.15	45,45,45,45	0
57	MG	BA	3572	1/1	0.96	0.16	61,61,61,61	0
57	MG	BA	3460	1/1	0.96	0.10	62,62,62,62	0
57	MG	DA	3580	1/1	0.96	0.16	36,36,36,36	0
57	MG	BA	3491	1/1	0.96	0.15	45,45,45,45	0
57	MG	BA	3153	1/1	0.96	0.31	47,47,47,47	0
57	MG	BA	3197	1/1	0.96	0.30	41,41,41,41	0
57	MG	BA	3244	1/1	0.96	0.22	53,53,53,53	0
57	MG	DA	3057	1/1	0.96	0.20	42,42,42,42	0
57	MG	BA	3547	1/1	0.96	0.23	39,39,39,39	0
57	MG	DA	3040	1/1	0.96	0.12	31,31,31,31	0
57	MG	DA	3220	1/1	0.96	0.16	46,46,46,46	0
57	MG	DA	3299	1/1	0.96	0.20	55,55,55,55	0
57	MG	BA	3462	1/1	0.96	0.19	36,36,36,36	0
57	MG	DA	3193	1/1	0.96	0.13	57,57,57,57	0
57	MG	BA	3676	1/1	0.96	0.21	33,33,33,33	0
57	MG	BA	3012	1/1	0.96	0.20	39,39,39,39	0
57	MG	BW	203	1/1	0.96	0.20	44,44,44,44	0
57	MG	BA	3492	1/1	0.96	0.13	46,46,46,46	0
57	MG	BA	3804	1/1	0.96	0.42	53,53,53,53	0
57	MG	DA	3374	1/1	0.96	0.16	56,56,56,56	0
57	MG	BA	3251	1/1	0.96	0.19	44,44,44,44	0
57	MG	BB	213	1/1	0.96	0.19	60,60,60,60	0
57	MG	BA	3694	1/1	0.96	0.10	51,51,51,51	0
57	MG	DA	3156	1/1	0.96	0.09	51,51,51,51	0
57	MG	BA	3091	1/1	0.96	0.40	56,56,56,56	0
57	MG	BA	3059	1/1	0.96	0.21	26,26,26,26	0
57	MG	DA	3059	1/1	0.96	0.26	43,43,43,43	0
57	MG	BA	3248	1/1	0.96	0.30	42,42,42,42	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	DA	3109	1/1	0.96	0.15	40,40,40,40	0
57	MG	DA	3596	1/1	0.96	0.10	56,56,56,56	0
57	MG	DA	3395	1/1	0.96	0.12	47,47,47,47	0
57	MG	BA	3778	1/1	0.96	0.16	48,48,48,48	0
57	MG	BA	3665	1/1	0.96	0.16	49,49,49,49	0
57	MG	DA	3416	1/1	0.96	0.12	50,50,50,50	0
57	MG	DA	3454	1/1	0.96	0.16	56,56,56,56	0
57	MG	AA	3087	1/1	0.96	0.11	41,41,41,41	0
57	MG	BA	3191	1/1	0.96	0.18	43,43,43,43	0
57	MG	BA	3414	1/1	0.96	0.18	41,41,41,41	0
57	MG	BA	3691	1/1	0.96	0.16	55,55,55,55	0
57	MG	BA	3689	1/1	0.96	0.17	42,42,42,42	0
57	MG	BA	3208	1/1	0.96	0.16	44,44,44,44	0
57	MG	BA	3582	1/1	0.96	0.16	74,74,74,74	0
57	MG	BA	3336	1/1	0.96	0.15	64,64,64,64	0
57	MG	DA	3306	1/1	0.96	0.13	55,55,55,55	0
57	MG	DA	3341	1/1	0.96	0.13	51,51,51,51	0
57	MG	DA	3111	1/1	0.96	0.19	61,61,61,61	0
57	MG	DA	3169	1/1	0.96	0.24	47,47,47,47	0
57	MG	CA	3049	1/1	0.96	0.20	63,63,63,63	0
57	MG	BN	3001	1/1	0.96	0.31	53,53,53,53	0
57	MG	DA	3204	1/1	0.96	0.31	46,46,46,46	0
57	MG	BA	3469	1/1	0.96	0.15	49,49,49,49	0
57	MG	BF	303	1/1	0.96	0.54	49,49,49,49	0
57	MG	DA	3269	1/1	0.96	0.06	49,49,49,49	0
57	MG	DB	3007	1/1	0.96	0.20	58,58,58,58	0
57	MG	AA	3074	1/1	0.96	0.09	50,50,50,50	0
57	MG	BA	3763	1/1	0.96	0.19	24,24,24,24	0
57	MG	BG	203	1/1	0.96	0.16	42,42,42,42	0
57	MG	DA	3509	1/1	0.96	0.12	59,59,59,59	0
57	MG	BV	202	1/1	0.96	0.17	50,50,50,50	0
57	MG	BA	3488	1/1	0.96	0.19	60,60,60,60	0
57	MG	BB	207	1/1	0.96	0.22	54,54,54,54	0
57	MG	BA	3370	1/1	0.96	0.20	39,39,39,39	0
57	MG	BA	3711	1/1	0.96	0.19	54,54,54,54	0
57	MG	BA	3184	1/1	0.96	0.32	43,43,43,43	0
57	MG	DA	3619	1/1	0.96	0.11	69,69,69,69	0
57	MG	DA	3084	1/1	0.96	0.08	39,39,39,39	0
57	MG	DA	3282	1/1	0.96	0.06	52,52,52,52	0
57	MG	DA	3648	1/1	0.96	0.14	57,57,57,57	0
57	MG	DA	3597	1/1	0.96	0.06	51,51,51,51	0
57	MG	BA	3107	1/1	0.96	0.16	53,53,53,53	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	BA	3574	1/1	0.96	0.19	66,66,66,66	0
57	MG	BA	3613	1/1	0.96	0.41	42,42,42,42	0
57	MG	BA	3657	1/1	0.96	0.26	47,47,47,47	0
57	MG	BA	3699	1/1	0.96	0.23	35,35,35,35	0
57	MG	BA	3408	1/1	0.96	0.20	36,36,36,36	0
57	MG	DA	3022	1/1	0.96	0.27	51,51,51,51	0
57	MG	DA	3346	1/1	0.96	0.12	48,48,48,48	0
57	MG	DA	3365	1/1	0.96	0.08	36,36,36,36	0
57	MG	BA	3041	1/1	0.96	0.24	40,40,40,40	0
57	MG	BW	202	1/1	0.96	0.22	54,54,54,54	0
57	MG	DA	3012	1/1	0.96	0.12	33,33,33,33	0
57	MG	DE	302	1/1	0.96	0.17	33,33,33,33	0
57	MG	CA	3045	1/1	0.96	0.24	54,54,54,54	0
57	MG	DA	3493	1/1	0.96	0.30	66,66,66,66	0
57	MG	CA	3069	1/1	0.96	0.12	60,60,60,60	0
57	MG	B0	103	1/1	0.96	0.08	53,53,53,53	0
57	MG	BA	3132	1/1	0.96	0.14	40,40,40,40	0
57	MG	BA	3753	1/1	0.96	0.15	33,33,33,33	0
57	MG	AA	3048	1/1	0.96	0.22	57,57,57,57	0
57	MG	BA	3076	1/1	0.96	0.17	43,43,43,43	0
57	MG	DA	3445	1/1	0.96	0.10	32,32,32,32	0
57	MG	DA	3253	1/1	0.96	0.13	45,45,45,45	0
57	MG	AA	3180	1/1	0.96	0.10	73,73,73,73	0
57	MG	DD	301	1/1	0.96	0.15	47,47,47,47	0
57	MG	BA	3356	1/1	0.96	0.16	37,37,37,37	0
57	MG	BA	3349	1/1	0.96	0.09	56,56,56,56	0
57	MG	BA	3140	1/1	0.96	0.14	47,47,47,47	0
57	MG	CA	3056	1/1	0.96	0.10	64,64,64,64	0
57	MG	CA	3048	1/1	0.96	0.12	67,67,67,67	0
57	MG	AA	3011	1/1	0.96	0.34	57,57,57,57	0
57	MG	DA	3052	1/1	0.96	0.13	61,61,61,61	0
57	MG	BA	3660	1/1	0.96	0.11	61,61,61,61	0
57	MG	CA	3162	1/1	0.96	0.10	66,66,66,66	0
57	MG	BA	3696	1/1	0.96	0.14	33,33,33,33	0
57	MG	DA	3296	1/1	0.96	0.12	28,28,28,28	0
57	MG	DA	3464	1/1	0.96	0.10	46,46,46,46	0
57	MG	BA	3094	1/1	0.96	0.21	36,36,36,36	0
57	MG	AA	3173	1/1	0.96	0.15	54,54,54,54	0
57	MG	BA	3112	1/1	0.96	0.23	30,30,30,30	0
57	MG	BA	3701	1/1	0.96	0.15	43,43,43,43	0
57	MG	DA	3663	1/1	0.96	0.13	60,60,60,60	0
57	MG	BA	3468	1/1	0.96	0.17	62,62,62,62	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	BV	205	1/1	0.96	0.09	38,38,38,38	0
57	MG	BA	3806	1/1	0.96	0.16	30,30,30,30	0
57	MG	AA	3043	1/1	0.96	0.23	51,51,51,51	0
57	MG	AA	3203	1/1	0.96	0.13	59,59,59,59	0
57	MG	BA	3160	1/1	0.96	0.32	55,55,55,55	0
57	MG	BA	3644	1/1	0.96	0.14	35,35,35,35	0
57	MG	BA	3603	1/1	0.96	0.13	53,53,53,53	0
57	MG	BA	3083	1/1	0.96	0.15	56,56,56,56	0
57	MG	AA	3212	1/1	0.96	0.13	42,42,42,42	0
57	MG	BA	3034	1/1	0.96	0.25	56,56,56,56	0
57	MG	AA	3113	1/1	0.96	0.12	58,58,58,58	0
57	MG	BA	3441	1/1	0.96	0.13	35,35,35,35	0
57	MG	AA	3151	1/1	0.96	0.14	45,45,45,45	0
57	MG	CA	3005	1/1	0.96	0.15	62,62,62,62	0
57	MG	BA	3169	1/1	0.96	0.17	45,45,45,45	0
57	MG	DA	3574	1/1	0.96	0.11	53,53,53,53	0
57	MG	DA	3101	1/1	0.96	0.16	49,49,49,49	0
57	MG	BA	3375	1/1	0.96	0.13	68,68,68,68	0
57	MG	DA	3569	1/1	0.96	0.23	49,49,49,49	0
57	MG	AX	3005	1/1	0.97	0.14	47,47,47,47	0
57	MG	CA	3050	1/1	0.97	0.20	61,61,61,61	0
57	MG	BF	301	1/1	0.97	0.16	35,35,35,35	0
57	MG	BA	3776	1/1	0.97	0.20	43,43,43,43	0
57	MG	AA	3208	1/1	0.97	0.17	60,60,60,60	0
57	MG	BA	3299	1/1	0.97	0.16	25,25,25,25	0
57	MG	BA	3330	1/1	0.97	0.23	37,37,37,37	0
57	MG	BA	3752	1/1	0.97	0.19	32,32,32,32	0
57	MG	AA	3158	1/1	0.97	0.14	45,45,45,45	0
57	MG	BD	305	1/1	0.97	0.16	35,35,35,35	0
57	MG	BA	3390	1/1	0.97	0.26	38,38,38,38	0
57	MG	BD	303	1/1	0.97	0.14	39,39,39,39	0
57	MG	BA	3113	1/1	0.97	0.25	53,53,53,53	0
57	MG	BF	306	1/1	0.97	0.28	31,31,31,31	0
57	MG	DA	3072	1/1	0.97	0.14	47,47,47,47	0
57	MG	BA	3222	1/1	0.97	0.18	37,37,37,37	0
57	MG	DA	3187	1/1	0.97	0.11	42,42,42,42	0
57	MG	BA	3428	1/1	0.97	0.19	46,46,46,46	0
57	MG	BF	307	1/1	0.97	0.24	37,37,37,37	0
57	MG	AA	3105	1/1	0.97	0.32	69,69,69,69	0
57	MG	DA	3168	1/1	0.97	0.29	45,45,45,45	0
57	MG	DA	3257	1/1	0.97	0.18	50,50,50,50	0
57	MG	BA	3311	1/1	0.97	0.27	48,48,48,48	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	BG	201	1/1	0.97	0.20	58,58,58,58	0
57	MG	BA	3011	1/1	0.97	0.19	35,35,35,35	0
57	MG	BA	3731	1/1	0.97	0.30	37,37,37,37	0
57	MG	DA	3042	1/1	0.97	0.17	38,38,38,38	0
57	MG	BA	3379	1/1	0.97	0.18	31,31,31,31	0
57	MG	BA	3214	1/1	0.97	0.17	41,41,41,41	0
57	MG	BA	3653	1/1	0.97	0.21	39,39,39,39	0
57	MG	DA	3166	1/1	0.97	0.11	55,55,55,55	0
57	MG	BA	3674	1/1	0.97	0.15	63,63,63,63	0
57	MG	AA	3099	1/1	0.97	0.20	51,51,51,51	0
57	MG	DA	3466	1/1	0.97	0.11	41,41,41,41	0
57	MG	AA	3137	1/1	0.97	0.15	51,51,51,51	0
57	MG	DA	3369	1/1	0.97	0.15	28,28,28,28	0
57	MG	CA	3123	1/1	0.97	0.14	58,58,58,58	0
57	MG	BA	3481	1/1	0.97	0.18	41,41,41,41	0
60	K	CX	3001	1/1	0.97	0.19	82,82,82,82	0
57	MG	DA	3599	1/1	0.97	0.20	36,36,36,36	0
57	MG	BA	3549	1/1	0.97	0.29	39,39,39,39	0
57	MG	DA	3019	1/1	0.97	0.29	37,37,37,37	0
57	MG	BA	3089	1/1	0.97	0.17	19,19,19,19	0
57	MG	BA	3410	1/1	0.97	0.16	27,27,27,27	0
57	MG	BA	3029	1/1	0.97	0.48	37,37,37,37	0
57	MG	BE	302	1/1	0.97	0.23	39,39,39,39	0
57	MG	DA	3542	1/1	0.97	0.17	24,24,24,24	0
57	MG	DD	307	1/1	0.97	0.32	43,43,43,43	0
57	MG	BA	3474	1/1	0.97	0.18	55,55,55,55	0
57	MG	AA	3112	1/1	0.97	0.17	63,63,63,63	0
57	MG	BA	3420	1/1	0.97	0.16	40,40,40,40	0
57	MG	BA	3630	1/1	0.97	0.14	58,58,58,58	0
57	MG	DA	3552	1/1	0.97	0.12	54,54,54,54	0
57	MG	DW	3004	1/1	0.97	0.22	52,52,52,52	0
57	MG	BA	3263	1/1	0.97	0.34	49,49,49,49	0
57	MG	AA	3147	1/1	0.97	0.10	70,70,70,70	0
57	MG	DA	3171	1/1	0.97	0.12	31,31,31,31	0
57	MG	DA	3191	1/1	0.97	0.17	37,37,37,37	0
57	MG	DA	3155	1/1	0.97	0.25	48,48,48,48	0
57	MG	BA	3787	1/1	0.97	0.23	45,45,45,45	0
57	MG	DA	3349	1/1	0.97	0.07	52,52,52,52	0
57	MG	BA	3565	1/1	0.97	0.17	40,40,40,40	0
57	MG	DA	3278	1/1	0.97	0.06	43,43,43,43	0
57	MG	DA	3266	1/1	0.97	0.09	57,57,57,57	0
57	MG	AA	3148	1/1	0.97	0.22	57,57,57,57	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	AX	3006	1/1	0.97	0.10	65,65,65,65	0
57	MG	BA	3067	1/1	0.97	0.15	41,41,41,41	0
57	MG	BA	3425	1/1	0.97	0.15	40,40,40,40	0
57	MG	DA	3601	1/1	0.97	0.10	44,44,44,44	0
57	MG	DA	3105	1/1	0.97	0.19	48,48,48,48	0
57	MG	DA	3265	1/1	0.97	0.12	30,30,30,30	0
57	MG	DA	3305	1/1	0.97	0.20	50,50,50,50	0
57	MG	BA	3677	1/1	0.97	0.17	60,60,60,60	0
57	MG	BA	3103	1/1	0.97	0.17	38,38,38,38	0
57	MG	BA	3483	1/1	0.97	0.15	28,28,28,28	0
57	MG	BA	3260	1/1	0.97	0.30	39,39,39,39	0
57	MG	BA	3193	1/1	0.97	0.20	48,48,48,48	0
57	MG	BA	3082	1/1	0.97	0.22	39,39,39,39	0
57	MG	AA	3125	1/1	0.97	0.24	37,37,37,37	0
57	MG	BA	3245	1/1	0.97	0.23	34,34,34,34	0
57	MG	DA	3228	1/1	0.97	0.30	38,38,38,38	0
57	MG	BA	3093	1/1	0.97	0.26	56,56,56,56	0
57	MG	BA	3116	1/1	0.97	0.28	50,50,50,50	0
57	MG	DA	3345	1/1	0.97	0.09	44,44,44,44	0
59	ZN	D9	501	1/1	0.97	0.12	68,68,68,68	0
57	MG	BA	3036	1/1	0.97	0.17	40,40,40,40	0
57	MG	BA	3326	1/1	0.97	0.19	20,20,20,20	0
57	MG	DA	3028	1/1	0.97	0.36	52,52,52,52	0
57	MG	DA	3449	1/1	0.97	0.10	54,54,54,54	0
57	MG	BA	3774	1/1	0.97	0.07	46,46,46,46	0
57	MG	BA	3766	1/1	0.97	0.15	28,28,28,28	0
57	MG	DA	3261	1/1	0.97	0.12	49,49,49,49	0
57	MG	BA	3270	1/1	0.97	0.17	48,48,48,48	0
57	MG	DA	3307	1/1	0.97	0.09	42,42,42,42	0
57	MG	BA	3137	1/1	0.97	0.24	39,39,39,39	0
57	MG	CA	3134	1/1	0.97	0.16	69,69,69,69	0
57	MG	BN	3003	1/1	0.97	0.19	48,48,48,48	0
57	MG	BA	3158	1/1	0.97	0.20	41,41,41,41	0
57	MG	DA	3613	1/1	0.97	0.15	54,54,54,54	0
57	MG	DA	3192	1/1	0.97	0.10	60,60,60,60	0
57	MG	BA	3042	1/1	0.97	0.20	43,43,43,43	0
57	MG	DA	3390	1/1	0.97	0.11	43,43,43,43	0
57	MG	CA	3072	1/1	0.97	0.17	54,54,54,54	0
57	MG	BA	3139	1/1	0.97	0.33	40,40,40,40	0
57	MG	DA	3370	1/1	0.97	0.14	51,51,51,51	0
57	MG	DA	3089	1/1	0.97	0.39	52,52,52,52	0
57	MG	BA	3393	1/1	0.97	0.18	51,51,51,51	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	BA	3280	1/1	0.97	0.14	37,37,37,37	0
57	MG	DA	3143	1/1	0.97	0.18	38,38,38,38	0
57	MG	BA	3254	1/1	0.97	0.22	25,25,25,25	0
57	MG	BA	3358	1/1	0.97	0.21	49,49,49,49	0
57	MG	CA	3137	1/1	0.97	0.16	56,56,56,56	0
57	MG	BB	212	1/1	0.97	0.13	55,55,55,55	0
57	MG	CA	3167	1/1	0.97	0.17	60,60,60,60	0
57	MG	BA	3371	1/1	0.97	0.14	35,35,35,35	0
57	MG	BA	3046	1/1	0.97	0.28	41,41,41,41	0
57	MG	DA	3099	1/1	0.97	0.17	32,32,32,32	0
57	MG	BB	203	1/1	0.97	0.24	43,43,43,43	0
57	MG	DA	3664	1/1	0.97	0.39	48,48,48,48	0
57	MG	DA	3086	1/1	0.97	0.09	43,43,43,43	0
57	MG	BA	3115	1/1	0.97	0.24	59,59,59,59	0
57	MG	BA	3489	1/1	0.97	0.07	59,59,59,59	0
57	MG	BA	3698	1/1	0.97	0.22	31,31,31,31	0
57	MG	BA	3725	1/1	0.97	0.14	44,44,44,44	0
57	MG	BA	3338	1/1	0.97	0.13	40,40,40,40	0
57	MG	BB	204	1/1	0.97	0.18	41,41,41,41	0
57	MG	DA	3020	1/1	0.97	0.16	55,55,55,55	0
57	MG	DA	3231	1/1	0.97	0.09	62,62,62,62	0
57	MG	CA	3034	1/1	0.97	0.14	59,59,59,59	0
57	MG	DA	3579	1/1	0.97	0.10	48,48,48,48	0
57	MG	DA	3310	1/1	0.97	0.13	38,38,38,38	0
57	MG	DA	3175	1/1	0.97	0.12	41,41,41,41	0
57	MG	DA	3506	1/1	0.97	0.09	42,42,42,42	0
57	MG	BA	3518	1/1	0.97	0.20	44,44,44,44	0
57	MG	DA	3384	1/1	0.97	0.10	49,49,49,49	0
57	MG	AA	3154	1/1	0.97	0.11	69,69,69,69	0
57	MG	DW	3001	1/1	0.97	0.40	54,54,54,54	0
57	MG	BA	3111	1/1	0.97	0.13	54,54,54,54	0
57	MG	BA	3232	1/1	0.97	0.20	52,52,52,52	0
57	MG	BA	3479	1/1	0.97	0.07	50,50,50,50	0
57	MG	BA	3188	1/1	0.97	0.30	49,49,49,49	0
57	MG	BA	3611	1/1	0.97	0.17	46,46,46,46	0
57	MG	DA	3460	1/1	0.97	0.13	41,41,41,41	0
57	MG	BA	3345	1/1	0.97	0.14	38,38,38,38	0
57	MG	BA	3475	1/1	0.97	0.13	42,42,42,42	0
57	MG	BA	3786	1/1	0.97	0.13	35,35,35,35	0
57	MG	AA	3186	1/1	0.97	0.12	42,42,42,42	0
57	MG	DV	3002	1/1	0.97	0.30	49,49,49,49	0
57	MG	BA	3048	1/1	0.97	0.13	47,47,47,47	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	BA	3144	1/1	0.97	0.19	41,41,41,41	0
57	MG	BA	3789	1/1	0.97	0.18	12,12,12,12	0
57	MG	BA	3553	1/1	0.97	0.10	59,59,59,59	0
57	MG	DA	3322	1/1	0.97	0.19	51,51,51,51	0
57	MG	DA	3184	1/1	0.97	0.16	47,47,47,47	0
57	MG	BA	3756	1/1	0.97	0.20	48,48,48,48	0
57	MG	BA	3343	1/1	0.97	0.15	53,53,53,53	0
57	MG	DA	3529	1/1	0.97	0.08	38,38,38,38	0
57	MG	BA	3152	1/1	0.97	0.30	43,43,43,43	0
57	MG	DA	3016	1/1	0.97	0.34	50,50,50,50	0
57	MG	DA	3644	1/1	0.97	0.08	55,55,55,55	0
57	MG	BA	3181	1/1	0.97	0.25	43,43,43,43	0
57	MG	CA	3131	1/1	0.97	0.07	55,55,55,55	0
57	MG	BA	3368	1/1	0.97	0.20	40,40,40,40	0
57	MG	AA	3092	1/1	0.97	0.14	63,63,63,63	0
57	MG	BN	3005	1/1	0.97	0.17	36,36,36,36	0
57	MG	DA	3142	1/1	0.97	0.13	47,47,47,47	0
57	MG	BA	3363	1/1	0.97	0.15	22,22,22,22	0
57	MG	BB	208	1/1	0.97	0.14	45,45,45,45	0
57	MG	CA	3071	1/1	0.97	0.15	68,68,68,68	0
57	MG	DA	3561	1/1	0.97	0.04	57,57,57,57	0
57	MG	DA	3338	1/1	0.97	0.15	61,61,61,61	0
57	MG	BA	3331	1/1	0.97	0.17	49,49,49,49	0
57	MG	DA	3352	1/1	0.97	0.19	63,63,63,63	0
57	MG	DA	3436	1/1	0.97	0.12	54,54,54,54	0
57	MG	DA	3046	1/1	0.97	0.16	47,47,47,47	0
57	MG	BA	3476	1/1	0.97	0.15	55,55,55,55	0
57	MG	DA	3647	1/1	0.97	0.11	54,54,54,54	0
57	MG	BA	3221	1/1	0.97	0.17	37,37,37,37	0
57	MG	DF	3003	1/1	0.97	0.40	43,43,43,43	0
57	MG	DA	3096	1/1	0.97	0.23	42,42,42,42	0
57	MG	BA	3643	1/1	0.97	0.13	46,46,46,46	0
57	MG	DA	3058	1/1	0.97	0.14	29,29,29,29	0
57	MG	BA	3086	1/1	0.97	0.21	22,22,22,22	0
57	MG	BA	3028	1/1	0.97	0.22	51,51,51,51	0
57	MG	AK	3001	1/1	0.97	0.18	44,44,44,44	0
57	MG	BA	3004	1/1	0.97	0.19	33,33,33,33	0
57	MG	DA	3435	1/1	0.97	0.15	50,50,50,50	0
57	MG	BF	309	1/1	0.97	0.15	53,53,53,53	0
57	MG	CA	3155	1/1	0.97	0.12	53,53,53,53	0
57	MG	DA	3326	1/1	0.97	0.16	43,43,43,43	0
57	MG	BA	3097	1/1	0.97	0.14	44,44,44,44	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	AA	3018	1/1	0.97	0.24	56,56,56,56	0
57	MG	BA	3490	1/1	0.97	0.10	54,54,54,54	0
57	MG	B7	103	1/1	0.97	0.16	42,42,42,42	0
57	MG	AA	3207	1/1	0.97	0.09	65,65,65,65	0
57	MG	BD	306	1/1	0.97	0.25	38,38,38,38	0
57	MG	DA	3373	1/1	0.97	0.15	44,44,44,44	0
57	MG	AA	3164	1/1	0.97	0.10	61,61,61,61	0
57	MG	BA	3309	1/1	0.97	0.18	41,41,41,41	0
57	MG	BA	3159	1/1	0.97	0.25	50,50,50,50	0
57	MG	BA	3360	1/1	0.97	0.16	41,41,41,41	0
57	MG	AA	3024	1/1	0.97	0.12	54,54,54,54	0
57	MG	BA	3286	1/1	0.97	0.21	34,34,34,34	0
57	MG	BA	3168	1/1	0.97	0.17	47,47,47,47	0
57	MG	BA	3380	1/1	0.97	0.10	48,48,48,48	0
57	MG	BA	3334	1/1	0.97	0.14	37,37,37,37	0
57	MG	AA	3182	1/1	0.97	0.14	49,49,49,49	0
57	MG	BA	3202	1/1	0.97	0.19	60,60,60,60	0
57	MG	BA	3435	1/1	0.97	0.27	45,45,45,45	0
57	MG	BA	3105	1/1	0.97	0.18	37,37,37,37	0
57	MG	DA	3182	1/1	0.97	0.24	51,51,51,51	0
57	MG	B8	101	1/1	0.97	0.21	44,44,44,44	0
57	MG	DA	3455	1/1	0.97	0.10	47,47,47,47	0
57	MG	CA	3147	1/1	0.97	0.12	64,64,64,64	0
57	MG	CA	3084	1/1	0.97	0.13	60,60,60,60	0
57	MG	DB	3010	1/1	0.97	0.17	57,57,57,57	0
57	MG	BA	3102	1/1	0.97	0.19	44,44,44,44	0
57	MG	DA	3189	1/1	0.97	0.20	41,41,41,41	0
57	MG	AA	3120	1/1	0.97	0.19	45,45,45,45	0
57	MG	B7	101	1/1	0.97	0.24	39,39,39,39	0
57	MG	BA	3784	1/1	0.97	0.21	33,33,33,33	0
57	MG	BA	3449	1/1	0.98	0.21	35,35,35,35	0
57	MG	BA	3544	1/1	0.98	0.22	44,44,44,44	0
57	MG	DA	3508	1/1	0.98	0.10	44,44,44,44	0
57	MG	DA	3281	1/1	0.98	0.16	53,53,53,53	0
57	MG	BA	3060	1/1	0.98	0.20	30,30,30,30	0
57	MG	BA	3187	1/1	0.98	0.25	29,29,29,29	0
57	MG	BA	3705	1/1	0.98	0.11	62,62,62,62	0
57	MG	BA	3085	1/1	0.98	0.27	35,35,35,35	0
57	MG	BA	3339	1/1	0.98	0.21	23,23,23,23	0
57	MG	BA	3050	1/1	0.98	0.20	38,38,38,38	0
57	MG	BA	3281	1/1	0.98	0.28	60,60,60,60	0
57	MG	DA	3010	1/1	0.98	0.17	47,47,47,47	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	DA	3161	1/1	0.98	0.19	38,38,38,38	0
57	MG	DQ	3001	1/1	0.98	0.13	47,47,47,47	0
57	MG	BA	3625	1/1	0.98	0.18	39,39,39,39	0
57	MG	BA	3135	1/1	0.98	0.20	43,43,43,43	0
57	MG	AA	3090	1/1	0.98	0.21	66,66,66,66	0
57	MG	DA	3363	1/1	0.98	0.16	29,29,29,29	0
57	MG	BA	3080	1/1	0.98	0.17	60,60,60,60	0
58	SF4	CD	302	8/8	0.98	0.16	60,68,83,86	0
57	MG	BA	3467	1/1	0.98	0.23	50,50,50,50	0
57	MG	DF	3002	1/1	0.98	0.18	48,48,48,48	0
57	MG	BA	3772	1/1	0.98	0.19	33,33,33,33	0
57	MG	DA	3412	1/1	0.98	0.20	50,50,50,50	0
57	MG	BA	3416	1/1	0.98	0.21	21,21,21,21	0
57	MG	BA	3521	1/1	0.98	0.20	39,39,39,39	0
57	MG	BA	3472	1/1	0.98	0.16	20,20,20,20	0
57	MG	BA	3039	1/1	0.98	0.20	32,32,32,32	0
57	MG	BA	3588	1/1	0.98	0.23	31,31,31,31	0
57	MG	DA	3115	1/1	0.98	0.24	40,40,40,40	0
57	MG	DA	3471	1/1	0.98	0.23	50,50,50,50	0
59	ZN	AN	501	1/1	0.98	0.19	69,69,69,69	0
57	MG	CA	3099	1/1	0.98	0.15	44,44,44,44	0
57	MG	BA	3313	1/1	0.98	0.07	53,53,53,53	0
57	MG	DA	3491	1/1	0.98	0.16	51,51,51,51	0
57	MG	BA	3025	1/1	0.98	0.16	27,27,27,27	0
57	MG	BA	3792	1/1	0.98	0.14	54,54,54,54	0
57	MG	AA	3040	1/1	0.98	0.11	60,60,60,60	0
57	MG	AA	3053	1/1	0.98	0.20	61,61,61,61	0
57	MG	BA	3124	1/1	0.98	0.21	19,19,19,19	0
57	MG	CA	3133	1/1	0.98	0.21	59,59,59,59	0
57	MG	DA	3330	1/1	0.98	0.11	45,45,45,45	0
57	MG	AA	3062	1/1	0.98	0.28	51,51,51,51	0
57	MG	AA	3082	1/1	0.98	0.13	46,46,46,46	0
57	MG	DA	3442	1/1	0.98	0.12	39,39,39,39	0
57	MG	BA	3556	1/1	0.98	0.21	36,36,36,36	0
57	MG	DA	3357	1/1	0.98	0.07	50,50,50,50	0
57	MG	DA	3258	1/1	0.98	0.14	48,48,48,48	0
57	MG	BA	3148	1/1	0.98	0.33	44,44,44,44	0
57	MG	BA	3247	1/1	0.98	0.16	25,25,25,25	0
57	MG	BA	3609	1/1	0.98	0.11	39,39,39,39	0
57	MG	DA	3555	1/1	0.98	0.29	53,53,53,53	0
57	MG	DA	3399	1/1	0.98	0.13	59,59,59,59	0
57	MG	BA	3038	1/1	0.98	0.25	35,35,35,35	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	BA	3287	1/1	0.98	0.14	42,42,42,42	0
57	MG	BA	3450	1/1	0.98	0.13	48,48,48,48	0
57	MG	BA	3234	1/1	0.98	0.15	38,38,38,38	0
57	MG	BA	3558	1/1	0.98	0.14	32,32,32,32	0
57	MG	BA	3719	1/1	0.98	0.18	53,53,53,53	0
57	MG	DA	3453	1/1	0.98	0.22	60,60,60,60	0
57	MG	DA	3198	1/1	0.98	0.13	40,40,40,40	0
57	MG	BA	3230	1/1	0.98	0.20	53,53,53,53	0
57	MG	BA	3737	1/1	0.98	0.29	43,43,43,43	0
57	MG	AA	3168	1/1	0.98	0.11	59,59,59,59	0
57	MG	AA	3086	1/1	0.98	0.07	57,57,57,57	0
57	MG	BA	3010	1/1	0.98	0.16	39,39,39,39	0
57	MG	BA	3605	1/1	0.98	0.17	43,43,43,43	0
59	ZN	B6	103	1/1	0.98	0.24	49,49,49,49	0
57	MG	BA	3791	1/1	0.98	0.18	28,28,28,28	0
57	MG	BA	3367	1/1	0.98	0.25	29,29,29,29	0
57	MG	AA	3077	1/1	0.98	0.25	56,56,56,56	0
57	MG	BA	3762	1/1	0.98	0.20	46,46,46,46	0
57	MG	DA	3003	1/1	0.98	0.15	27,27,27,27	0
57	MG	BA	3534	1/1	0.98	0.21	44,44,44,44	0
57	MG	CA	3148	1/1	0.98	0.11	70,70,70,70	0
57	MG	DA	3500	1/1	0.98	0.10	49,49,49,49	0
57	MG	BA	3327	1/1	0.98	0.18	38,38,38,38	0
57	MG	BA	3040	1/1	0.98	0.36	35,35,35,35	0
59	ZN	CN	501	1/1	0.98	0.08	93,93,93,93	0
57	MG	DA	3665	1/1	0.98	0.14	42,42,42,42	0
57	MG	DA	3190	1/1	0.98	0.20	54,54,54,54	0
57	MG	BU	203	1/1	0.98	0.21	47,47,47,47	0
57	MG	CA	3103	1/1	0.98	0.13	46,46,46,46	0
57	MG	BR	202	1/1	0.98	0.14	31,31,31,31	0
57	MG	DA	3144	1/1	0.98	0.11	38,38,38,38	0
57	MG	DA	3459	1/1	0.98	0.19	47,47,47,47	0
57	MG	DA	3525	1/1	0.98	0.13	59,59,59,59	0
57	MG	CA	3105	1/1	0.98	0.18	52,52,52,52	0
57	MG	BA	3235	1/1	0.98	0.16	42,42,42,42	0
57	MG	DD	305	1/1	0.98	0.12	36,36,36,36	0
57	MG	CA	3085	1/1	0.98	0.13	54,54,54,54	0
57	MG	BA	3167	1/1	0.98	0.12	41,41,41,41	0
57	MG	BP	203	1/1	0.98	0.15	33,33,33,33	0
57	MG	BA	3487	1/1	0.98	0.14	50,50,50,50	0
58	SF4	AD	501	8/8	0.98	0.16	62,68,73,86	0
57	MG	BA	3241	1/1	0.98	0.19	36,36,36,36	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	BA	3278	1/1	0.98	0.18	34,34,34,34	0
57	MG	DA	3534	1/1	0.98	0.15	55,55,55,55	0
57	MG	BA	3332	1/1	0.98	0.18	38,38,38,38	0
57	MG	DA	3034	1/1	0.98	0.18	38,38,38,38	0
57	MG	BB	217	1/1	0.98	0.18	29,29,29,29	0
57	MG	DA	3177	1/1	0.98	0.15	42,42,42,42	0
57	MG	BA	3044	1/1	0.98	0.22	20,20,20,20	0
57	MG	DA	3008	1/1	0.98	0.09	36,36,36,36	0
57	MG	BA	3498	1/1	0.98	0.18	36,36,36,36	0
57	MG	DA	3294	1/1	0.98	0.16	43,43,43,43	0
57	MG	DA	3289	1/1	0.98	0.10	53,53,53,53	0
57	MG	BF	305	1/1	0.98	0.09	49,49,49,49	0
57	MG	DA	3157	1/1	0.98	0.11	47,47,47,47	0
57	MG	DU	3001	1/1	0.98	0.32	55,55,55,55	0
57	MG	DA	3292	1/1	0.98	0.17	30,30,30,30	0
59	ZN	BY	501	1/1	0.98	0.15	58,58,58,58	0
57	MG	BA	3174	1/1	0.98	0.18	37,37,37,37	0
57	MG	BA	3454	1/1	0.98	0.23	27,27,27,27	0
57	MG	BA	3364	1/1	0.98	0.27	60,60,60,60	0
57	MG	DA	3021	1/1	0.98	0.09	31,31,31,31	0
57	MG	DA	3393	1/1	0.98	0.10	50,50,50,50	0
57	MG	BA	3049	1/1	0.98	0.21	36,36,36,36	0
57	MG	DA	3197	1/1	0.98	0.14	55,55,55,55	0
57	MG	DD	308	1/1	0.98	0.29	48,48,48,48	0
57	MG	BA	3735	1/1	0.98	0.43	57,57,57,57	0
57	MG	CA	3043	1/1	0.98	0.11	47,47,47,47	0
57	MG	BA	3736	1/1	0.98	0.16	42,42,42,42	0
57	MG	CA	3089	1/1	0.98	0.12	47,47,47,47	0
57	MG	CA	3065	1/1	0.98	0.17	49,49,49,49	0
57	MG	DA	3512	1/1	0.98	0.09	47,47,47,47	0
57	MG	B0	101	1/1	0.98	0.17	36,36,36,36	0
57	MG	CA	3047	1/1	0.98	0.14	53,53,53,53	0
57	MG	DE	301	1/1	0.98	0.40	46,46,46,46	0
57	MG	BA	3744	1/1	0.98	0.14	39,39,39,39	0
57	MG	BV	201	1/1	0.98	0.31	33,33,33,33	0
57	MG	DN	5001	1/1	0.98	0.11	66,66,66,66	0
57	MG	B6	101	1/1	0.98	0.17	48,48,48,48	0
57	MG	DA	3404	1/1	0.98	0.12	48,48,48,48	0
57	MG	BA	3142	1/1	0.98	0.17	49,49,49,49	0
57	MG	BA	3563	1/1	0.98	0.17	36,36,36,36	0
57	MG	AA	3126	1/1	0.98	0.09	49,49,49,49	0
57	MG	DA	3094	1/1	0.98	0.22	50,50,50,50	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	BA	3141	1/1	0.98	0.28	42,42,42,42	0
57	MG	BA	3497	1/1	0.98	0.14	28,28,28,28	0
57	MG	BA	3607	1/1	0.98	0.24	38,38,38,38	0
57	MG	BA	3259	1/1	0.98	0.21	25,25,25,25	0
57	MG	BA	3569	1/1	0.99	0.19	49,49,49,49	0
57	MG	DA	3347	1/1	0.99	0.20	27,27,27,27	0
57	MG	DA	3480	1/1	0.99	0.10	40,40,40,40	0
57	MG	BA	3458	1/1	0.99	0.18	18,18,18,18	0
57	MG	BA	3392	1/1	0.99	0.17	53,53,53,53	0
57	MG	DA	3027	1/1	0.99	0.57	51,51,51,51	0
57	MG	BA	3726	1/1	0.99	0.19	63,63,63,63	0
59	ZN	B5	102	1/1	0.99	0.22	48,48,48,48	0
57	MG	DA	3026	1/1	0.99	0.56	59,59,59,59	0
57	MG	BA	3374	1/1	0.99	0.17	40,40,40,40	0
57	MG	BA	3216	1/1	0.99	0.23	37,37,37,37	0
57	MG	DA	3535	1/1	0.99	0.18	56,56,56,56	0
57	MG	BA	3069	1/1	0.99	0.27	22,22,22,22	0
57	MG	BA	3045	1/1	0.99	0.21	36,36,36,36	0
57	MG	BD	307	1/1	0.99	0.21	40,40,40,40	0
57	MG	DA	3315	1/1	0.99	0.08	42,42,42,42	0
57	MG	DA	3671	1/1	0.99	0.13	74,74,74,74	0
59	ZN	B9	501	1/1	0.99	0.18	38,38,38,38	0
57	MG	BA	3422	1/1	0.99	0.24	33,33,33,33	0
57	MG	BA	3233	1/1	0.99	0.30	56,56,56,56	0
59	ZN	D5	501	1/1	0.99	0.20	58,58,58,58	0
59	ZN	D6	501	1/1	0.99	0.17	71,71,71,71	0
57	MG	DF	3004	1/1	0.99	0.38	44,44,44,44	0
57	MG	BA	3198	1/1	0.99	0.24	37,37,37,37	0
57	MG	BA	3597	1/1	0.99	0.21	25,25,25,25	0
57	MG	BA	3384	1/1	0.99	0.19	41,41,41,41	0
57	MG	DA	3560	1/1	0.99	0.07	40,40,40,40	0
57	MG	DA	3285	1/1	0.99	0.13	32,32,32,32	0
57	MG	BA	3378	1/1	0.99	0.12	28,28,28,28	0
57	MG	BA	3013	1/1	0.99	0.14	32,32,32,32	0
57	MG	DA	3344	1/1	0.99	0.16	31,31,31,31	0
57	MG	DA	3031	1/1	0.99	0.43	43,43,43,43	0
57	MG	DA	3297	1/1	0.99	0.11	39,39,39,39	0
57	MG	DA	3005	1/1	0.99	0.22	57,57,57,57	0
57	MG	BU	206	1/1	0.99	0.40	35,35,35,35	0
57	MG	BA	3037	1/1	1.00	0.24	34,34,34,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.