Full wwPDB X-ray Structure Validation Report (i)

Aug 3, 2026 – 10:19 AM EDT

PDB ID	:	4WPO / pdb_00004wpo
Title	:	Crystal structure of the Thermus thermophilus 70S ribosome in complex with elongation factor G in the pre-translocational state
Authors	:	Lin, J.; Gagnon, M.G.; Steitz, T.A.
Deposited on	:	2014-10-20
Resolution	:	2.80 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

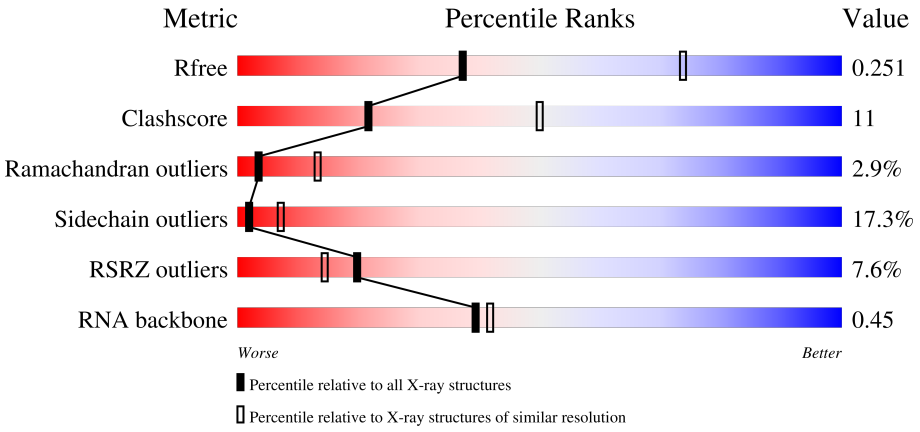
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.80 Å.

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



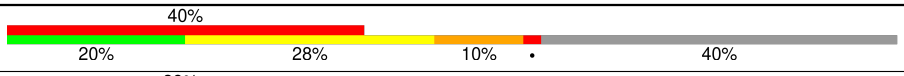
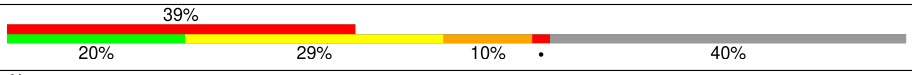
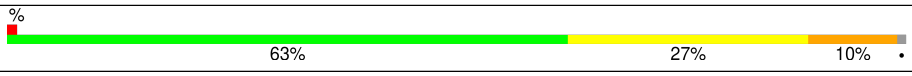
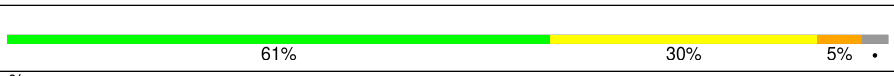
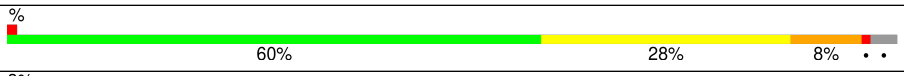
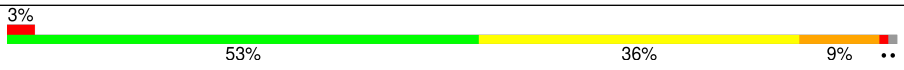
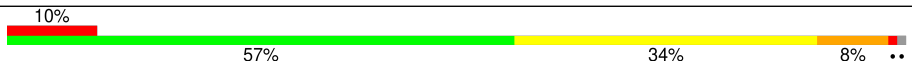
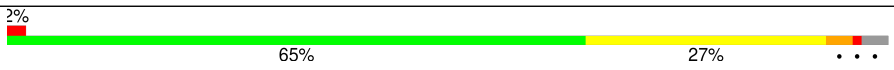
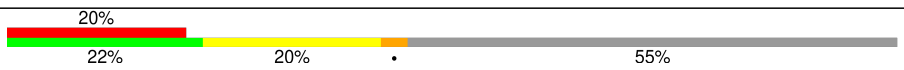
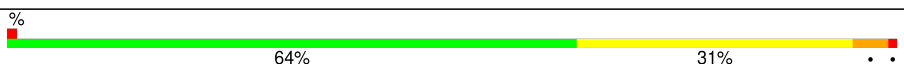
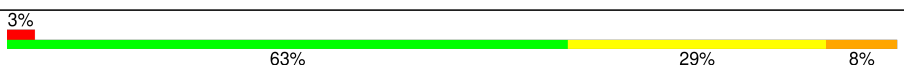
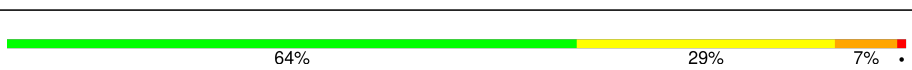
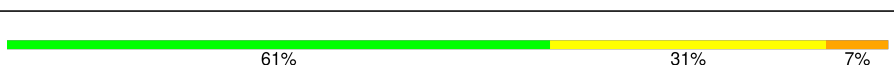
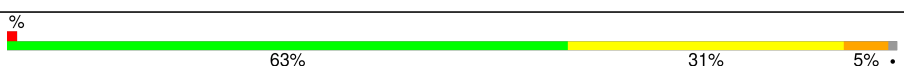
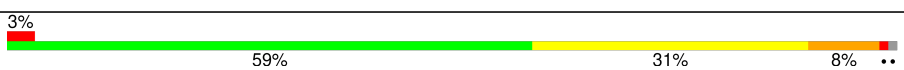
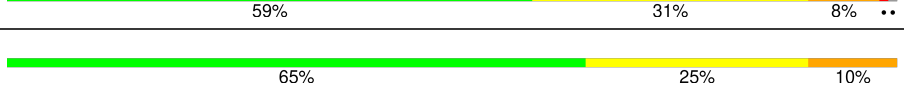
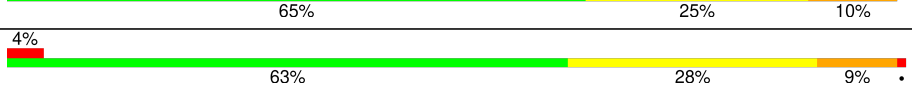
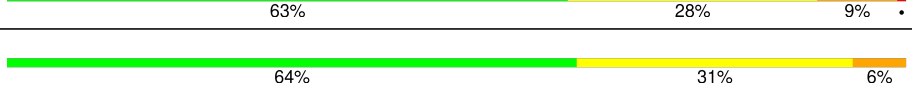
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)
RNA backbone	3983	1114 (3.00-2.60)

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

Mol	Chain	Length	Quality of chain
1	AA	2915	% 62% 30% 7% .
1	CA	2915	3% 57% 33% 8% .
2	AB	121	74% 25% .
2	CB	121	% 62% 31% 6% .

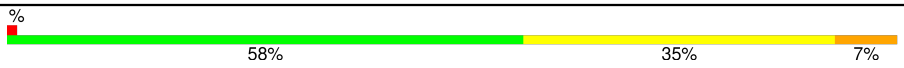
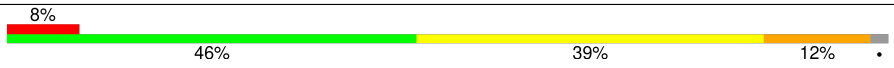
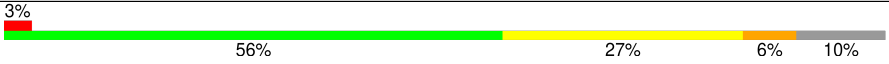
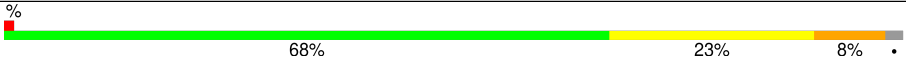
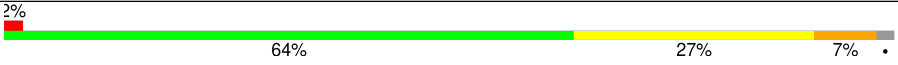
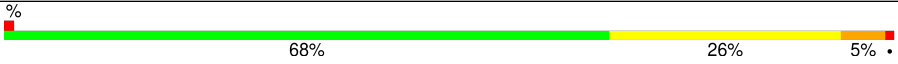
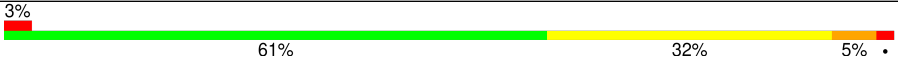
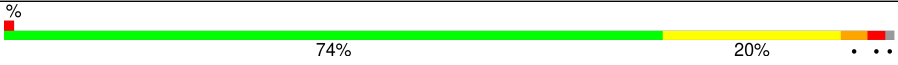
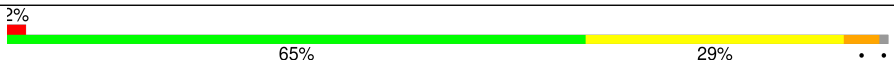
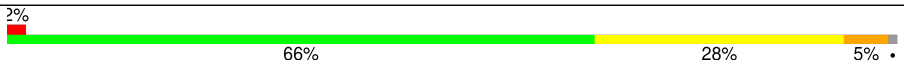
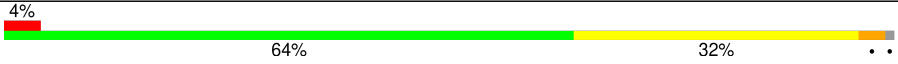
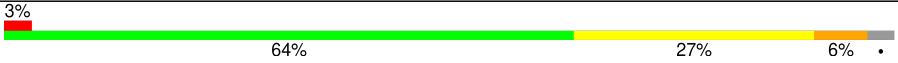
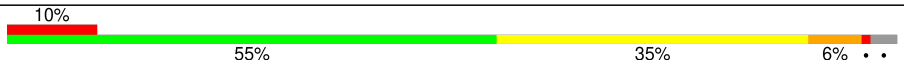
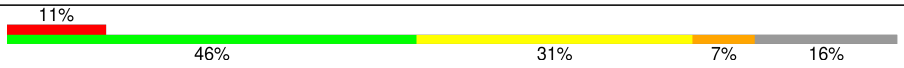
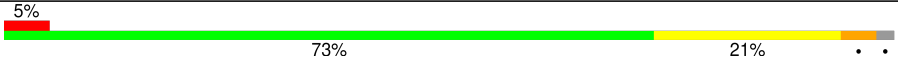
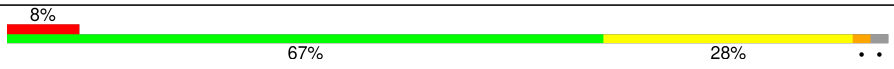
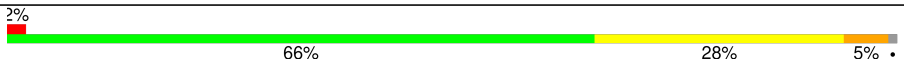
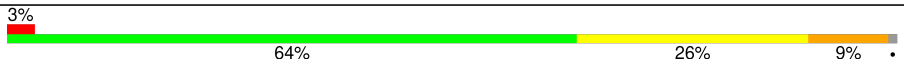
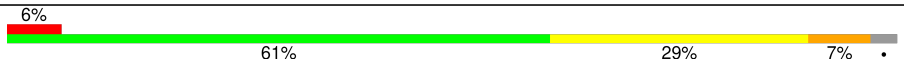
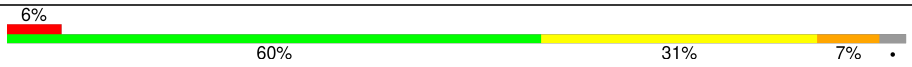
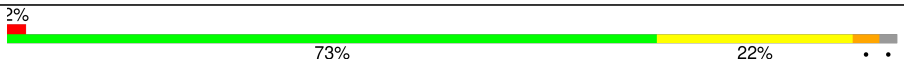
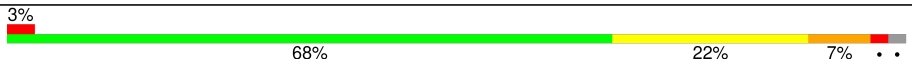
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	AC	228	
3	CC	228	
4	AD	276	
4	CD	276	
5	AE	206	
5	CE	206	
6	AF	210	
6	CF	210	
7	AG	182	
7	CG	182	
8	AH	180	
8	CH	180	
9	AK	173	
9	CK	173	
10	AL	147	
10	CL	147	
11	AN	140	
11	CN	140	
12	AO	122	
12	CO	122	
13	AP	150	
13	CP	150	
14	AQ	141	
14	CQ	141	
15	AR	118	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
15	CR	118	
16	AS	112	
16	CS	112	
17	AT	146	
17	CT	146	
18	AU	118	
18	CU	118	
19	AV	101	
19	CV	101	
20	AW	113	
20	CW	113	
21	AX	96	
21	CX	96	
22	AY	110	
22	CY	110	
23	AZ	206	
23	CZ	206	
24	A0	85	
24	C0	85	
25	A1	98	
25	C1	98	
26	A2	72	
26	C2	72	
27	A3	60	
27	C3	60	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
28	A4	71	13% 35% 51% 8%
28	C4	71	23% 51% 34% 13%
29	A5	60	73% 18% 7%
29	C5	60	77% 17% 5%
30	A6	54	2% 56% 30% 13%
30	C6	54	2% 61% 30% 7%
31	A7	49	6% 63% 29% 6%
31	C7	49	10% 65% 27% 6%
32	A8	65	2% 46% 42% 11%
32	C8	65	5% 63% 29% 6%
33	A9	37	3% 68% 24% 8%
33	C9	37	8% 59% 35% 5%
34	BA	1521	2% 54% 37% 7%
34	DA	1521	3% 50% 39% 9%
35	BB	256	14% 38% 38% 14% 10%
35	DB	256	20% 38% 40% 12% 10%
36	BC	239	11% 52% 27% 7% 14%
36	DC	239	19% 44% 34% 8% 14%
37	BD	209	12% 60% 30% 8%
37	DD	209	6% 61% 31% 7%
38	BE	162	2% 47% 39% 6% 9%
38	DE	162	7% 44% 38% 9% 9%
39	BF	101	% 58% 34% 7%
39	DF	101	% 64% 29% 6%
40	BG	156	8% 71% 22% 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
40	DG	156	13% 69% 26%
41	BH	138	2% 57% 36% 6%
41	DH	138	13% 54% 33% 11%
42	BI	128	18% 54% 40% 5%
42	DI	128	43% 59% 34% 5%
43	BJ	105	30% 51% 34% 7% 8%
43	DJ	105	38% 43% 43% 5% 9%
44	BK	129	4% 51% 33% 12%
44	DK	129	7% 57% 27% 12%
45	BL	132	3% 75% 16% 8%
45	DL	132	7% 64% 25% 8%
46	BM	126	10% 56% 34% 7%
46	DM	126	28% 48% 40% 10%
47	BN	61	25% 52% 33% 11%
47	DN	61	70% 43% 46% 10%
48	BO	89	4% 55% 38% 6%
48	DO	89	3% 61% 35%
49	BP	88	9% 47% 41% 6% 7%
49	DP	88	3% 53% 31% 7% 7%
50	BQ	105	4% 58% 25% 10% 6%
50	DQ	105	6% 58% 30% 6% 6%
51	BR	88	42% 26% 8% 23%
51	DR	88	2% 47% 25% 6% 23%
52	BS	93	26% 43% 42% 5% 10%
52	DS	93	40% 52% 35% 11%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
53	BT	106	13% 47% 36% 6% 9%
53	DT	106	9% 54% 27% 8% 9%
54	BU	27	26% 56% 26% 15%
54	DU	27	41% 56% 26% 15%
55	BV	24	25% 33% 17% 46%
55	DV	24	21% 38% 8% 50%
56	BW	76	9% 43% 39% 13%
56	DW	76	9% 37% 42% 14% 5%
57	BX	77	% 60% 34% 5%
57	DX	77	3% 51% 34% 14%
58	BY	76	11% 42% 36% 20%
58	DY	76	12% 43% 39% 9%
59	BZ	758	13% 48% 35% 12%
59	DZ	758	16% 50% 36% 9%

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
60	MG	AA	3027	-	-	-	X
60	MG	AA	3108	-	-	-	X
60	MG	AA	3183	-	-	-	X
60	MG	AA	3203	-	-	-	X
60	MG	AA	3770	-	-	-	X
60	MG	AA	3805	-	-	-	X
60	MG	BA	1800	-	-	-	X
60	MG	CA	3031	-	-	-	X
60	MG	CA	3042	-	-	-	X
60	MG	CA	3122	-	-	-	X
60	MG	CA	3220	-	-	-	X
60	MG	DA	1651	-	-	-	X

2 Entry composition (i)

There are 65 unique types of molecules in this entry. The entry contains 313372 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 23S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	2872	Total	C	N	O	P	0	0	0
			61861	27532	11574	19884	2871			
1	CA	2868	Total	C	N	O	P	0	0	0
			61771	27492	11554	19858	2867			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			
2	CB	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			

- Molecule 3 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	137	Total	C	N	O	S	0	0	0
			1063	669	201	192	1			
3	CC	137	Total	C	N	O	S	0	0	0
			1063	669	201	192	1			

- Molecule 4 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AD	275	Total	C	N	O	S	0	0	0
			2136	1349	423	361	3			
4	CD	275	Total	C	N	O	S	0	0	0
			2142	1352	426	361	3			

- Molecule 5 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AE	204	Total	C	N	O	S	0	0	0
			1559	985	298	270	6			
5	CE	204	Total	C	N	O	S	0	0	0
			1559	985	298	270	6			

- Molecule 6 is a protein called 50S ribosomal protein L4.

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

- Molecule 7 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AG	181	Total	C	N	O	S	0	0	0
			1425	914	256	251	4			
7	CG	181	Total	C	N	O	S	0	0	0
			1424	911	258	251	4			

- Molecule 8 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AH	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			
8	CH	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			

- Molecule 9 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	AK	130	Total	C	N	O	0	0	0
			641	381	130	130			
9	CK	130	Total	C	N	O	0	0	0
			641	381	130	130			

- Molecule 10 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AL	66	Total	C	N	O	S	0	0	0
			498	310	93	92	3			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	CL	66	Total	C	N	O	S	0	0	0
			498	310	93	92	3			

- Molecule 11 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AN	140	Total	C	N	O	S	0	0	0
			1117	719	207	187	4			
11	CN	140	Total	C	N	O	S	0	0	0
			1117	719	207	187	4			

- Molecule 12 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			
12	CO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

- Molecule 13 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AP	149	Total	C	N	O	S	0	0	0
			1139	709	231	196	3			
13	CP	149	Total	C	N	O	S	0	0	0
			1135	706	230	196	3			

- Molecule 14 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			
14	CQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

- Molecule 15 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AR	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			
15	CR	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			

- Molecule 16 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AS	110	Total	C	N	O		0	0	0
			877	553	175	149				
16	CS	110	Total	C	N	O		0	0	0
			870	549	173	148				

- Molecule 17 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AT	131	Total	C	N	O	S	0	0	0
			1091	680	225	185	1			
17	CT	131	Total	C	N	O	S	0	0	0
			1083	675	224	183	1			

- Molecule 18 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	AU	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			
18	CU	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			

- Molecule 19 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AV	101	Total	C	N	O	S	0	0	0
			771	495	140	135	1			
19	CV	101	Total	C	N	O	S	0	0	0
			771	495	140	135	1			

- Molecule 20 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AW	112	Total	C	N	O	S	0	0	0
			886	557	174	153	2			
20	CW	112	Total	C	N	O	S	0	0	0
			886	557	174	153	2			

- Molecule 21 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	AX	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			
21	CX	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			

- Molecule 22 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AY	107	Total	C	N	O	S	0	0	0
			806	517	152	131	6			
22	CY	107	Total	C	N	O	S	0	0	0
			806	517	152	131	6			

- Molecule 23 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AZ	171	Total	C	N	O	S	0	0	0
			1349	862	243	242	2			
23	CZ	174	Total	C	N	O	S	0	0	0
			1360	870	243	245	2			

- Molecule 24 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	A0	83	Total	C	N	O	S	0	0	0
			653	404	139	109	1			
24	C0	83	Total	C	N	O	S	0	0	0
			653	404	139	109	1			

- Molecule 25 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	A1	97	Total	C	N	O	S	0	0	0
			755	475	148	131	1			
25	C1	97	Total	C	N	O	S	0	0	0
			755	475	148	131	1			

- Molecule 26 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	A2	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	C2	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			

- Molecule 27 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
27	A3	59	Total	C	N	O	0	0	0
			469	298	90	81			
27	C3	59	Total	C	N	O	0	0	0
			464	296	90	78			

- Molecule 28 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	A4	69	Total	C	N	O	S	0	0	0
			558	352	102	99	5			
28	C4	69	Total	C	N	O	S	0	0	0
			532	339	97	91	5			

- Molecule 29 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	A5	59	Total	C	N	O	S	0	0	0
			455	285	89	76	5			
29	C5	59	Total	C	N	O	S	0	0	0
			455	285	89	76	5			

- Molecule 30 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	A6	53	Total	C	N	O	S	0	0	0
			453	281	91	77	4			
30	C6	53	Total	C	N	O	S	0	0	0
			449	279	91	75	4			

- Molecule 31 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	A7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			
31	C7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			

- Molecule 32 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	A8	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			
32	C8	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			

- Molecule 33 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	A9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			
33	C9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

- Molecule 34 is a RNA chain called 16S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BA	1497	Total	C	N	O	P	0	0	0
			32185	14324	5968	10396	1497			
34	DA	1503	Total	C	N	O	P	0	0	0
			32312	14381	5990	10438	1503			

- Molecule 35 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BB	231	Total	C	N	O	S	0	0	0
			1846	1179	331	331	5			
35	DB	231	Total	C	N	O	S	0	0	0
			1825	1167	326	327	5			

- Molecule 36 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BC	206	Total	C	N	O	S	0	0	0
			1552	976	302	273	1			
36	DC	206	Total	C	N	O	S	0	0	0
			1544	970	300	273	1			

- Molecule 37 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BD	208	Total	C	N	O	S	0	0	0
			1659	1040	326	286	7			
37	DD	208	Total	C	N	O	S	0	0	0
			1678	1052	333	286	7			

- Molecule 38 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BE	148	Total	C	N	O	S	0	0	0
			1129	714	213	198	4			
38	DE	148	Total	C	N	O	S	0	0	0
			1133	716	214	199	4			

- Molecule 39 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BF	100	Total	C	N	O	S	0	0	0
			812	514	146	149	3			
39	DF	100	Total	C	N	O	S	0	0	0
			820	518	147	152	3			

- Molecule 40 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BG	155	Total	C	N	O	S	0	0	0
			1231	766	243	216	6			
40	DG	155	Total	C	N	O	S	0	0	0
			1235	769	244	216	6			

- Molecule 41 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BH	137	Total	C	N	O	S	0	0	0
			1088	689	206	191	2			
41	DH	137	Total	C	N	O	S	0	0	0
			1088	689	206	191	2			

- Molecule 42 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
42	BI	127	Total	C	N	O	0	0	0
			986	626	193	167			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
42	DI	127	Total 978	C 619	N 190	O 169	0	0	0

- Molecule 43 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
43	BJ	97	Total 709	C 440	N 138	O 131	0	0	0
43	DJ	96	Total 714	C 445	N 138	O 131	0	0	0

- Molecule 44 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BK	114	Total 833	C 519	N 156	O 155	S 3	0	0	0
44	DK	114	Total 833	C 519	N 156	O 155	S 3	0	0	0

- Molecule 45 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BL	122	Total 930	C 585	N 185	O 159	S 1	0	0	0
45	DL	122	Total 930	C 585	N 185	O 159	S 1	0	0	0

- Molecule 46 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BM	123	Total 966	C 598	N 200	O 166	S 2	0	0	0
46	DM	122	Total 950	C 586	N 197	O 165	S 2	0	0	0

- Molecule 47 is a protein called 30S ribosomal protein S14 type Z.

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

- Molecule 48 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	BO	88	Total	C	N	O	S	0	0	0
			728	456	144	126	2			
48	DO	88	Total	C	N	O	S	0	0	0
			728	456	144	126	2			

- Molecule 49 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	BP	82	Total	C	N	O	S	0	0	0
			681	433	134	113	1			
49	DP	82	Total	C	N	O	S	0	0	0
			677	430	133	113	1			

- Molecule 50 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	BQ	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			
50	DQ	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			

- Molecule 51 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
51	BR	68	Total	C	N	O	0	0	0
			555	355	108	92			
51	DR	68	Total	C	N	O	0	0	0
			555	355	108	92			

- Molecule 52 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	BS	84	Total	C	N	O	S	0	0	0
			661	423	122	114	2			
52	DS	83	Total	C	N	O	S	0	0	0
			646	412	119	113	2			

- Molecule 53 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	BT	96	Total	C	N	O	S	0	0	0
			728	446	156	124	2			
53	DT	96	Total	C	N	O	S	0	0	0
			731	449	156	124	2			

- Molecule 54 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
54	BU	23	Total	C	N	O	0	0	0
			199	122	48	29			
54	DU	23	Total	C	N	O	0	0	0
			199	122	48	29			

- Molecule 55 is a RNA chain called mRNA.

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

- Molecule 56 is a RNA chain called A-site tRNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
56	BW	74	Total	C	N	O	P	S	0	0	0
			1599	722	287	515	73	2			
56	DW	72	Total	C	N	O	P	S	0	0	0
			1552	697	280	502	72	1			

- Molecule 57 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
57	BX	76	Total	C	N	O	P	S	0	0	0
			1635	731	296	530	76	2			
57	DX	76	Total	C	N	O	P	S	0	0	0
			1635	731	296	530	76	2			

- Molecule 58 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
58	BY	74	Total	C	N	O	P	S	0	0	0
			1581	707	285	515	73	1			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
58	DY	73	Total	C	N	O	P	S	0	0	0
			1561	698	283	507	72	1			

- Molecule 59 is a protein called 50S ribosomal protein L9,Elongation factor G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
59	BZ	728	Total	C	N	O	S	0	0	0
			5663	3599	973	1072	19			
59	DZ	730	Total	C	N	O	S	0	0	0
			5682	3611	978	1074	19			

- Molecule 60 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	AA	817	Total	Mg	0	0
			817	817		
60	AB	23	Total	Mg	0	0
			23	23		
60	AD	11	Total	Mg	0	0
			11	11		
60	AE	5	Total	Mg	0	0
			5	5		
60	AF	8	Total	Mg	0	0
			8	8		
60	AG	3	Total	Mg	0	0
			3	3		
60	AH	1	Total	Mg	0	0
			1	1		
60	AN	3	Total	Mg	0	0
			3	3		
60	AO	1	Total	Mg	0	0
			1	1		
60	AP	3	Total	Mg	0	0
			3	3		
60	AQ	3	Total	Mg	0	0
			3	3		
60	AR	2	Total	Mg	0	0
			2	2		
60	AU	4	Total	Mg	0	0
			4	4		
60	AV	4	Total	Mg	0	0
			4	4		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	AW	4	Total Mg 4 4	0	0
60	AX	1	Total Mg 1 1	0	0
60	AY	1	Total Mg 1 1	0	0
60	AZ	1	Total Mg 1 1	0	0
60	A0	5	Total Mg 5 5	0	0
60	A1	2	Total Mg 2 2	0	0
60	A2	1	Total Mg 1 1	0	0
60	A4	1	Total Mg 1 1	0	0
60	A5	3	Total Mg 3 3	0	0
60	A6	2	Total Mg 2 2	0	0
60	A7	6	Total Mg 6 6	0	0
60	A8	2	Total Mg 2 2	0	0
60	A9	1	Total Mg 1 1	0	0
60	BA	213	Total Mg 213 213	0	0
60	BB	1	Total Mg 1 1	0	0
60	BD	1	Total Mg 1 1	0	0
60	BE	1	Total Mg 1 1	0	0
60	BF	1	Total Mg 1 1	0	0
60	BK	1	Total Mg 1 1	0	0
60	BL	2	Total Mg 2 2	0	0
60	BM	1	Total Mg 1 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	BN	2	Total Mg 2 2	0	0
60	BT	1	Total Mg 1 1	0	0
60	BV	1	Total Mg 1 1	0	0
60	BW	2	Total Mg 2 2	0	0
60	BX	15	Total Mg 15 15	0	0
60	BY	2	Total Mg 2 2	0	0
60	BZ	1	Total Mg 1 1	0	0
60	CA	664	Total Mg 664 664	0	0
60	CB	13	Total Mg 13 13	0	0
60	CD	4	Total Mg 4 4	0	0
60	CE	6	Total Mg 6 6	0	0
60	CF	6	Total Mg 6 6	0	0
60	CG	1	Total Mg 1 1	0	0
60	CN	1	Total Mg 1 1	0	0
60	CO	2	Total Mg 2 2	0	0
60	CP	1	Total Mg 1 1	0	0
60	CQ	4	Total Mg 4 4	0	0
60	CR	2	Total Mg 2 2	0	0
60	CU	1	Total Mg 1 1	0	0
60	CV	2	Total Mg 2 2	0	0
60	CY	1	Total Mg 1 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	C0	2	Total Mg 2 2	0	0
60	C3	1	Total Mg 1 1	0	0
60	C5	1	Total Mg 1 1	0	0
60	C7	1	Total Mg 1 1	0	0
60	C8	1	Total Mg 1 1	0	0
60	DA	168	Total Mg 168 168	0	0
60	DD	1	Total Mg 1 1	0	0
60	DE	2	Total Mg 2 2	0	0
60	DF	1	Total Mg 1 1	0	0
60	DJ	1	Total Mg 1 1	0	0
60	DK	2	Total Mg 2 2	0	0
60	DT	1	Total Mg 1 1	0	0
60	DW	1	Total Mg 1 1	0	0
60	DX	1	Total Mg 1 1	0	0
60	DZ	1	Total Mg 1 1	0	0

- Molecule 61 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	AA	1	Total K 1 1	0	0

- Molecule 62 is ZINC ION (CCD ID: ZN) (formula: Zn).

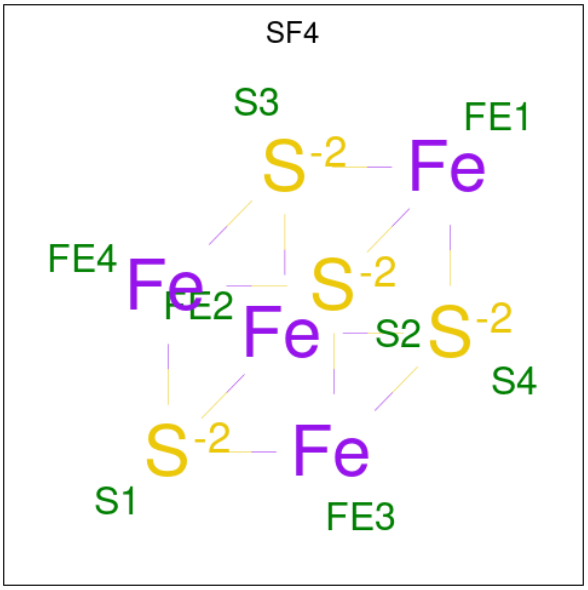
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	AY	1	Total Zn 1 1	0	0

Continued on next page...

Continued from previous page...

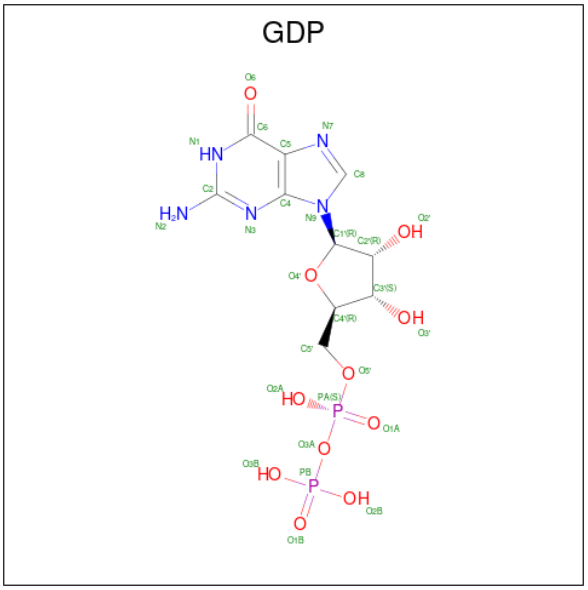
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	A4	1	Total Zn 1 1	0	0
62	A5	1	Total Zn 1 1	0	0
62	A6	1	Total Zn 1 1	0	0
62	A9	1	Total Zn 1 1	0	0
62	BN	1	Total Zn 1 1	0	0
62	CY	1	Total Zn 1 1	0	0
62	C4	1	Total Zn 1 1	0	0
62	C5	1	Total Zn 1 1	0	0
62	C6	1	Total Zn 1 1	0	0
62	C9	1	Total Zn 1 1	0	0
62	DN	1	Total Zn 1 1	0	0

- Molecule 63 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
63	BD	1	Total Fe S 8 4 4	0	0
63	DD	1	Total Fe S 8 4 4	0	0

- Molecule 64 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
64	BZ	1	Total C N O P 28 10 5 11 2	0	0
64	DZ	1	Total C N O P 28 10 5 11 2	0	0

- Molecule 65 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
65	AA	1408	Total O 1408 1408	0	0
65	AB	36	Total O 36 36	0	0
65	AD	15	Total O 15 15	0	0
65	AE	19	Total O 19 19	0	0
65	AF	7	Total O 7 7	0	0
65	AG	3	Total O 3 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
65	AH	1	Total O 1 1	0	0
65	AN	2	Total O 2 2	0	0
65	AO	1	Total O 1 1	0	0
65	AP	15	Total O 15 15	0	0
65	AQ	4	Total O 4 4	0	0
65	AR	2	Total O 2 2	0	0
65	AS	1	Total O 1 1	0	0
65	AT	2	Total O 2 2	0	0
65	AU	5	Total O 5 5	0	0
65	AV	2	Total O 2 2	0	0
65	AW	2	Total O 2 2	0	0
65	AX	3	Total O 3 3	0	0
65	AZ	1	Total O 1 1	0	0
65	A0	6	Total O 6 6	0	0
65	A1	1	Total O 1 1	0	0
65	A3	1	Total O 1 1	0	0
65	A5	3	Total O 3 3	0	0
65	A6	2	Total O 2 2	0	0
65	A7	4	Total O 4 4	0	0
65	A8	10	Total O 10 10	0	0
65	BA	212	Total O 212 212	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
65	BD	2	Total O 2 2	0	0
65	BE	2	Total O 2 2	0	0
65	BL	1	Total O 1 1	0	0
65	BM	1	Total O 1 1	0	0
65	BV	2	Total O 2 2	0	0
65	BW	3	Total O 3 3	0	0
65	BX	8	Total O 8 8	0	0
65	BY	1	Total O 1 1	0	0
65	BZ	2	Total O 2 2	0	0
65	CA	985	Total O 985 985	0	0
65	CB	9	Total O 9 9	0	0
65	CD	14	Total O 14 14	0	0
65	CE	13	Total O 13 13	0	0
65	CF	7	Total O 7 7	0	0
65	CN	2	Total O 2 2	0	0
65	CP	10	Total O 10 10	0	0
65	CQ	1	Total O 1 1	0	0
65	CR	1	Total O 1 1	0	0
65	CT	3	Total O 3 3	0	0
65	CU	2	Total O 2 2	0	0
65	CV	1	Total O 1 1	0	0

Continued on next page...

Continued from previous page...

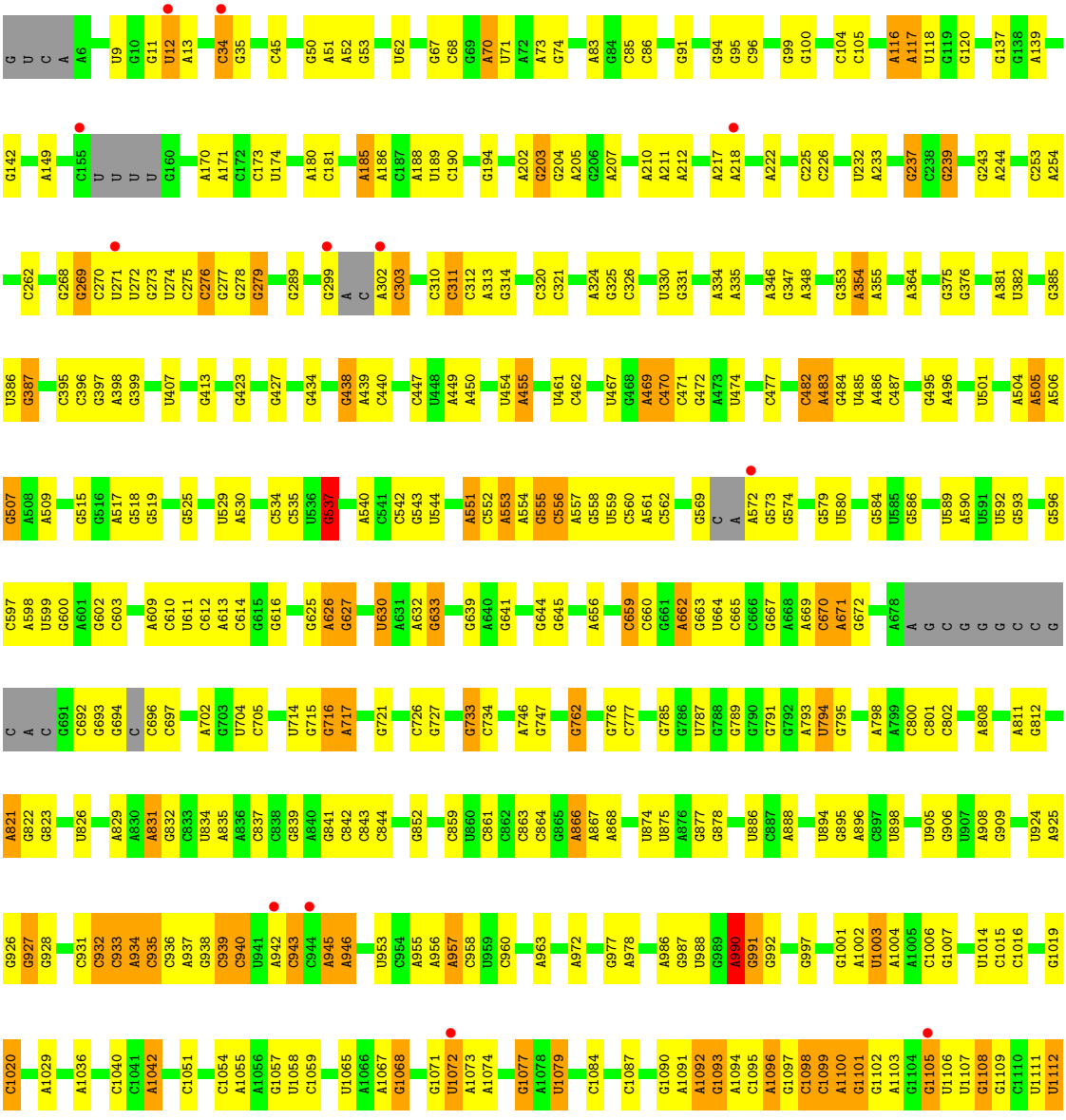
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
65	CY	1	Total O 1 1	0	0
65	C0	6	Total O 6 6	0	0
65	C1	2	Total O 2 2	0	0
65	C3	2	Total O 2 2	0	0
65	C6	1	Total O 1 1	0	0
65	C7	1	Total O 1 1	0	0
65	C8	3	Total O 3 3	0	0
65	DA	155	Total O 155 155	0	0
65	DE	4	Total O 4 4	0	0
65	DJ	1	Total O 1 1	0	0
65	DK	2	Total O 2 2	0	0
65	DL	1	Total O 1 1	0	0
65	DW	2	Total O 2 2	0	0
65	DX	1	Total O 1 1	0	0

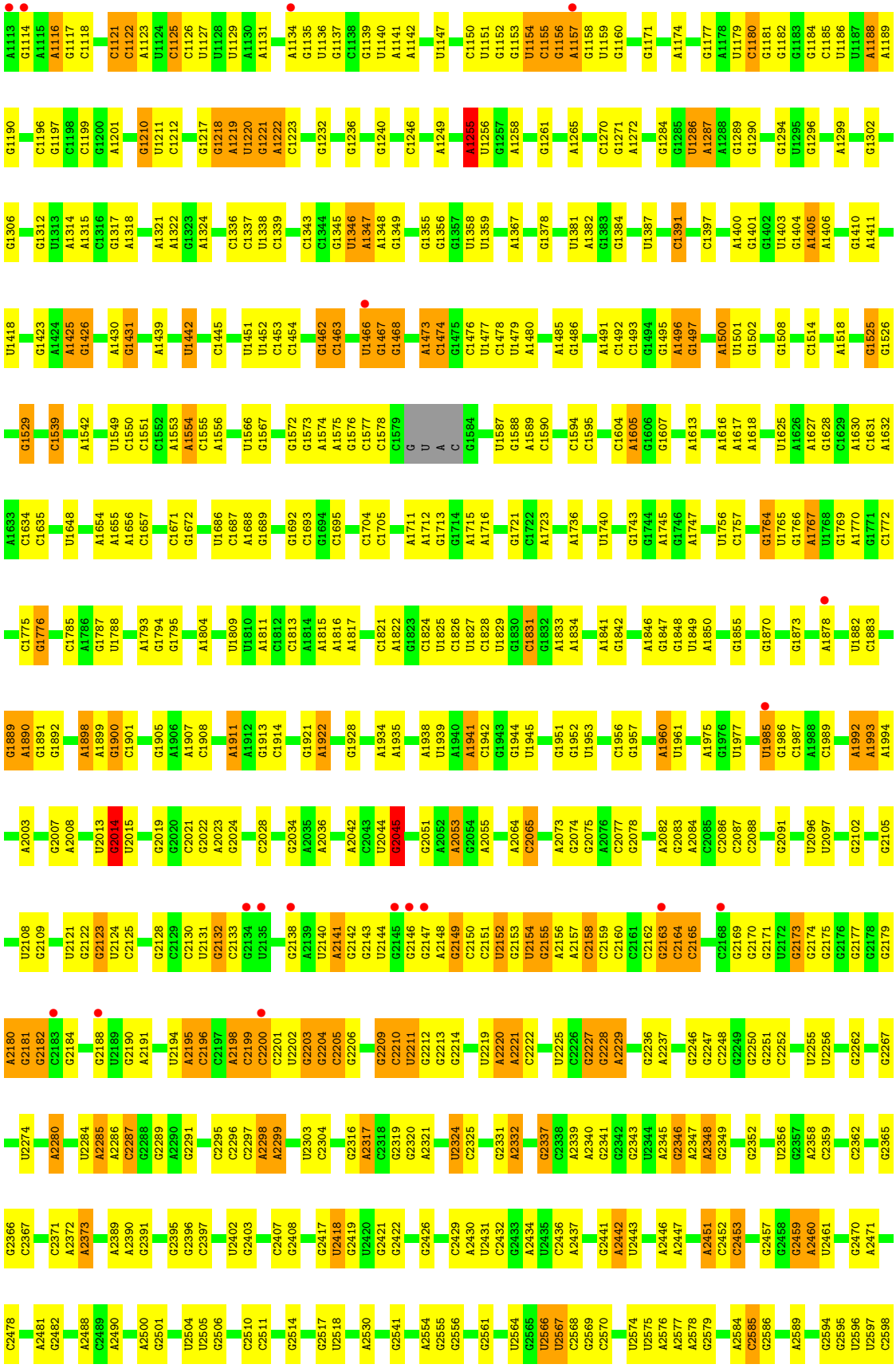
3 Residue-property plots (i)

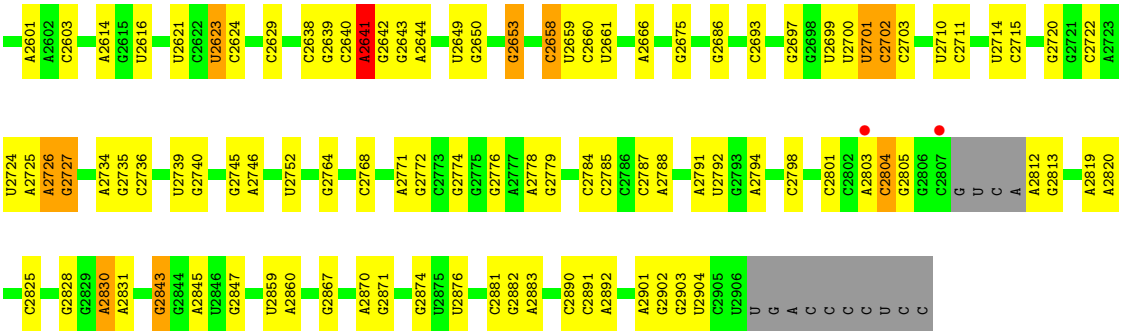
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: 23S Ribosomal RNA

Chain AA:

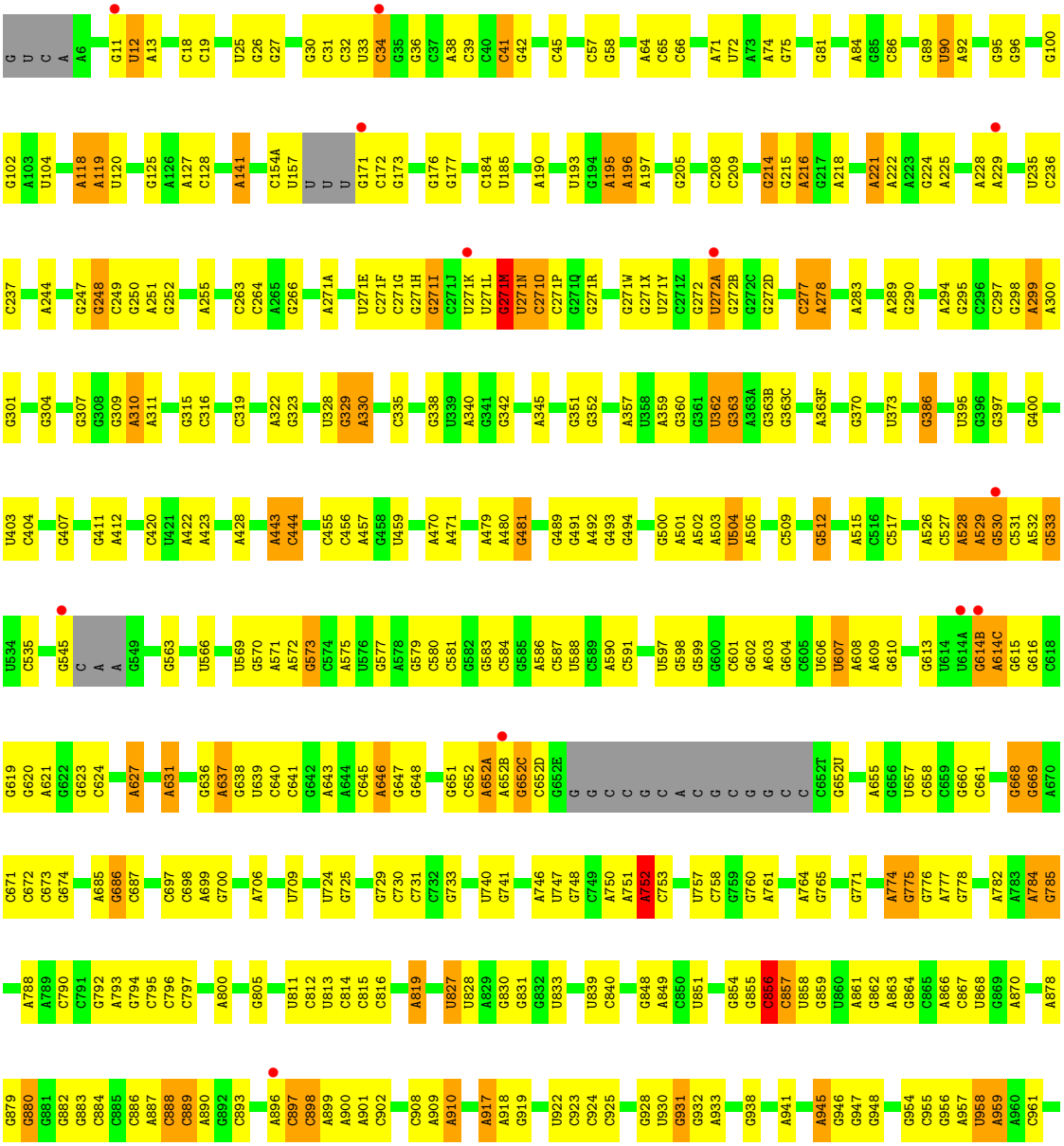


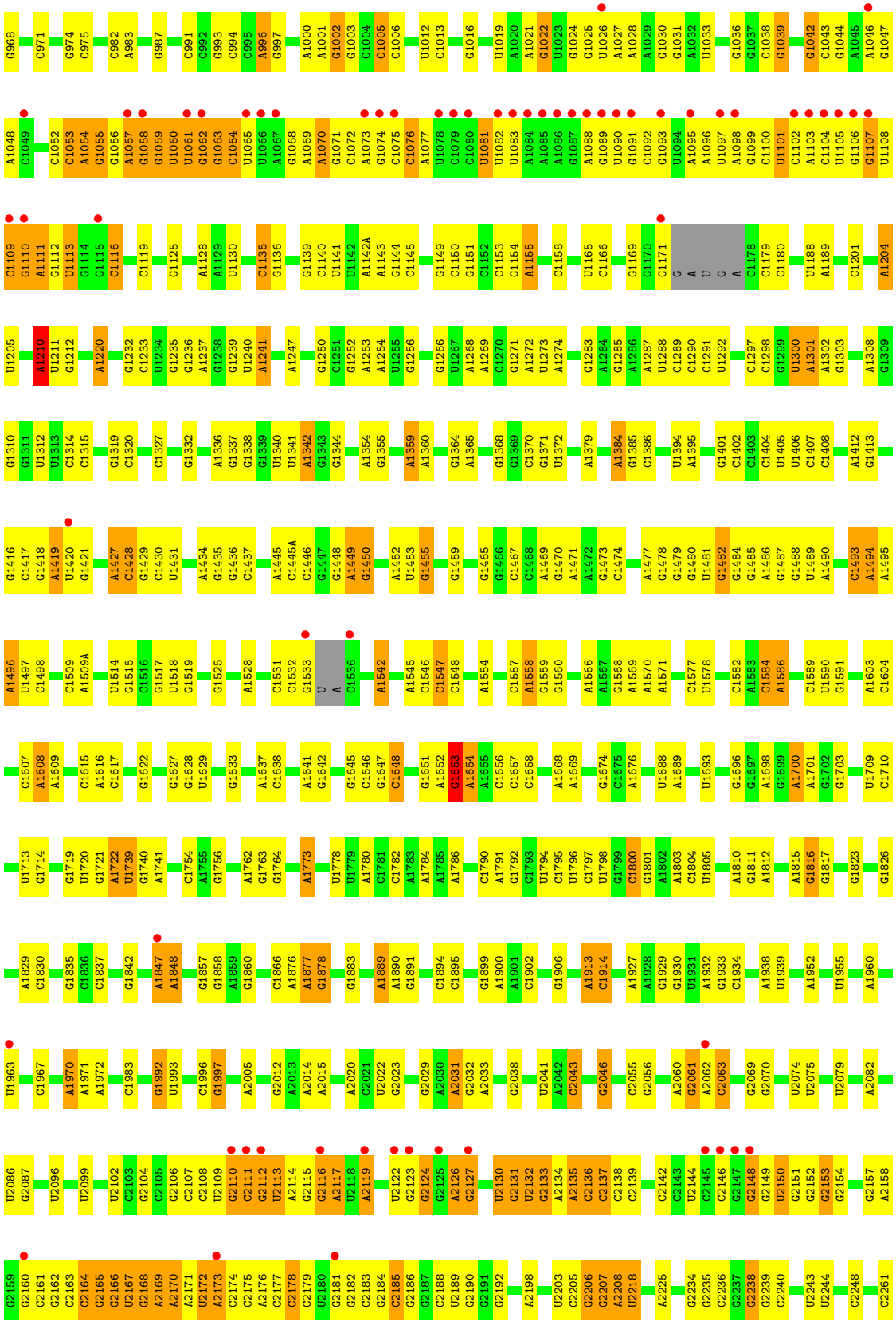


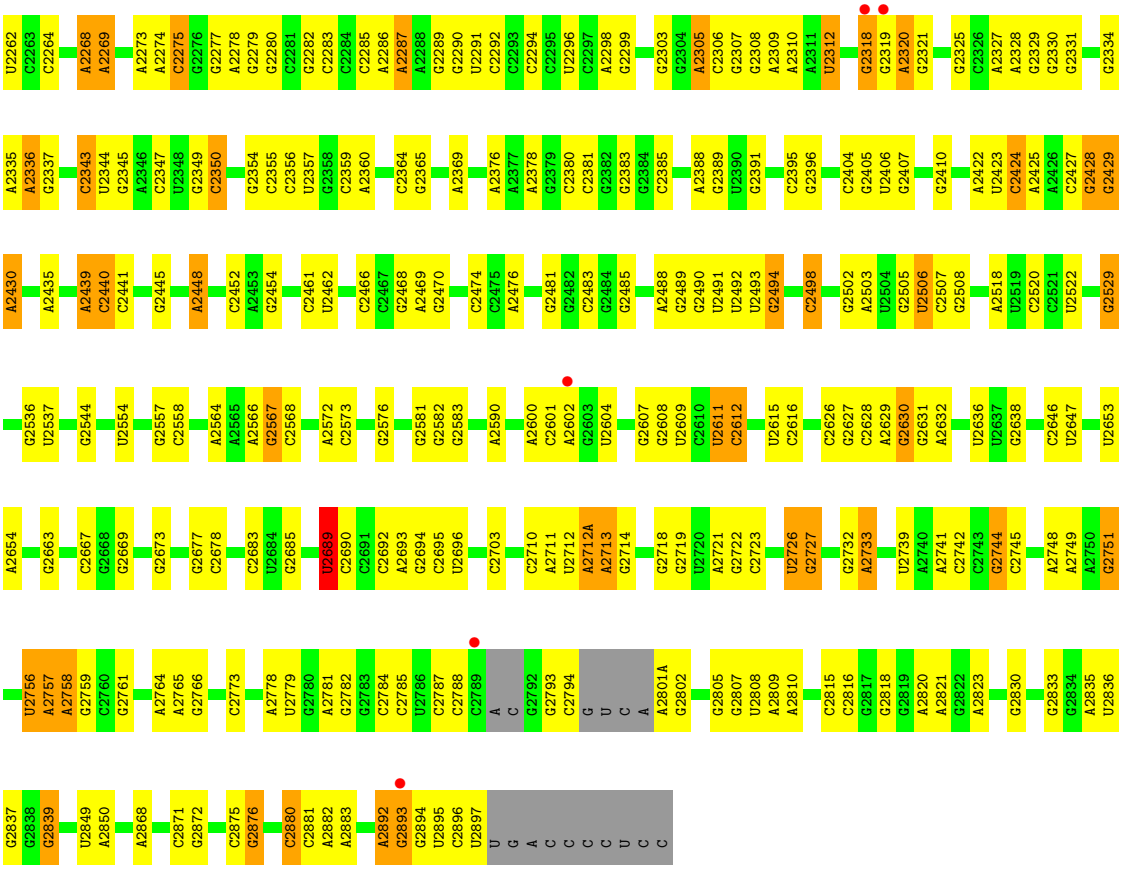


• Molecule 1: 23S Ribosomal RNA

Chain CA:

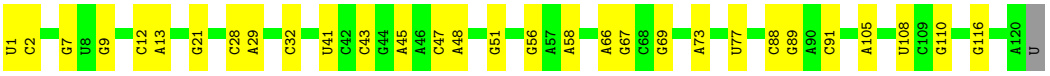



G968 C971 G974 C975 C982 A983 G987 C991 G992 G993 C994 C995 A996 G997 A1000 A1001 G1002 G1003 C1004 C1005 C1006 U1012 C1013 G1016 U1019 A1020 A1021 G1022 U1023 G1024 G1025 U1026 A1027 A1028 A1029 G1030 G1031 A1032 U1033 G1036 G1037 C1038 G1039 G1042 C1043 G1044 A1045 A1046 G1047
A1048 C1049 C1052 C1053 A1054 G1055 G1056 A1057 G1058 G1059 U1060 U1061 G1062 G1063 C1064 U1065 U1066 A1067 G1068 A1069 A1070 G1071 C1072 A1073 G1074 C1075 C1076 A1077 U1078 C1079 C1080 U1081 U1082 U1083 A1084 A1085 A1086 G1087 A1088 G1089 U1090 G1091 C1092 G1093 U1094 A1095 A1096 U1097 A1098 G1099 C1100 U1101 C1102 A1103 C1104 U1105 G1106 G1107 U1108
C1109 G1110 A1111 G1112 U1113 G1114 G1115 C1116 C1119 G1125 A1128 A1129 U1130 C1135 G1136 G1139 C1140 U1141 U1142 A1142A A1143 G1144 C1145 G1149 C1150 G1151 C1152 C1153 G1154 A1155 C1158 U1165 C1166 G1169 G1170 G1171 G A U G A C1178 C1179 C1180 U1188 A1189 C1201 A1204
U1205 A1210 U1211 G1212 A1220 G1232 C1233 U1234 G1235 G1236 A1237 G1238 G1239 U1240 A1241 A1247 G1250 C1251 G1252 A1253 A1254 U1255 G1256 G1266 U1267 A1268 A1269 C1270 G1271 A1272 U1273 A1274 G1283 A1284 G1285 A1286 A1287 U1288 C1289 C1290 C1291 U1292 C1297 C1298 G1299 U1300 A1301 A1302 G1303 A1308 G1309
G1310 G1311 U1312 U1313 C1314 C1315 G1319 C1320 C1327 G1332 A1336 G1337 G1338 G1339 U1340 U1341 A1342 G1343 G1344 A1354 G1355 A1359 A1360 G1364 A1365 G1368 G1369 C1370 G1371 U1372 A1379 A1384 G1385 C1386 U1394 A1395 G1401 C1402 C1403 C1404 U1405 U1406 C1407 C1408 A1412 G1413
G1416 C1417 G1418 A1419 U1420 G1421 A1427 C1428 G1429 C1430 U1431 A1434 G1435 G1436 C1437 A1445 C1445A C1446 G1447 G1448 A1449 G1450 A1452 U1453 G1455 G1459 G1465 G1466 C1467 C1468 A1469 G1470 A1471 A1472 G1473 C1474 A1477 G1478 G1479 G1480 U1481 G1482 G1484 G1485 A1486 G1487 G1488 U1489 A1490 C1493 A1494 A1495
A1496 U1497 C1498 C1509 A1509A U1514 G1515 C1516 G1517 U1518 G1519 C1525 A1528 C1531 C1532 G1533 U A C1536 A1542 A1545 C1546 C1547 C1548 A1554 C1557 A1558 G1559 G1560 A1566 A1567 G1568 A1569 A1570 A1571 C1577 U1578 C1582 A1583 C1584 A1586 C1589 U1590 G1591 A1603 C1604
C1607 A1608 A1609 C1615 A1616 C1617 G1622 G1627 G1628 U1629 G1633 A1637 C1638 A1641 G1642 G1645 C1646 G1647 C1648 G1651 A1652 G1653 A1654 A1655 C1656 C1657 C1658 A1668 A1669 G1674 C1675 A1676 U1688 A1689 U1693 G1696 G1697 A1698 G1699 A1700 A1701 G1702 G1703 U1709 C1710
U1713 G1714 G1719 U1720 G1721 A1722 U1739 G1740 A1741 C1754 A1755 G1756 A1762 G1763 G1764 A1773 U1778 U1779 A1780 C1781 C1782 A1783 A1784 A1785 A1786 C1790 A1791 G1792 C1793 U1794 C1795 U1796 C1797 U1798 C1799 C1800 G1801 A1802 A1803 C1804 U1805 A1810 G1811 A1812 A1815 G1816 G1817 G1823 G1826
A1829 C1830 G1835 C1836 C1837 G1842 A1847 A1848 G1857 G1858 A1859 G1860 C1866 A1876 A1877 G1878 G1883 A1889 A1890 G1891 C1894 C1895 G1899 A1900 A1901 C1902 G1906 A1913 C1914 A1927 A1928 G1929 G1930 U1931 A1932 G1933 C1934 A1938 U1939 A1952 U1955 A1960
U1963 C1967 A1970 A1971 A1972 C1983 G1992 U1993 C1996 G1997 A2005 G2012 A2013 A2014 A2015 A2020 C2021 U2022 G2023 G2029 A2030 A2031 G2032 A2033 G2038 U2041 A2042 C2043 G2046 C2055 G2056 A2060 G2061 A2062 C2063 G2069 G2070 U2074 U2075 U2079 A2082
U2086 G2087 U2096 U2099 U2102 C2103 G2104 C2105 G2106 C2107 C2108 U2109 G2110 C2111 G2112 U2113 A2114 G2115 G2116 A2117 U2118 A2119 U2122 G2123 G2124 G2125 A2126 G2127 U2130 G2131 U2132 G2133 A2134 A2135 C2136 C2137 C2138 C2139 C2142 G2143 U2144 C2145 C2146 G2147 G2148 G2149 U2150 G2151 G2152 G2153 G2154 G2157 A2158
G2159 G2160 C2161 G2162 C2163 C2164 G2165 G2166 U2167 G2168 A2169 A2170 A2171 U2172 A2173 C2174 C2175 A2176 C2177 C2178 C2179 U2180 G2181 A2182 C2183 G2184 C2185 G2186 G2187 C2188 U2189 G2190 G2191 G2192 A2198 U2203 C2205 G2206 G2207 A2208 U2218 A2225 G2234 G2235 C2236 G2237 G2238 G2239 C2240 U2243 U2244 C2248 C2261



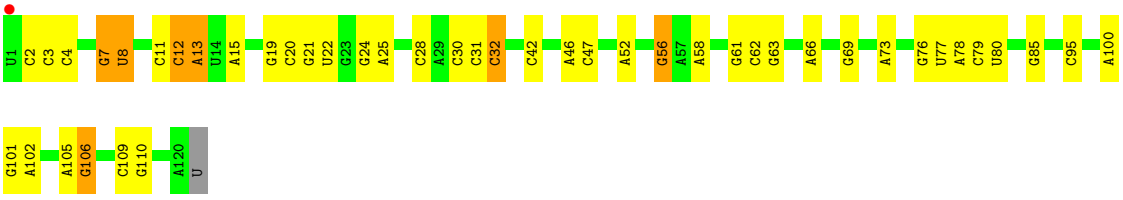
• Molecule 2: 5S Ribosomal RNA

Chain AB:



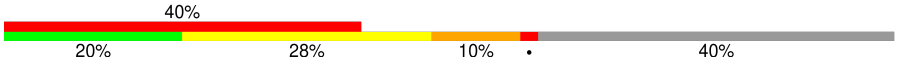
• Molecule 2: 5S Ribosomal RNA

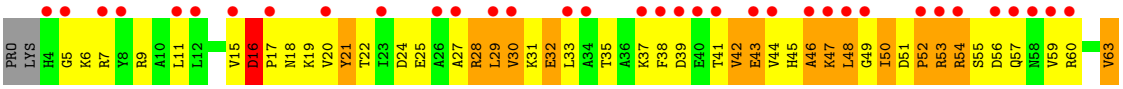
Chain CB:

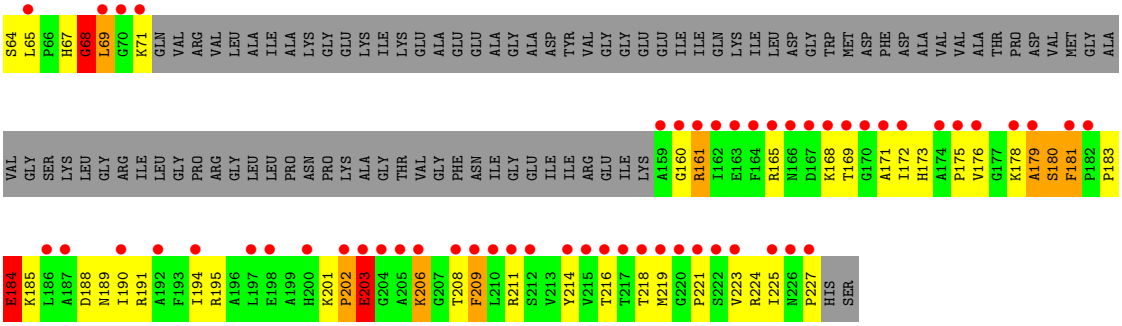


• Molecule 3: 50S ribosomal protein L1

Chain AC:

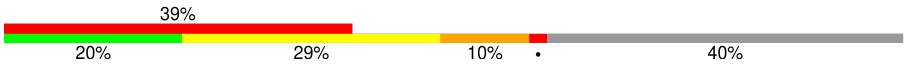


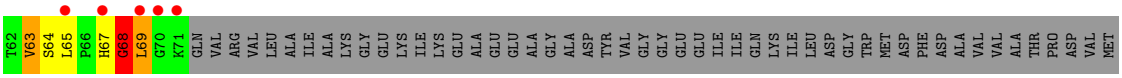


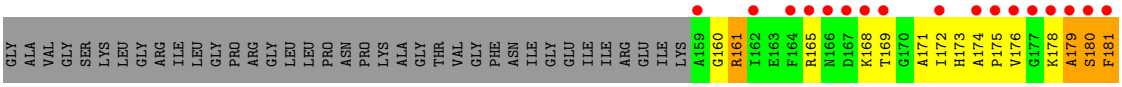


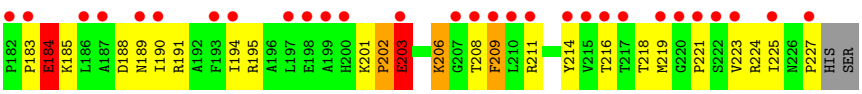
• Molecule 3: 50S ribosomal protein L1

Chain CC:



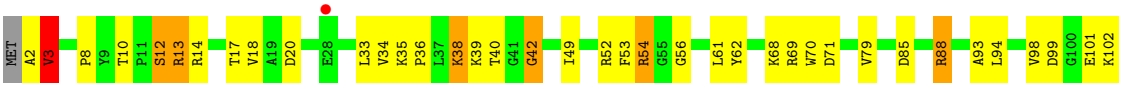


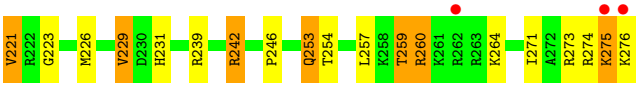




• Molecule 4: 50S ribosomal protein L2

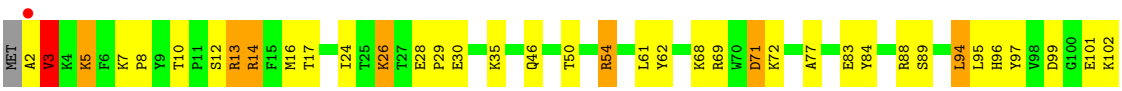
Chain AD:

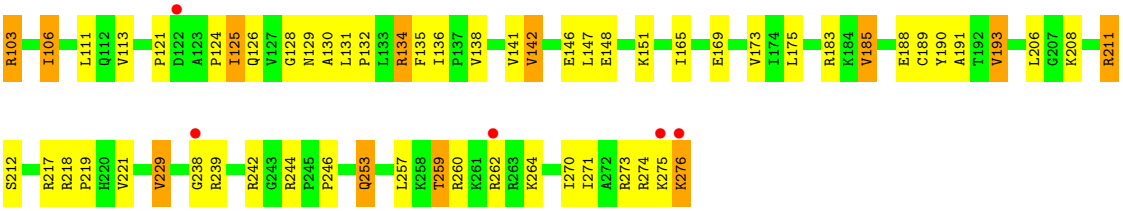




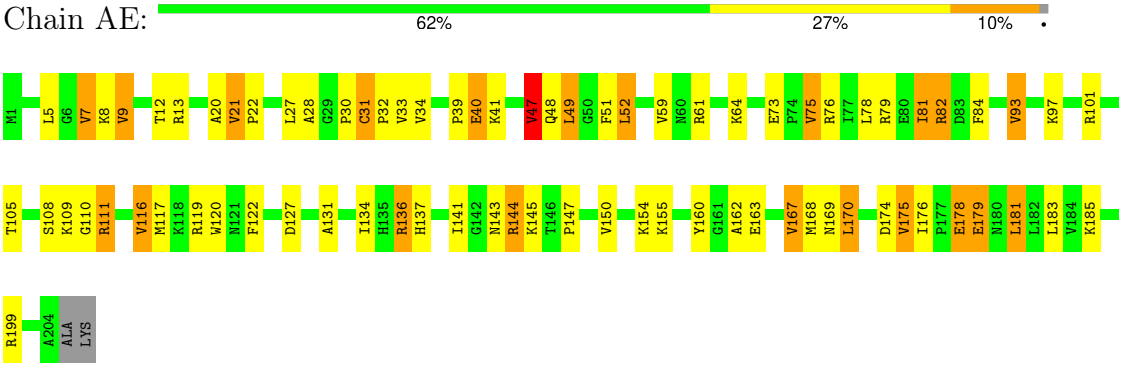
• Molecule 4: 50S ribosomal protein L2

Chain CD:

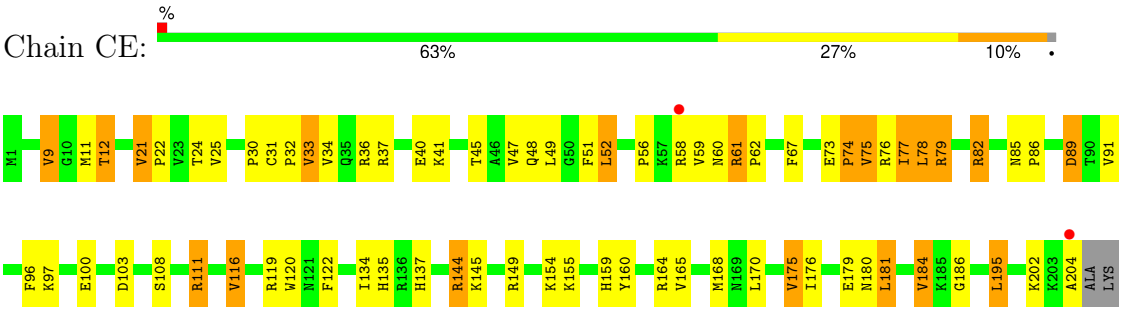




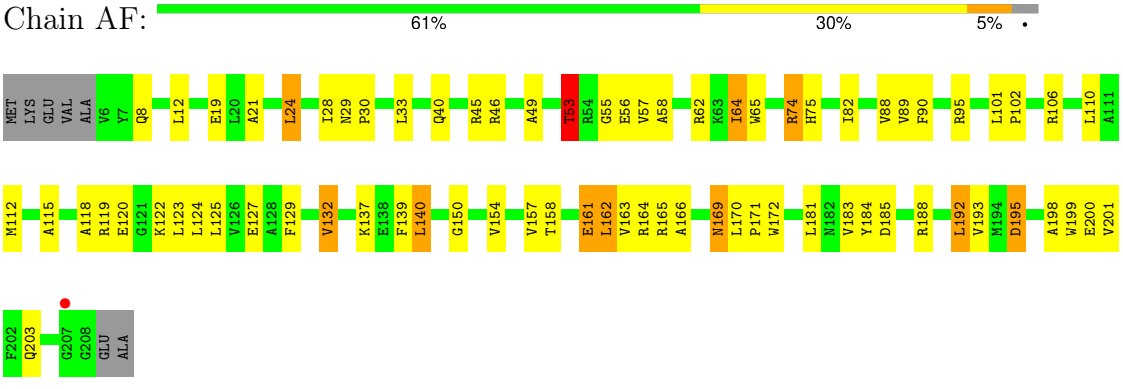
• Molecule 5: 50S ribosomal protein L3



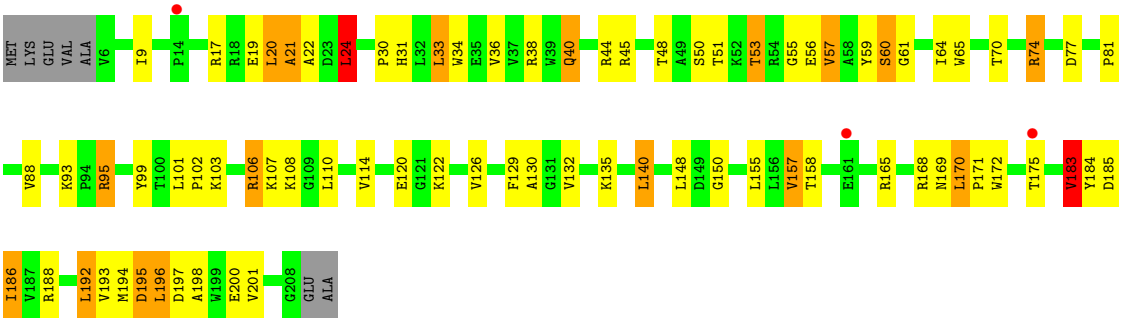
• Molecule 5: 50S ribosomal protein L3



• Molecule 6: 50S ribosomal protein L4

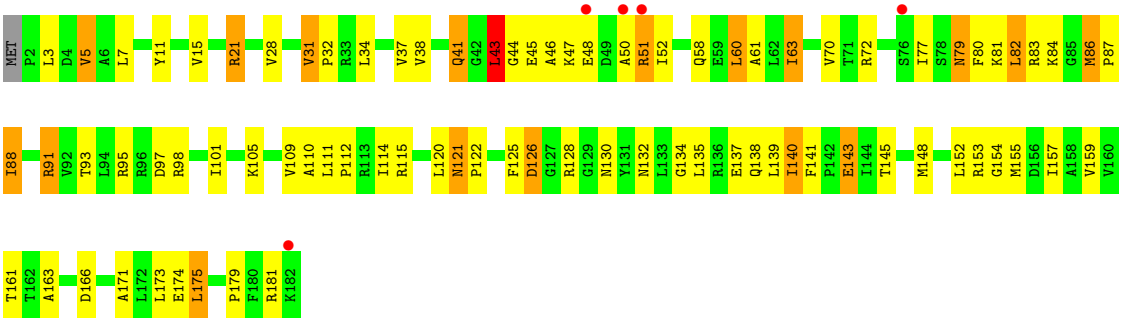


• Molecule 6: 50S ribosomal protein L4



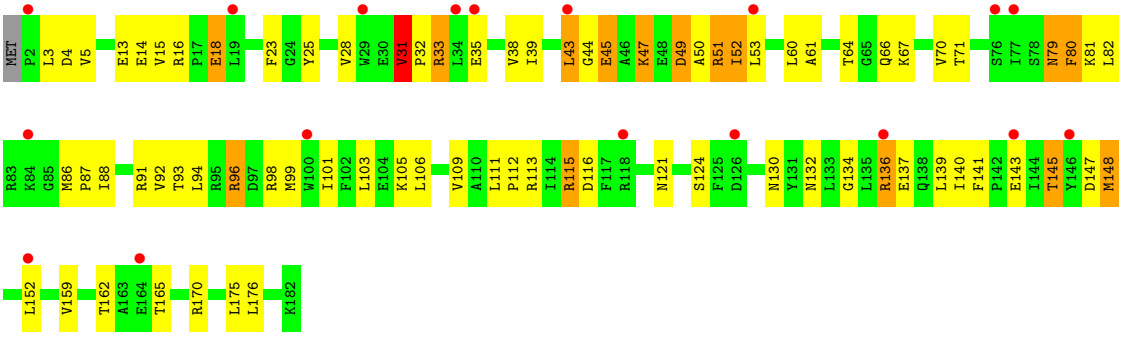
• Molecule 7: 50S ribosomal protein L5

Chain AG:



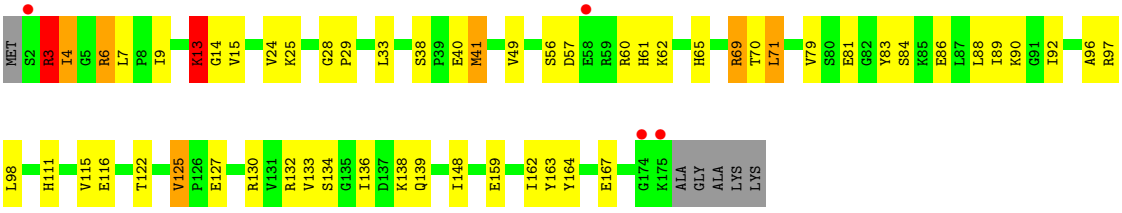
• Molecule 7: 50S ribosomal protein L5

Chain CG:



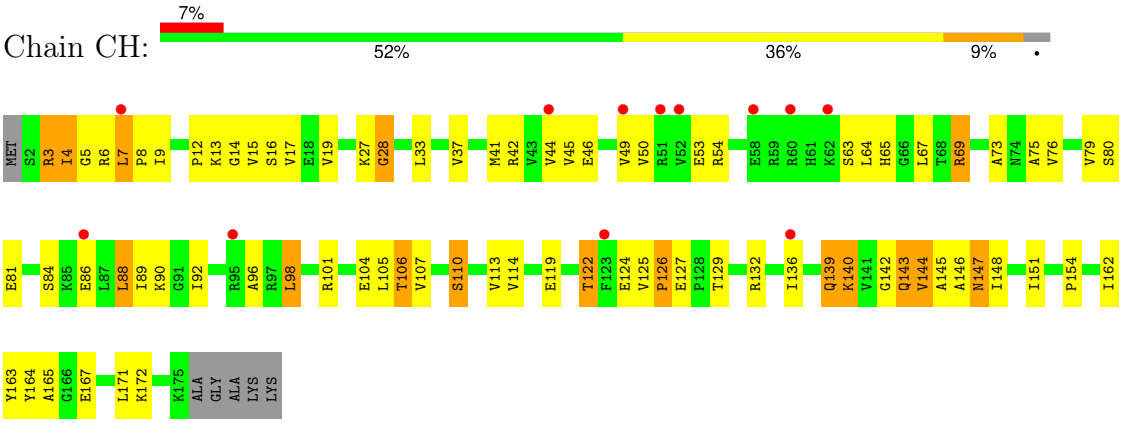
• Molecule 8: 50S ribosomal protein L6

Chain AH:



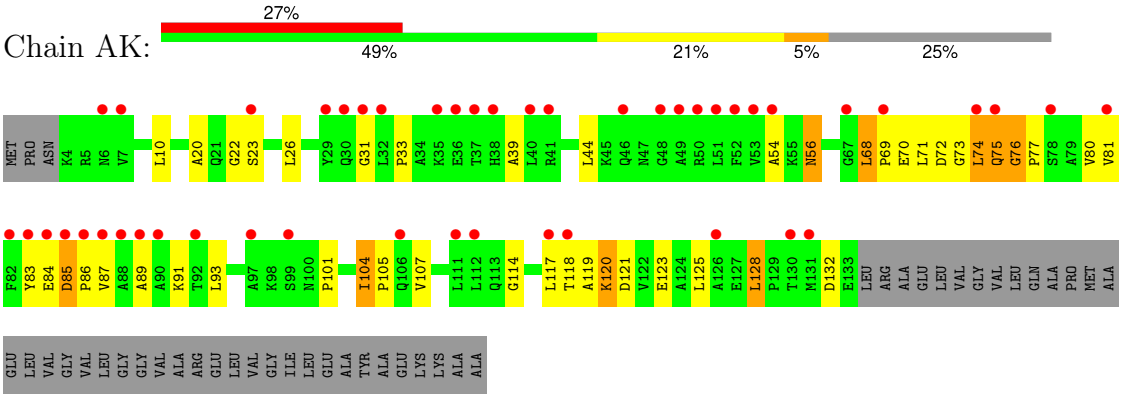
• Molecule 8: 50S ribosomal protein L6

Chain CH:



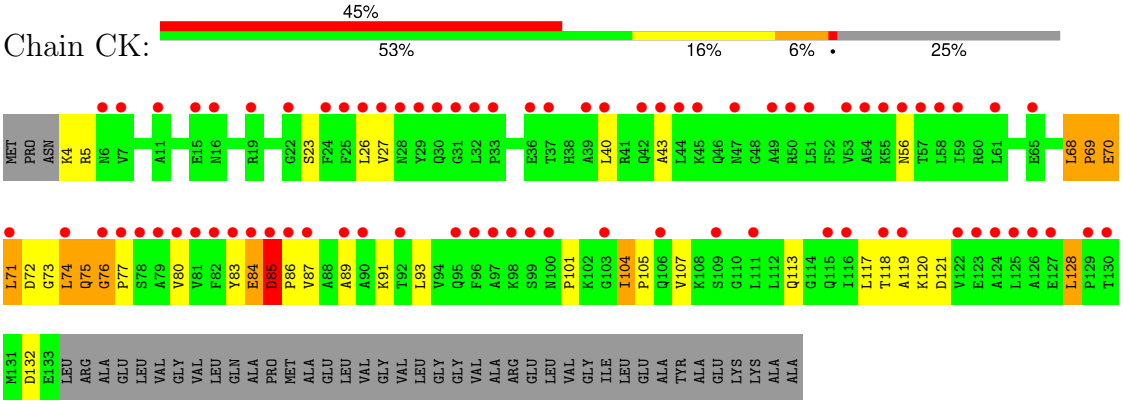
• Molecule 9: 50S ribosomal protein L10

Chain AK:



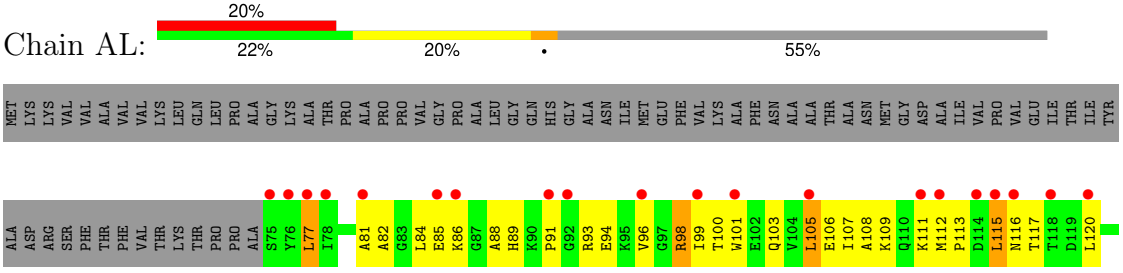
• Molecule 9: 50S ribosomal protein L10

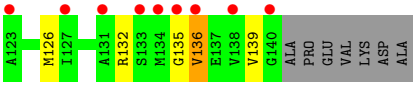
Chain CK:



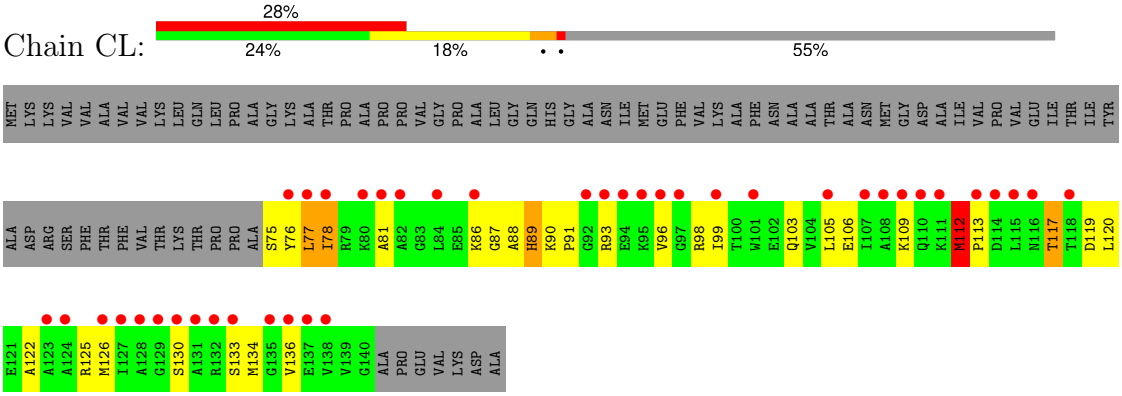
• Molecule 10: 50S ribosomal protein L11

Chain AL:

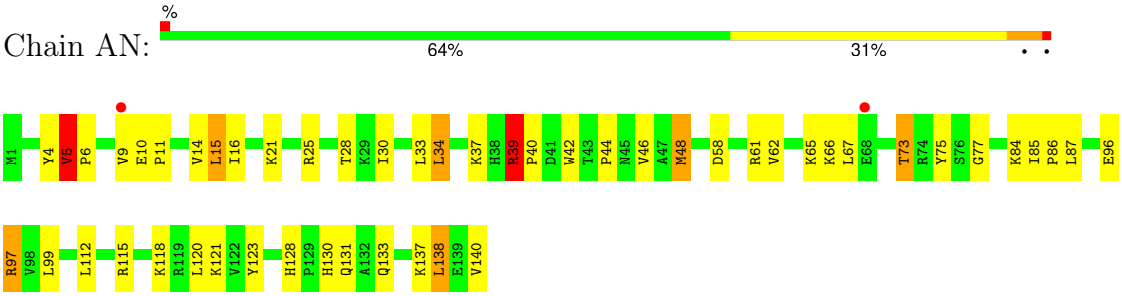




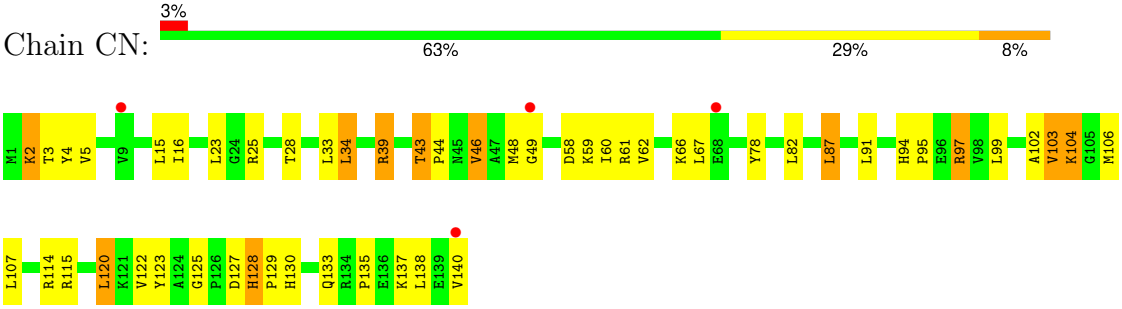
• Molecule 10: 50S ribosomal protein L11



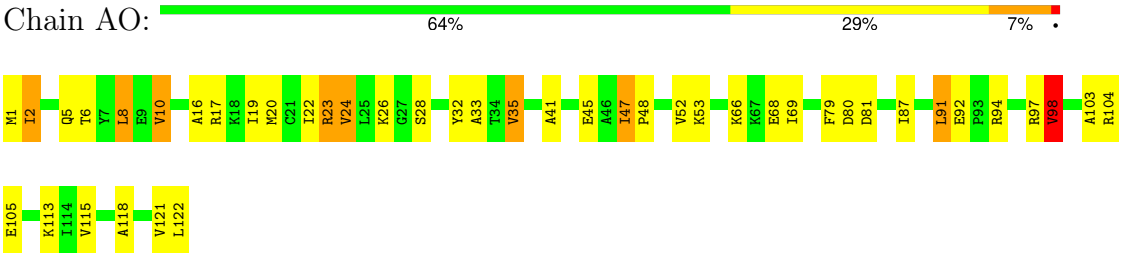
• Molecule 11: 50S ribosomal protein L13



• Molecule 11: 50S ribosomal protein L13

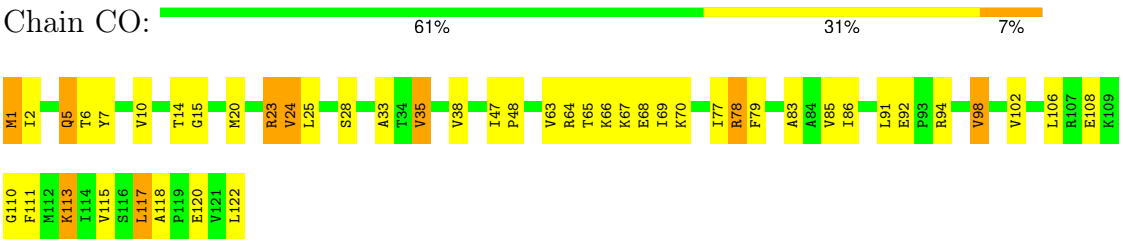


• Molecule 12: 50S ribosomal protein L14



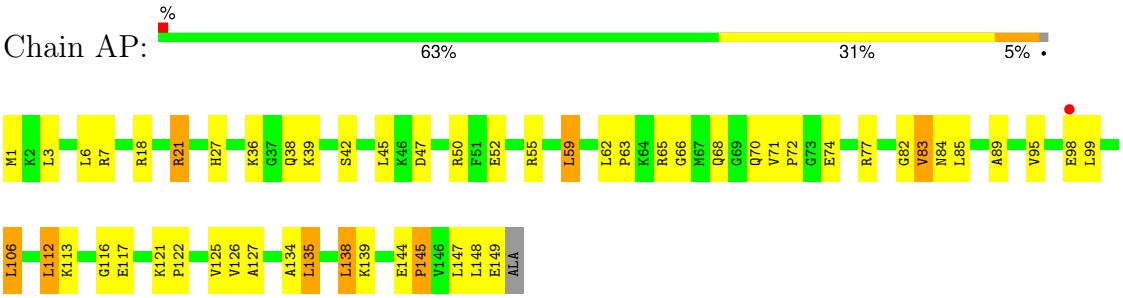
• Molecule 12: 50S ribosomal protein L14

Chain CO:



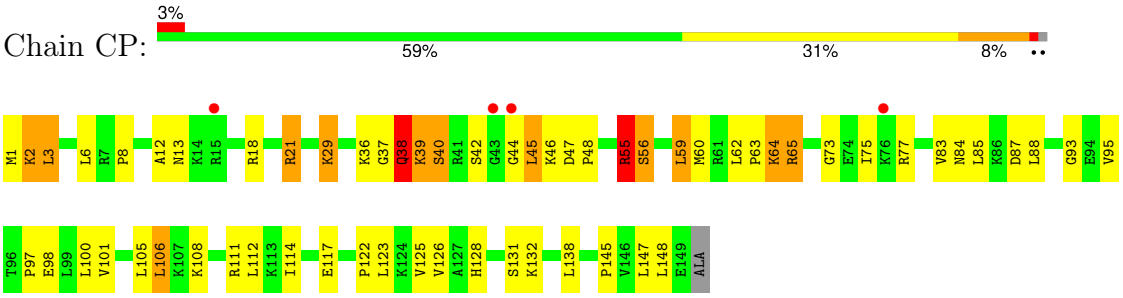
• Molecule 13: 50S ribosomal protein L15

Chain AP:



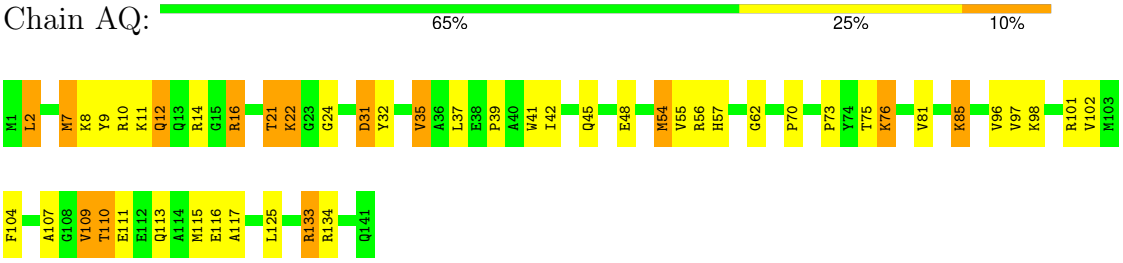
• Molecule 13: 50S ribosomal protein L15

Chain CP:



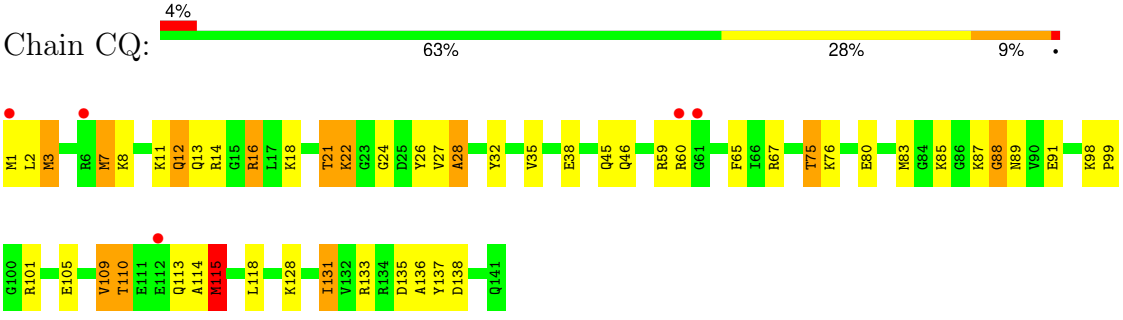
• Molecule 14: 50S ribosomal protein L16

Chain AQ:



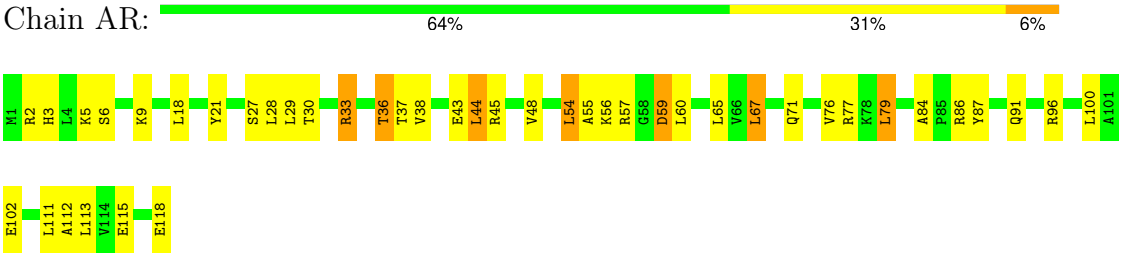
• Molecule 14: 50S ribosomal protein L16

Chain CQ:



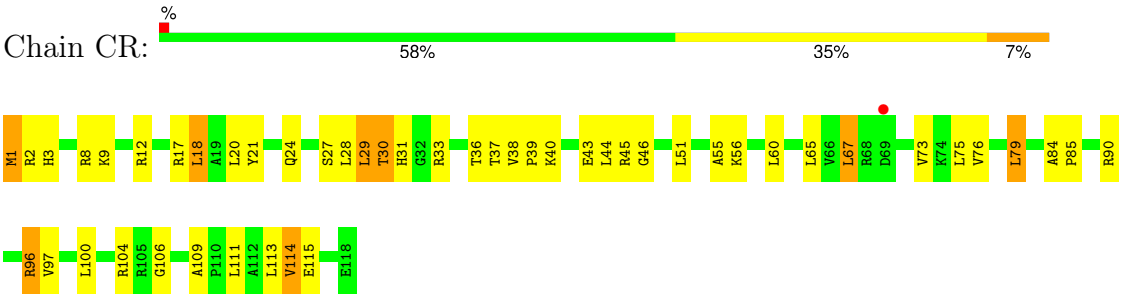
• Molecule 15: 50S ribosomal protein L17

Chain AR:



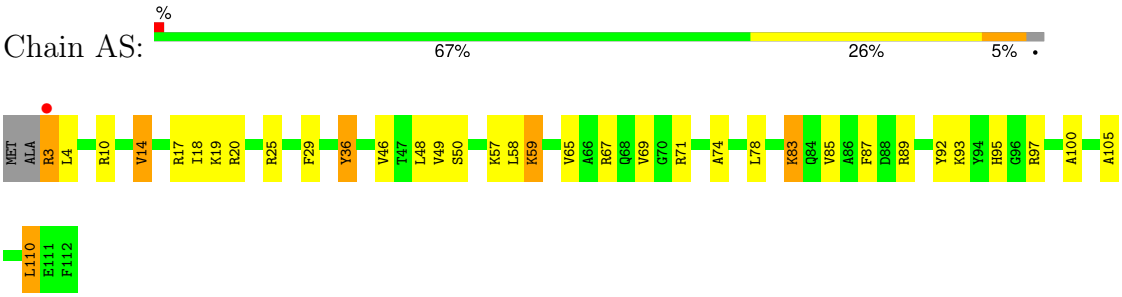
• Molecule 15: 50S ribosomal protein L17

Chain CR:



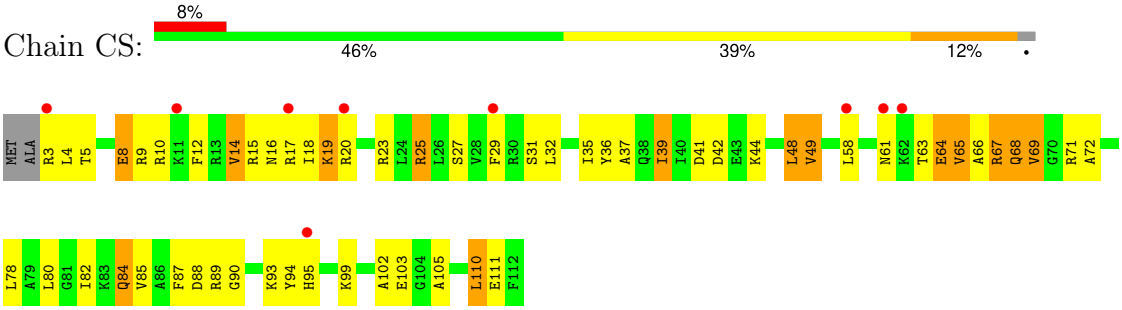
• Molecule 16: 50S ribosomal protein L18

Chain AS:



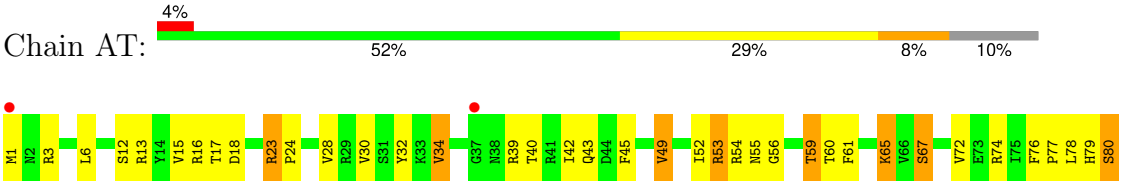
• Molecule 16: 50S ribosomal protein L18

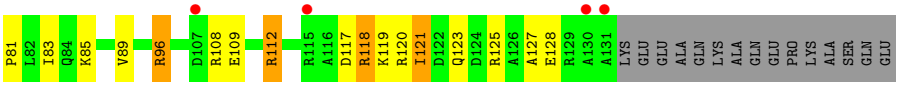
Chain CS:



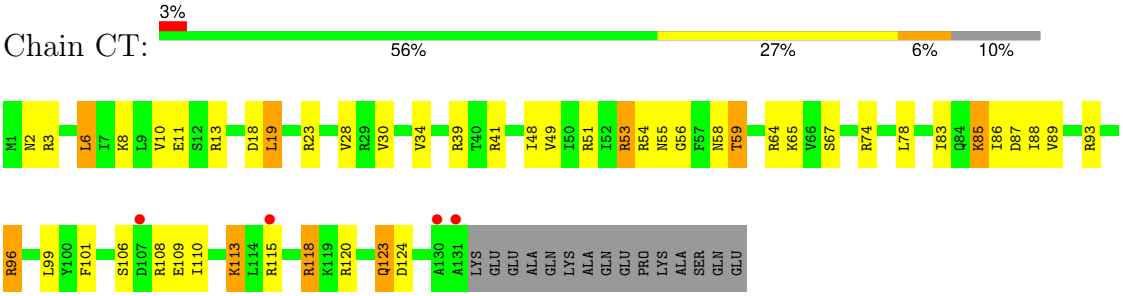
• Molecule 17: 50S ribosomal protein L19

Chain AT:

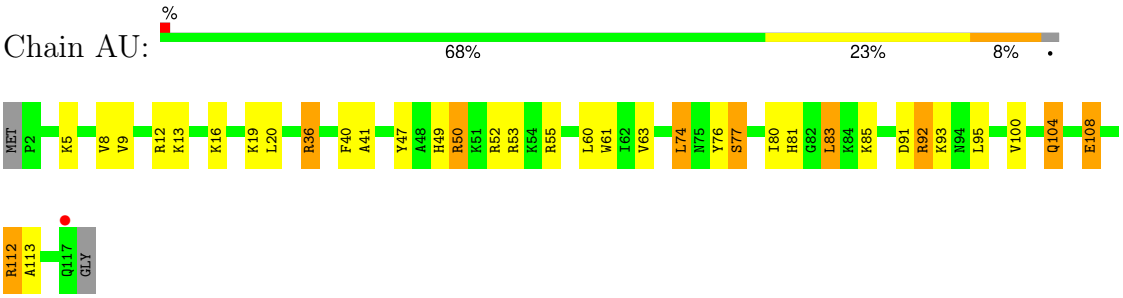




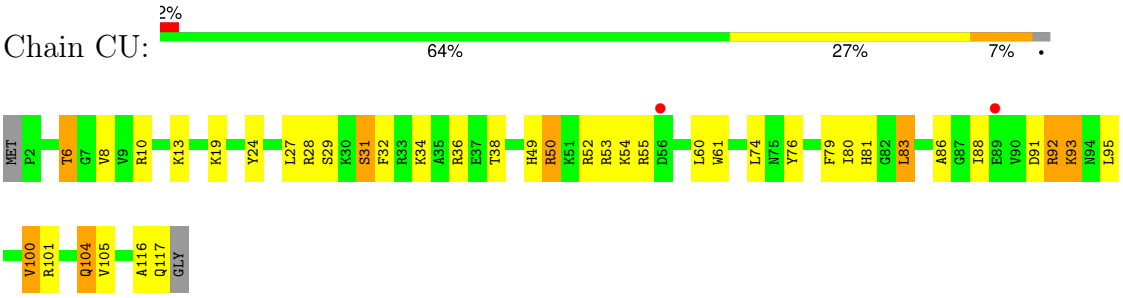
• Molecule 17: 50S ribosomal protein L19



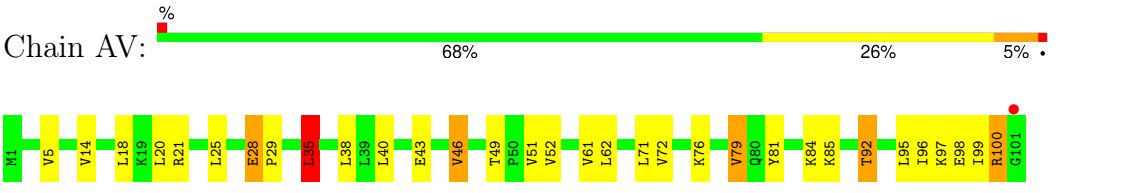
• Molecule 18: 50S ribosomal protein L20



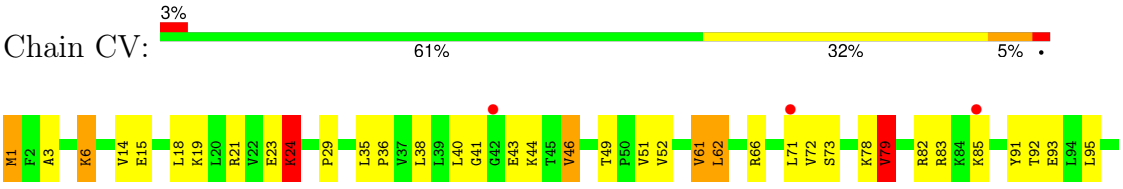
• Molecule 18: 50S ribosomal protein L20



• Molecule 19: 50S ribosomal protein L21

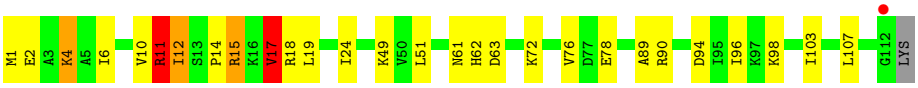


• Molecule 19: 50S ribosomal protein L21



• Molecule 20: 50S ribosomal protein L22

Chain AW:

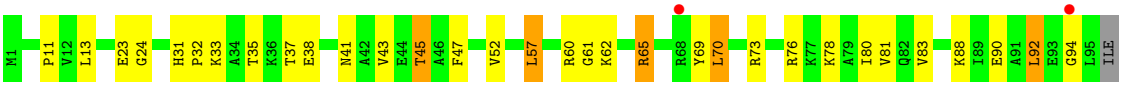


• Molecule 20: 50S ribosomal protein L22

Chain CW:

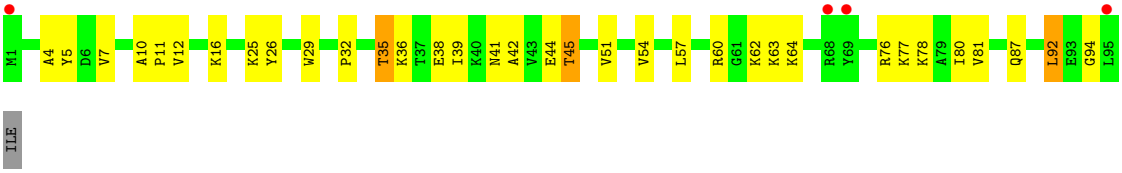
• Molecule 21: 50S ribosomal protein L23

Chain AX:



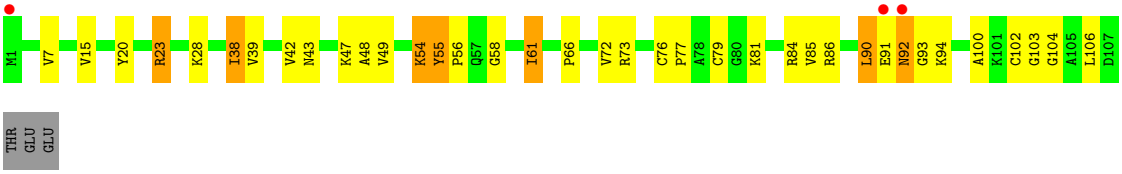
• Molecule 21: 50S ribosomal protein L23

Chain CX:



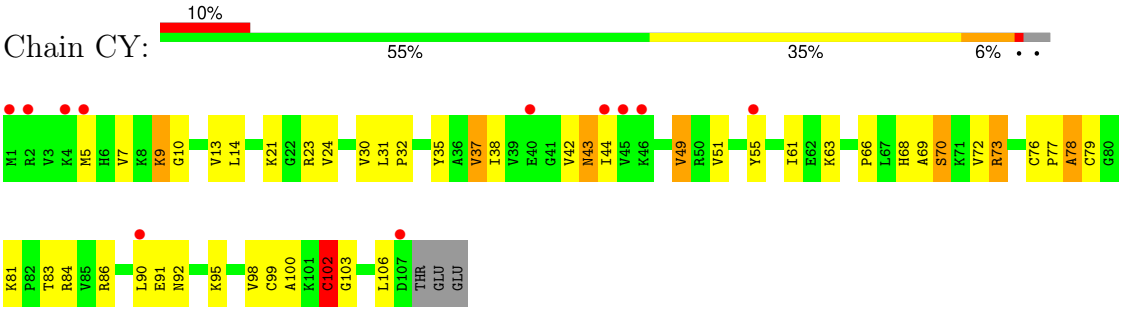
• Molecule 22: 50S ribosomal protein L24

Chain AY:



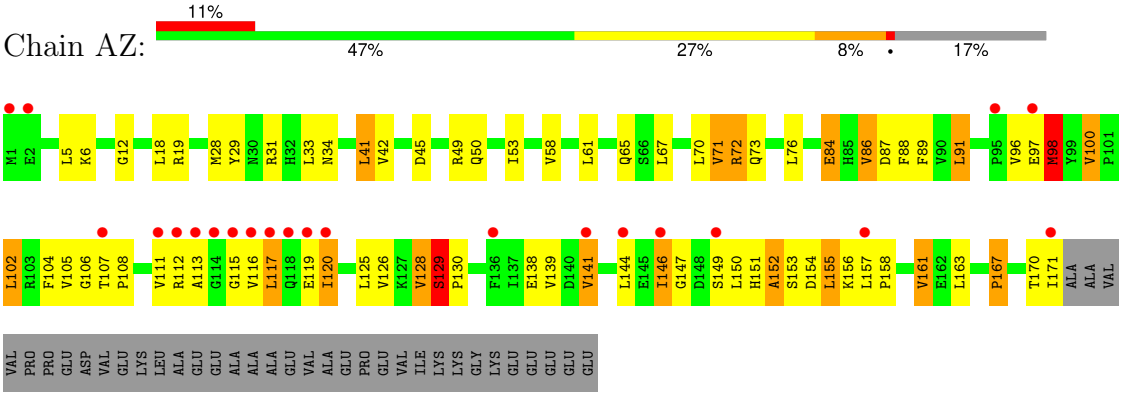
• Molecule 22: 50S ribosomal protein L24

Chain CY:



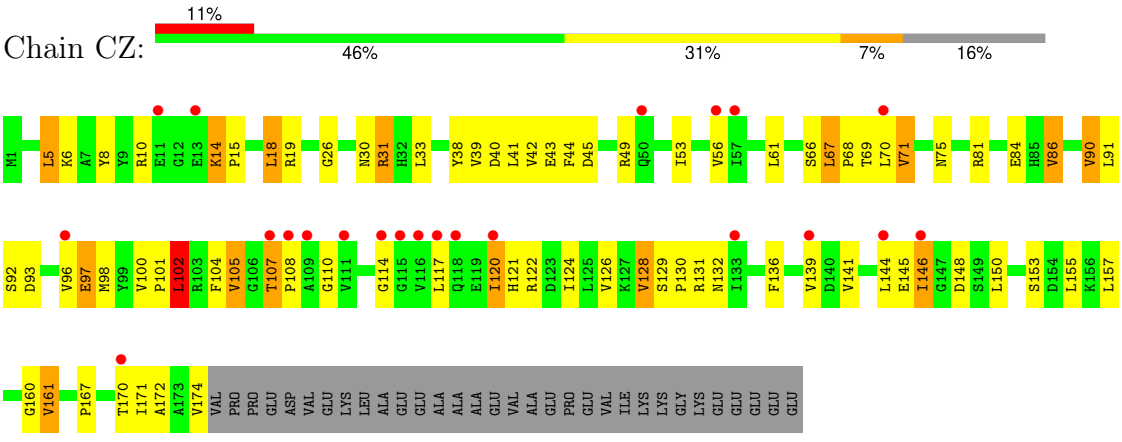
• Molecule 23: 50S ribosomal protein L25

Chain AZ:



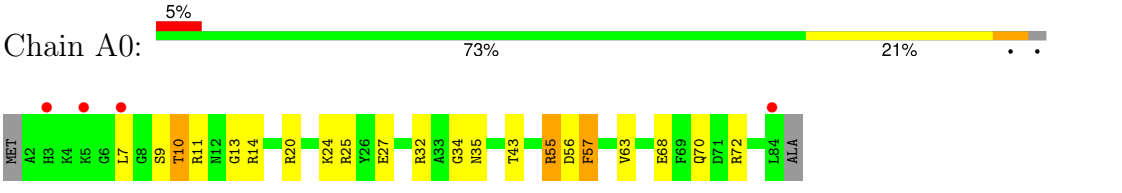
• Molecule 23: 50S ribosomal protein L25

Chain CZ:



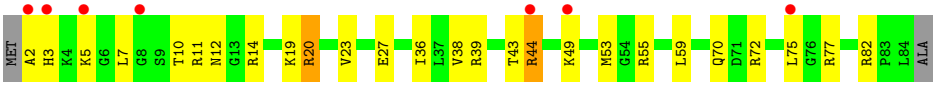
• Molecule 24: 50S ribosomal protein L27

Chain A0:



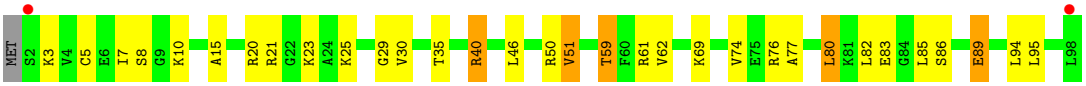
• Molecule 24: 50S ribosomal protein L27

Chain C0:



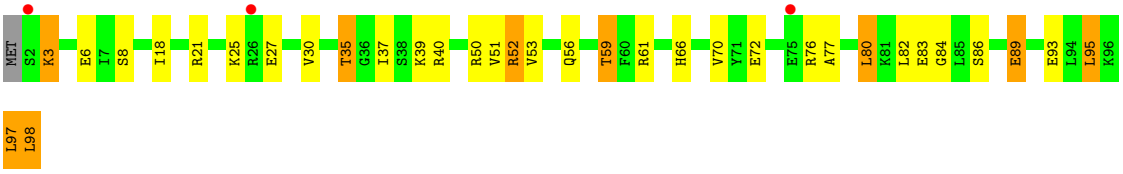
• Molecule 25: 50S ribosomal protein L28

Chain A1:



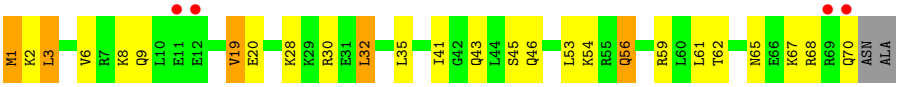
• Molecule 25: 50S ribosomal protein L28

Chain C1:



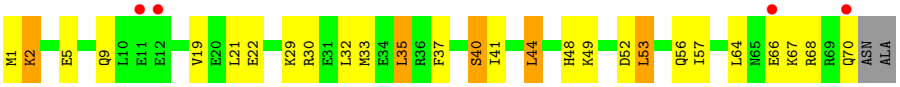
• Molecule 26: 50S ribosomal protein L29

Chain A2:



• Molecule 26: 50S ribosomal protein L29

Chain C2:

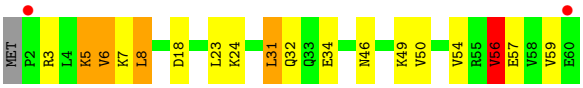


• Molecule 27: 50S ribosomal protein L30

Chain A3:

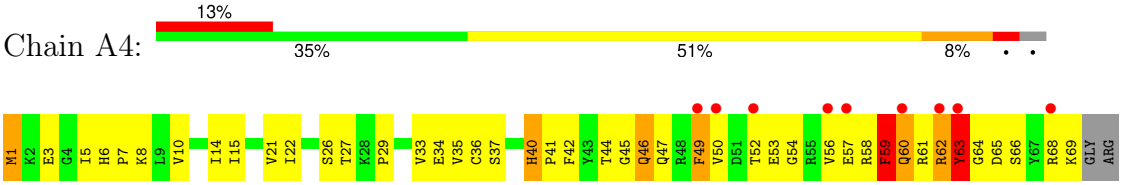
• Molecule 27: 50S ribosomal protein L30

Chain C3:



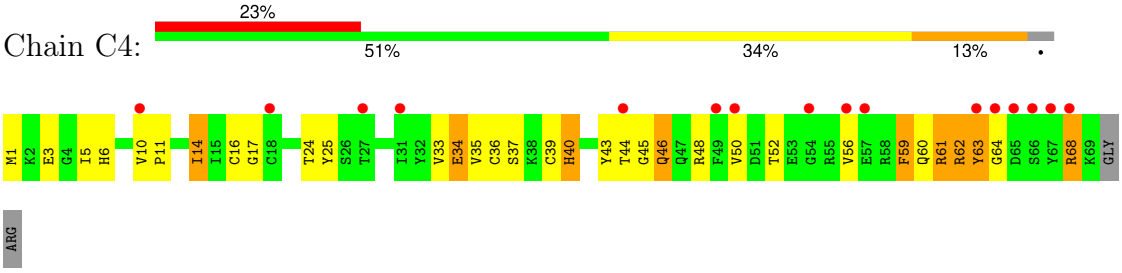
• Molecule 28: 50S ribosomal protein L31

Chain A4:



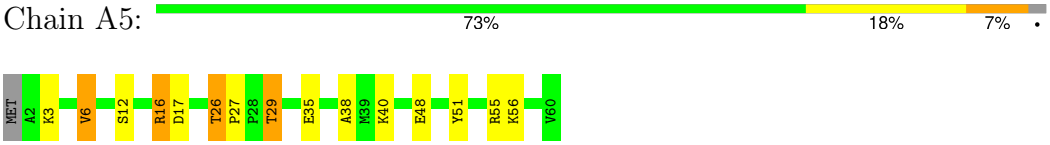
• Molecule 28: 50S ribosomal protein L31

Chain C4:



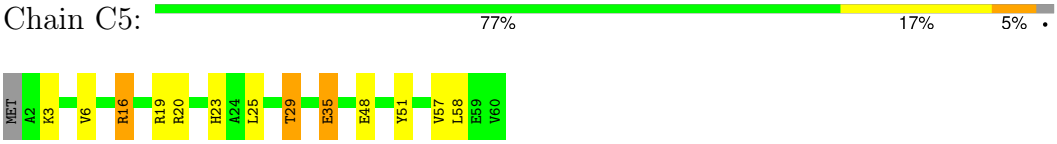
• Molecule 29: 50S ribosomal protein L32

Chain A5:



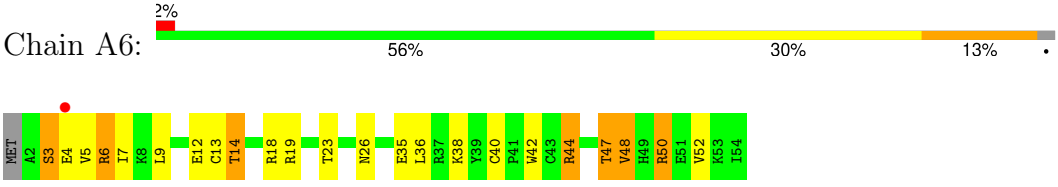
• Molecule 29: 50S ribosomal protein L32

Chain C5:



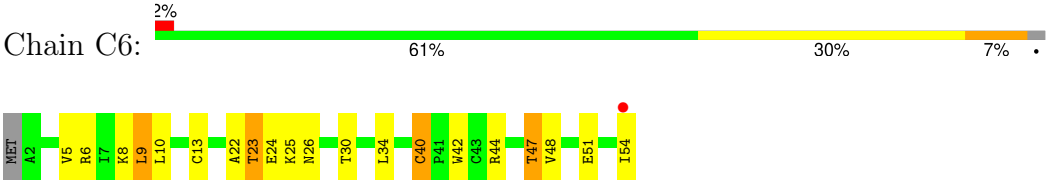
• Molecule 30: 50S ribosomal protein L33

Chain A6:



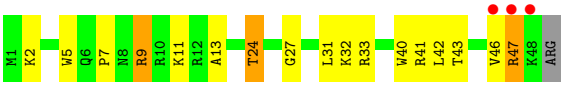
• Molecule 30: 50S ribosomal protein L33

Chain C6:



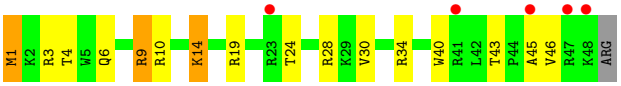
• Molecule 31: 50S ribosomal protein L34

Chain A7:



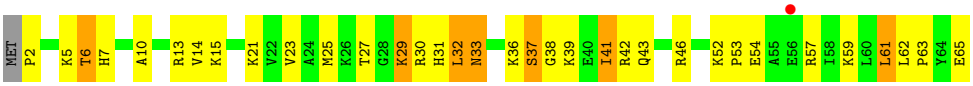
• Molecule 31: 50S ribosomal protein L34

Chain C7:



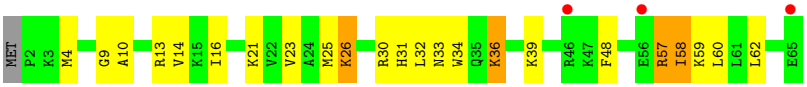
• Molecule 32: 50S ribosomal protein L35

Chain A8:



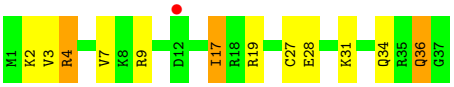
• Molecule 32: 50S ribosomal protein L35

Chain C8:



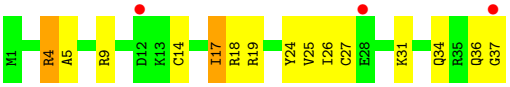
• Molecule 33: 50S ribosomal protein L36

Chain A9:



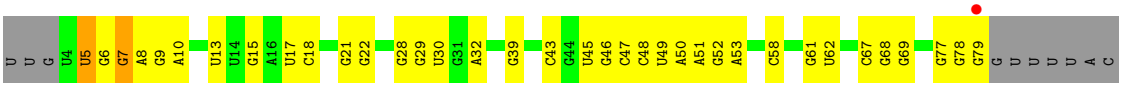
• Molecule 33: 50S ribosomal protein L36

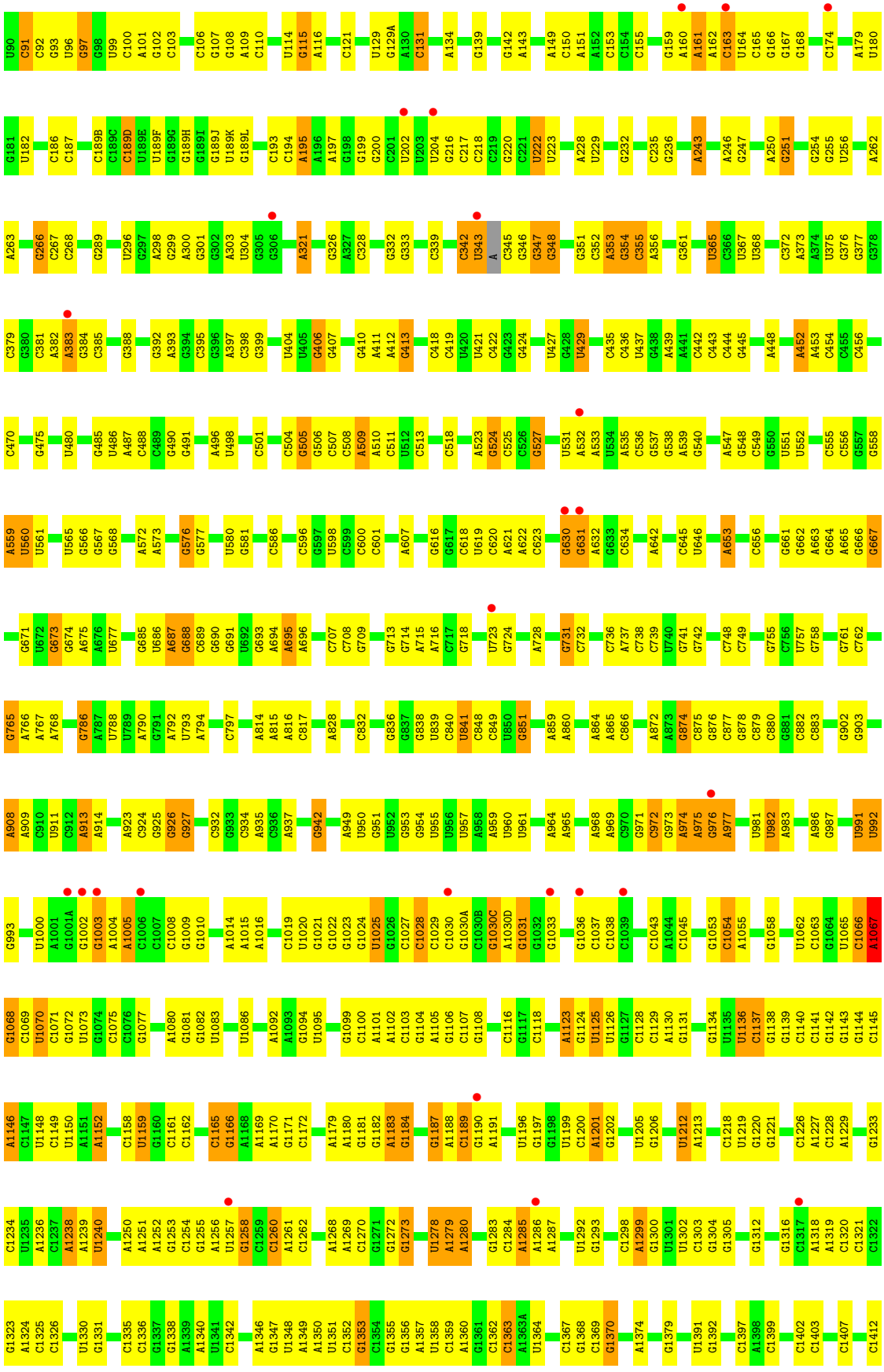
Chain C9:

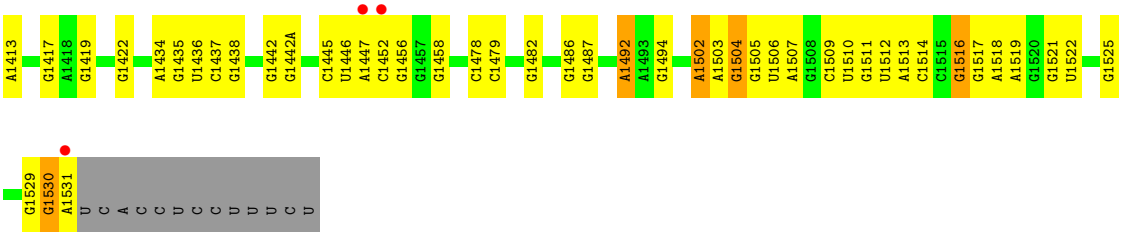


• Molecule 34: 16S Ribosomal RNA

Chain BA:

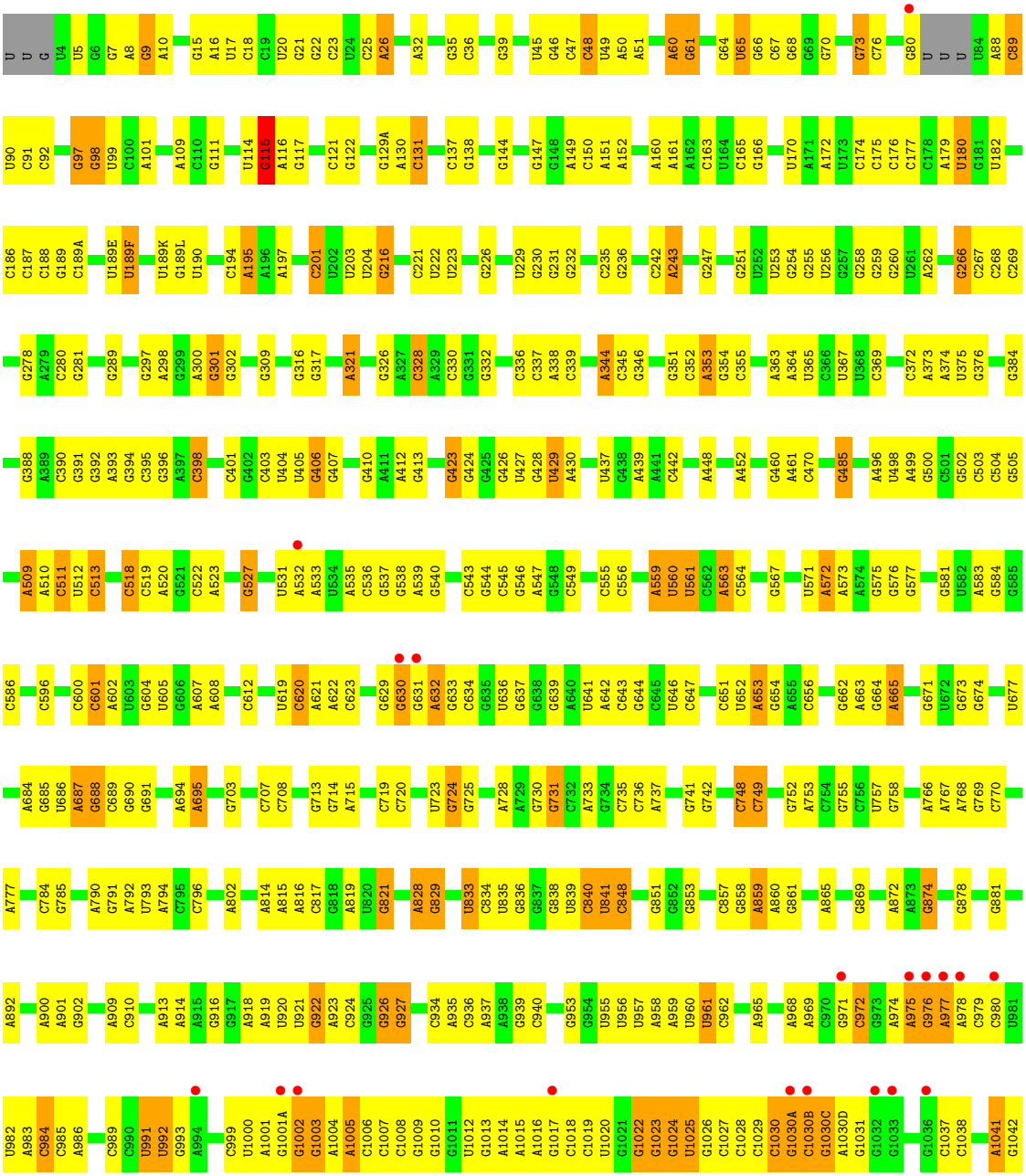


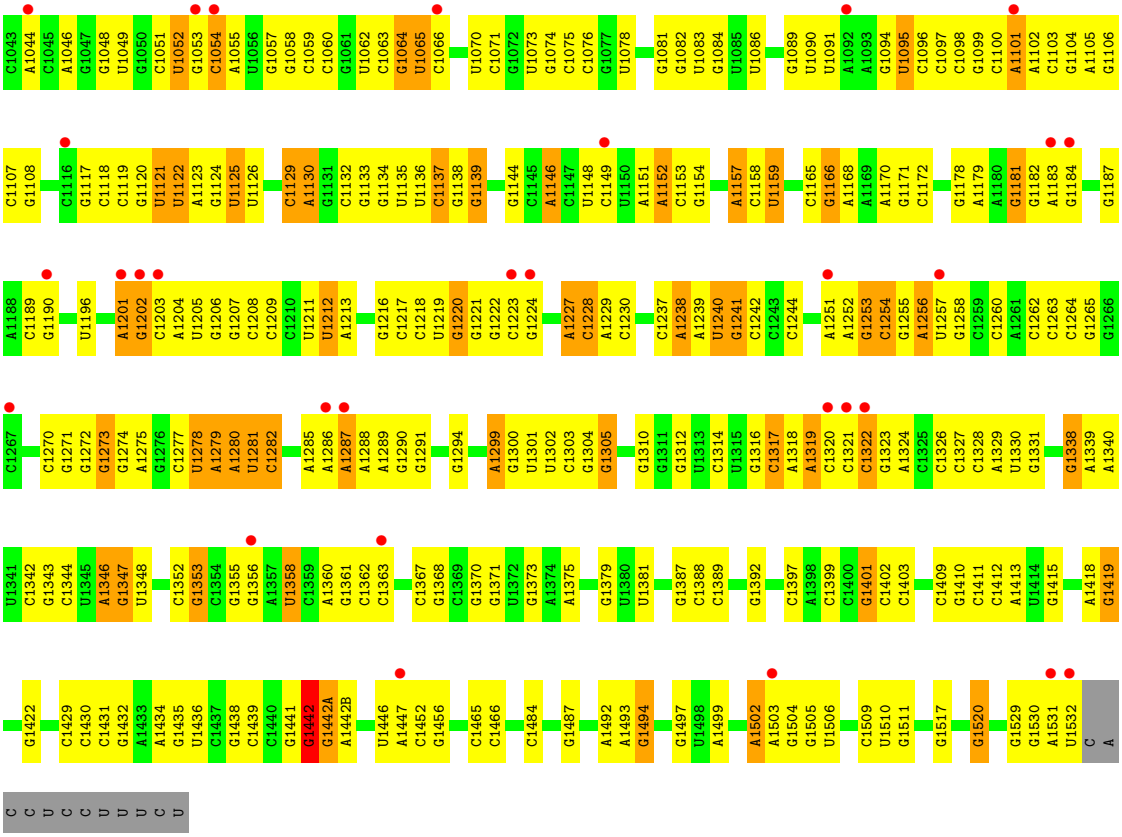

U90 C91 C92 G93 U96 G97 G98 U99 C100 A101 G102 C103 C106 C107 G108 A109 C110 U114 G115 A116 C121 U129 G129A A130 C131 A134 G139 G142 A143 A149 C150 A151 A152 C153 C154 C155 G159 A160 A161 A162 C163 U164 C165 G166 G167 G168 C174 A179 U180
G181 U182 C186 C187 C189B C189C C189D U189E U189F G189G G189H G189I G189J U189K G189L C193 C194 A195 A196 A197 G198 G199 G200 C201 U202 U203 U204 G216 C217 C218 C219 G220 C221 U222 U223 A228 U229 G232 C235 G236 A243 A246 G247 A250 G251 G254 G255 U256 A262
A263 G266 C267 C268 G289 U296 G297 A298 G299 A300 G301 G302 A303 U304 G305 G306 A321 G326 A327 C328 G332 G333 C339 C342 U343 A C345 G346 G347 G348 G351 C352 A353 G354 C355 A356 G361 U365 C366 U367 U368 C372 A373 A374 U375 G376 G377 G378
C379 G380 C381 A382 A383 G384 C385 G388 G392 A393 G394 C395 G396 A397 C398 G399 U404 U405 G406 G407 G410 A411 A412 G413 C418 C419 U420 U421 C422 G423 G424 U427 G428 U429 C435 C436 U437 G438 A439 A441 C442 C443 C444 G445 A448 A452 A453 C454 C455 C456
C470 G475 U480 G485 U486 A487 C488 C489 G490 G491 A496 U498 C501 C504 G505 G506 C507 C508 A509 A510 C511 U512 C513 C518 A523 G524 C525 C526 G527 U531 A532 A533 U534 A535 C536 G537 G538 A539 G540 A547 G548 C549 G550 U551 U552 C555 C556 G557 G558
A559 U560 U561 U565 G566 G567 G568 A572 A573 G576 G577 U580 G581 C586 C596 G597 U598 G599 C600 C601 A607 G616 G617 C618 U619 C620 A621 A622 C623 G630 G631 A632 G633 C634 A642 C645 U646 A653 C656 G661 G662 A663 G664 A665 G666 G667
G671 U672 G673 G674 A675 A676 U677 G685 U686 A687 G688 C689 G690 G691 U692 G693 A694 A695 A696 C707 C708 G709 G713 G714 A715 A716 C717 G718 U723 G724 A728 G731 C732 C736 A737 C738 C739 U740 G741 G742 C748 C749 G755 C756 U757 G758 G761 C762
G765 A766 A767 A768 G786 A787 U788 U789 A790 G791 A792 U793 A794 C797 A814 A815 A816 C817 A828 C832 G836 G837 G838 U839 C840 U841 C848 C849 U850 C851 A859 A860 A864 A865 C866 A872 A873 G874 C875 G876 C877 C878 C879 C880 G881 C882 C883 G902 G903
A908 A909 C910 U911 C912 A913 A914 A923 C924 G925 G926 G927 C932 G933 C934 A935 C936 A937 G942 A949 U950 G951 U952 G953 G954 U955 U956 U957 A958 A959 U960 U961 A964 A965 A968 A969 C970 G971 C972 G973 A974 A975 G976 A977 U981 U982 A983 A986 G987 U991 U992
G993 U1000 A1001 G1001A G1002 G1003 A1004 A1005 C1006 C1007 C1008 G1009 G1010 A1014 A1015 A1016 C1019 U1020 G1021 G1022 G1023 G1024 U1025 C1026 C1027 C1028 C1029 C1030 G1030A C1030B G1030C A1030D G1031 G1032 G1033 G1036 C1037 C1038 C1039 C1043 A1044 C1045 G1053 C1054 A1055 G1058 U1062 C1063 G1064 U1065 C1066 A1067
G1068 C1069 U1070 C1071 G1072 U1073 G1074 C1075 C1076 G1077 A1080 G1081 G1082 U1083 U1086 A1092 A1093 G1094 U1095 G1099 C1100 A1101 A1102 C1103 G1104 A1105 G1106 C1107 G1108 C1116 G1117 C1118 A1123 G1124 U1125 U1126 G1127 C1128 C1129 A1130 G1131 G1134 U1135 U1136 C1137 G1138 G1139 C1140 C1141 G1142 G1143 G1144 C1145
A1146 C1147 U1148 C1149 U1150 A1151 A1152 C1158 U1159 G1160 C1161 C1162 C1165 G1166 A1168 A1169 A1170 G1171 C1172 A1179 A1180 G1181 G1182 A1183 G1184 G1187 A1188 C1189 G1190 A1191 U1196 G1197 G1198 U1199 C1200 A1201 G1202 U1205 G1206 U1212 A1213 C1218 U1219 G1220 G1221 C1226 A1227 C1228 A1229 G1233
C1234 U1235 A1236 C1237 A1238 A1239 U1240 A1250 A1251 A1252 G1253 C1254 G1255 A1256 U1257 G1258 C1259 C1260 A1261 C1262 A1268 A1269 C1270 G1271 G1272 G1273 U1278 A1279 A1280 G1283 C1284 A1285 A1286 A1287 U1292 G1293 C1298 A1299 G1300 U1301 U1302 C1303 G1304 G1305 G1312 G1316 C1317 A1318 A1319 C1320 C1321 C1322
G1323 A1324 C1325 C1326 U1330 G1331 C1335 C1336 G1337 G1338 A1339 A1340 U1341 C1342 A1346 G1347 U1348 A1349 A1350 U1351 C1352 G1353 C1354 G1355 G1356 A1357 U1358 C1359 A1360 G1361 C1362 C1363 A1363A U1364 C1367 G1368 C1369 G1370 A1374 G1379 U1391 G1392 C1397 A1398 C1399 C1402 C1403 C1407 C1412



• Molecule 34: 16S Ribosomal RNA

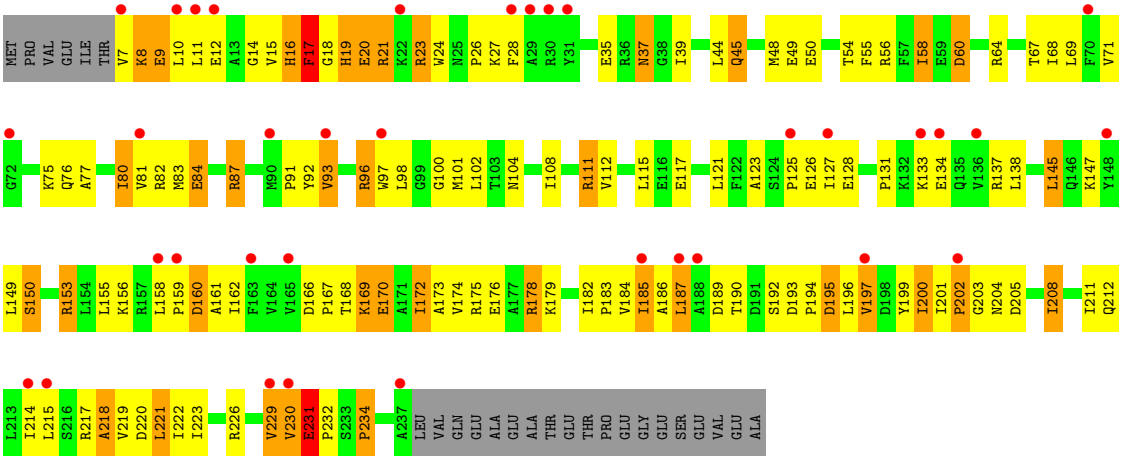
Chain DA:





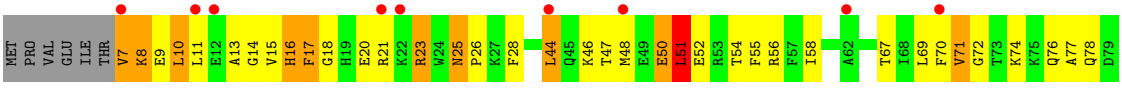
• Molecule 35: 30S ribosomal protein S2

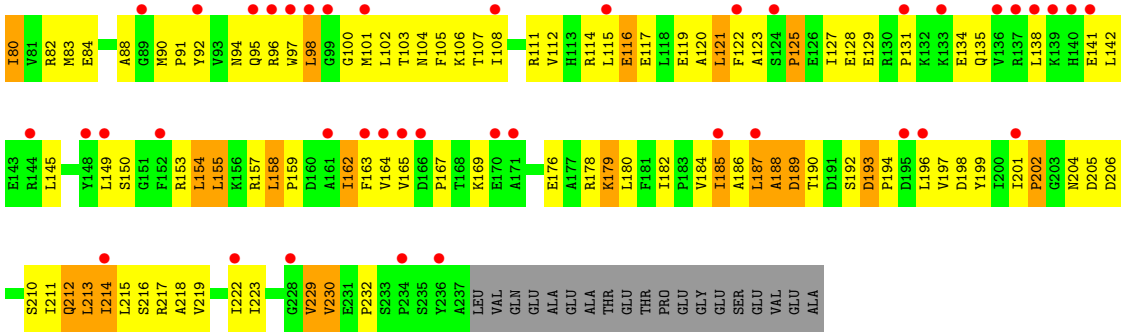
Chain BB:



• Molecule 35: 30S ribosomal protein S2

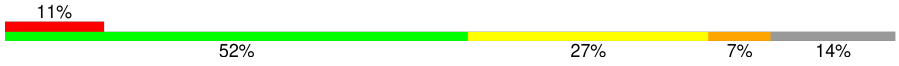
Chain DB:

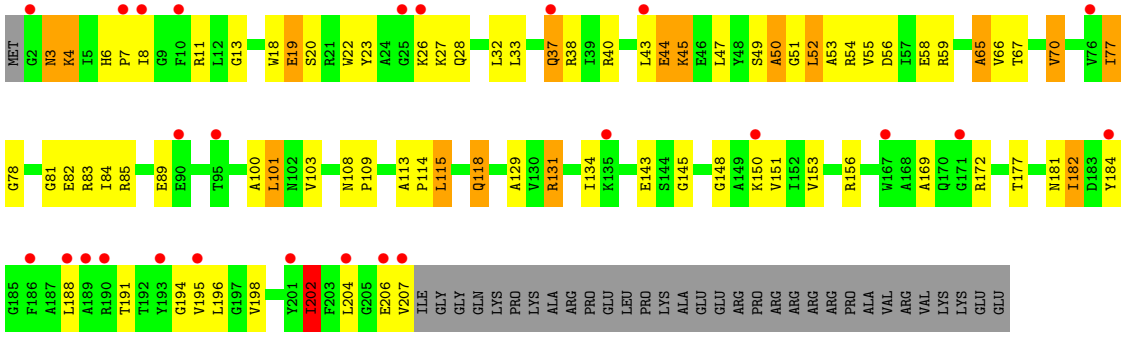




• Molecule 36: 30S ribosomal protein S3

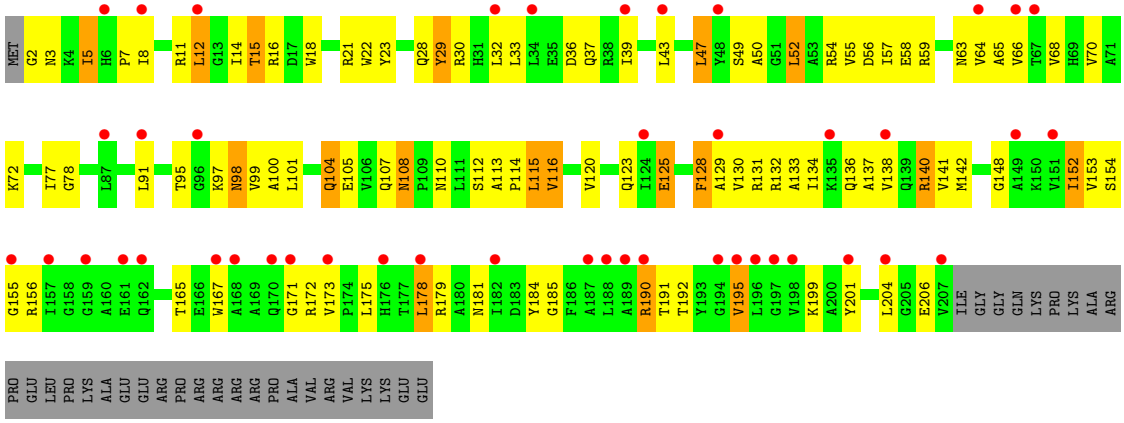
Chain BC:





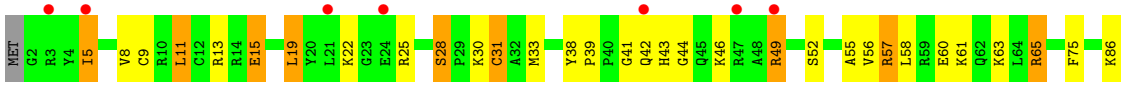
• Molecule 36: 30S ribosomal protein S3

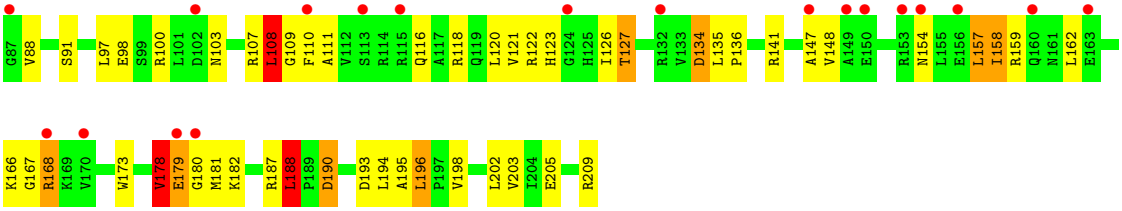
Chain DC:



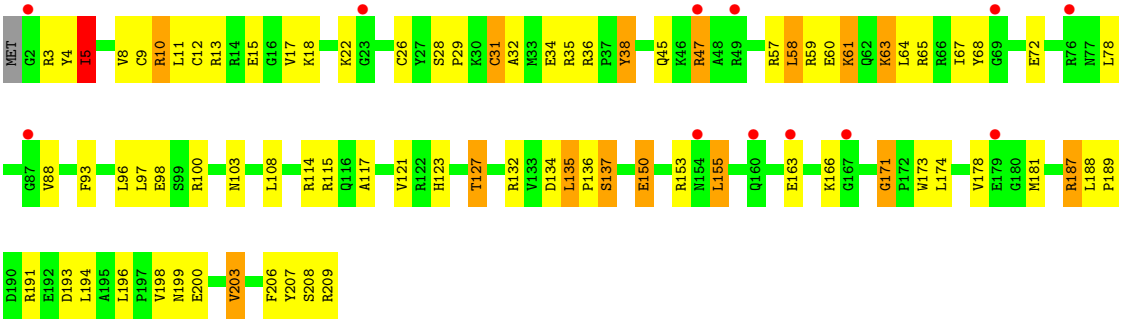
• Molecule 37: 30S ribosomal protein S4

Chain BD:

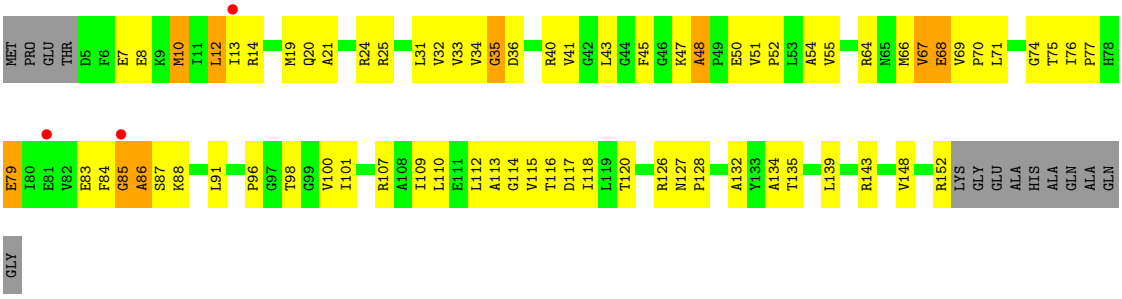




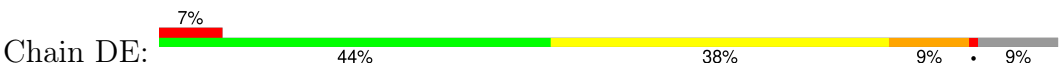
• Molecule 37: 30S ribosomal protein S4

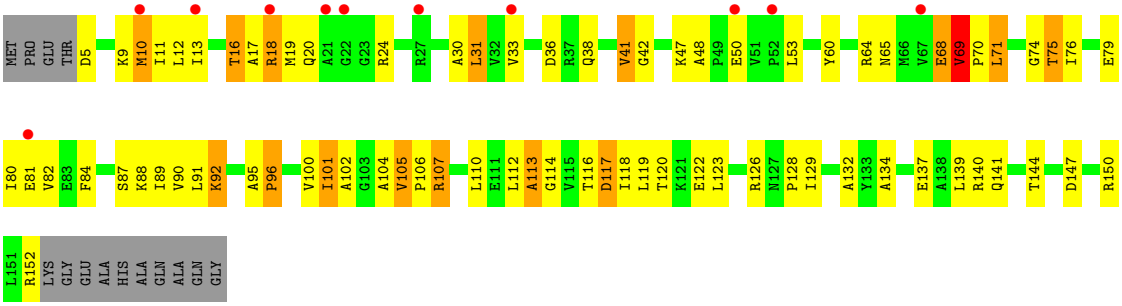


• Molecule 38: 30S ribosomal protein S5



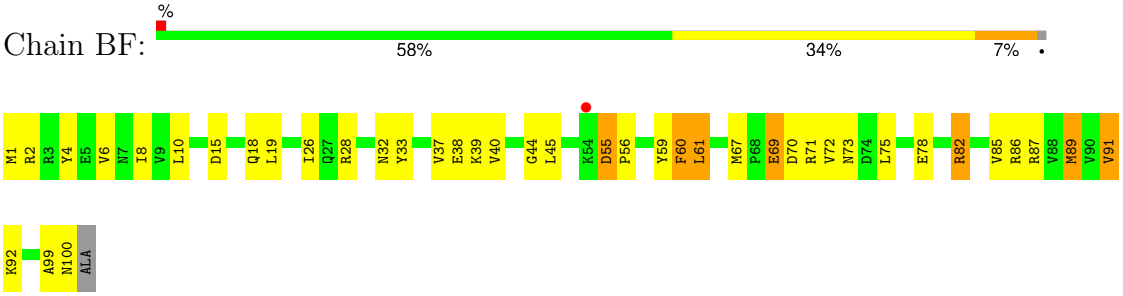
• Molecule 38: 30S ribosomal protein S5





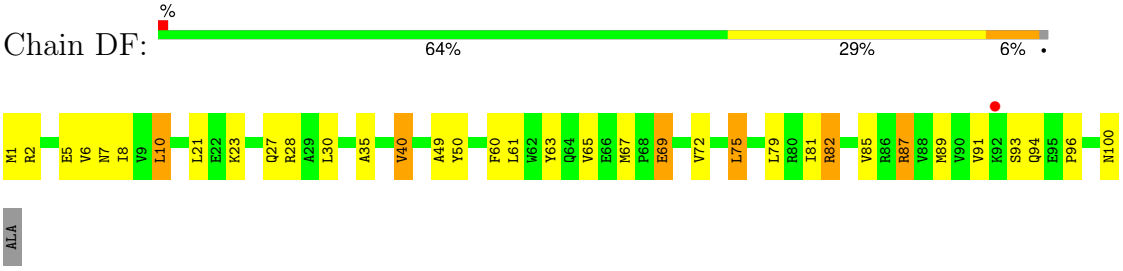
• Molecule 39: 30S ribosomal protein S6

Chain BF:



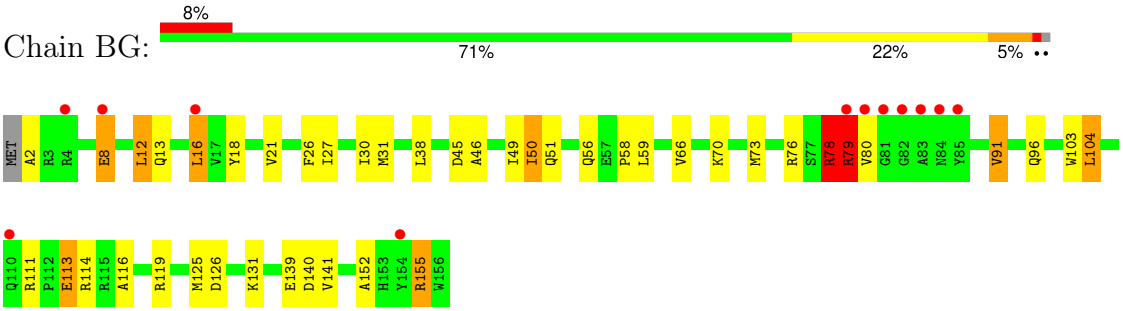
• Molecule 39: 30S ribosomal protein S6

Chain DF:



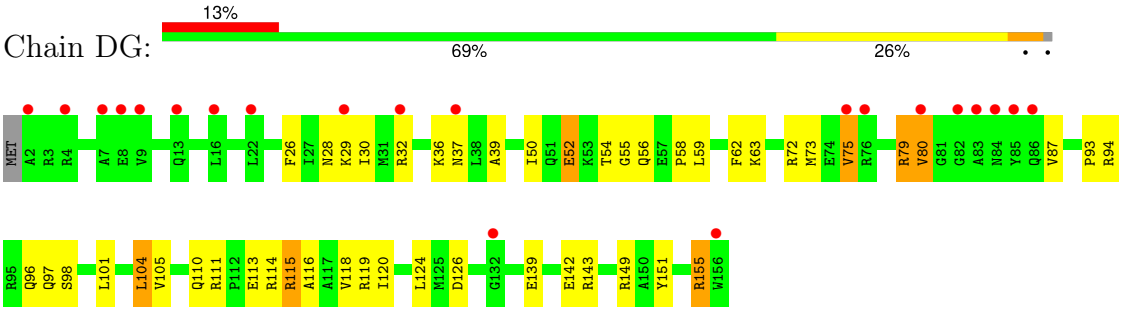
• Molecule 40: 30S ribosomal protein S7

Chain BG:



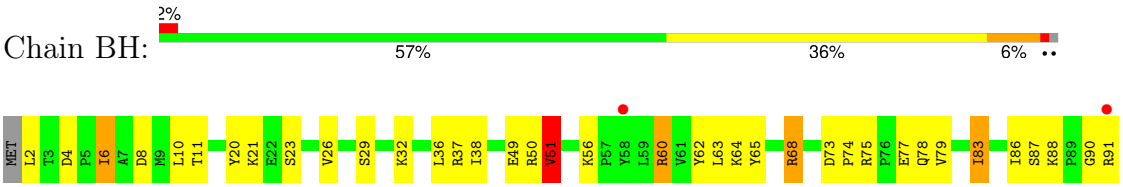
• Molecule 40: 30S ribosomal protein S7

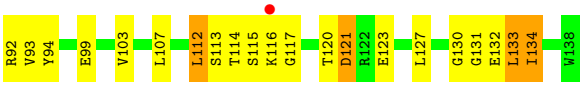
Chain DG:



• Molecule 41: 30S ribosomal protein S8

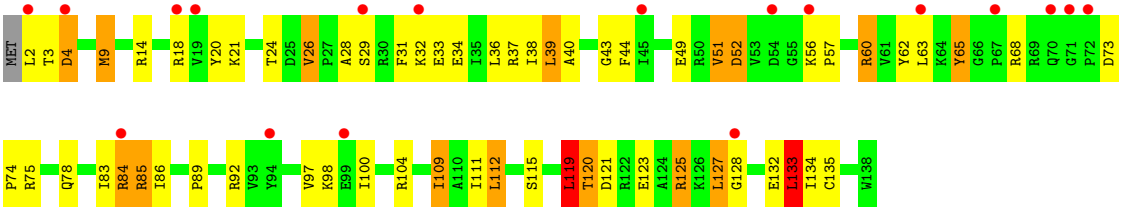
Chain BH:





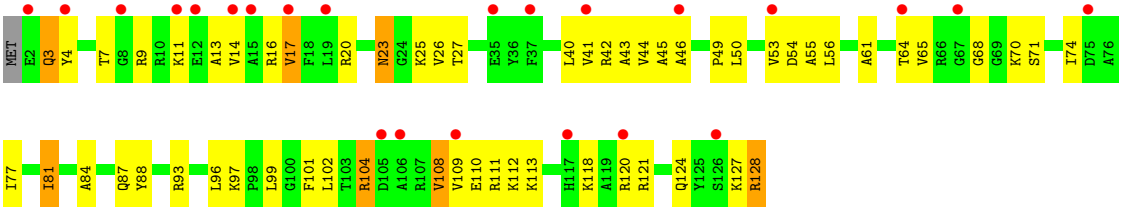
• Molecule 41: 30S ribosomal protein S8

Chain DH:



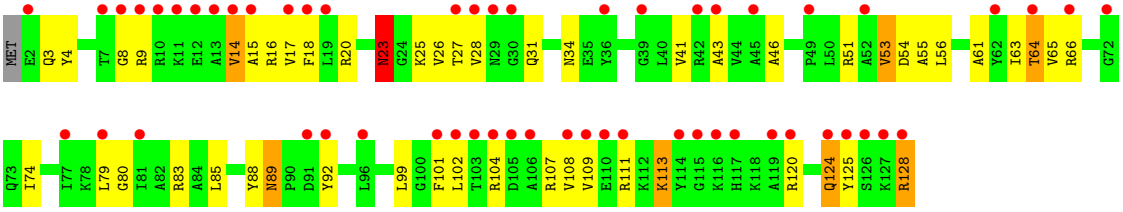
• Molecule 42: 30S ribosomal protein S9

Chain BI:



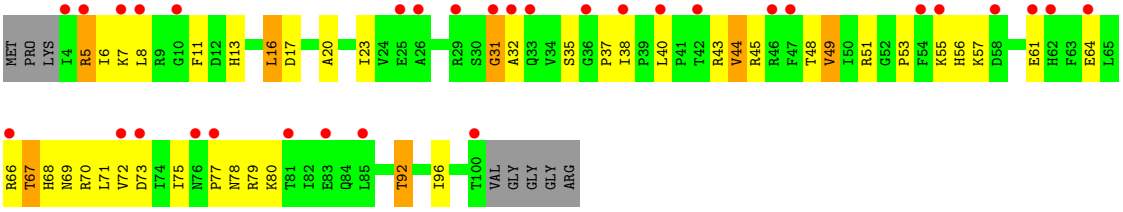
• Molecule 42: 30S ribosomal protein S9

Chain DI:



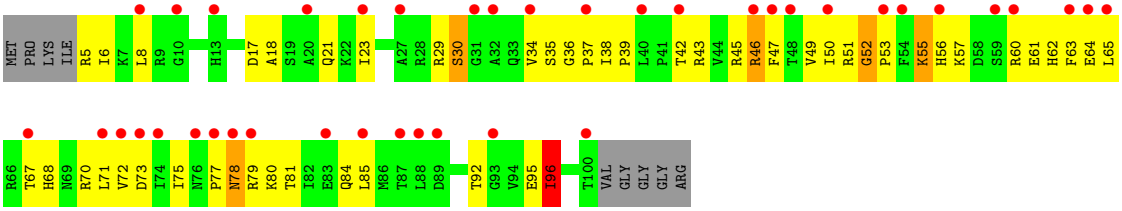
• Molecule 43: 30S ribosomal protein S10

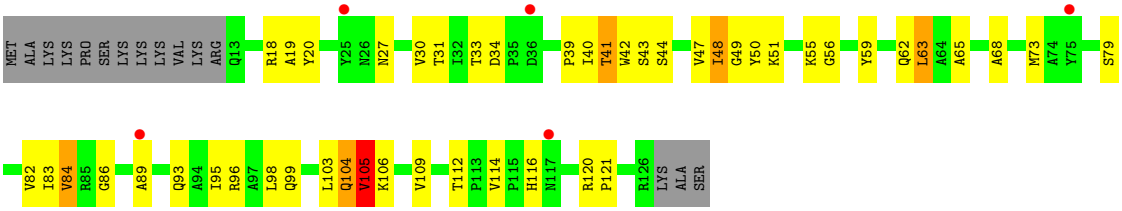
Chain BJ:



• Molecule 43: 30S ribosomal protein S10

Chain DJ:



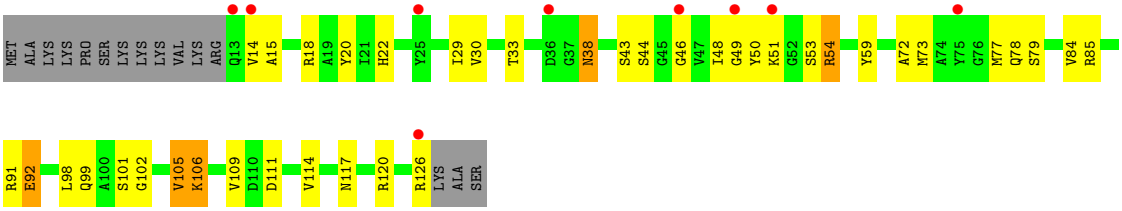


• Molecule 44: 30S ribosomal protein S11

Chain BK:

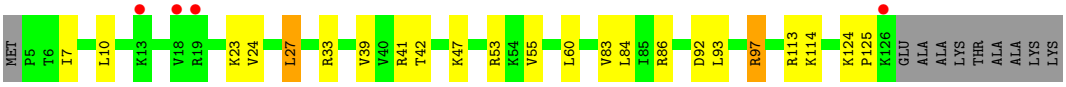
• Molecule 44: 30S ribosomal protein S11

Chain DK:



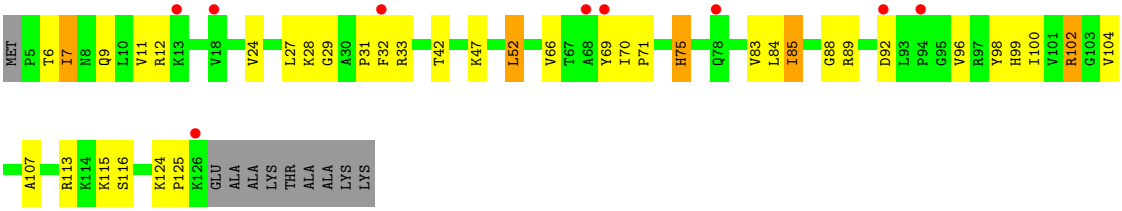
• Molecule 45: 30S ribosomal protein S12

Chain BL:



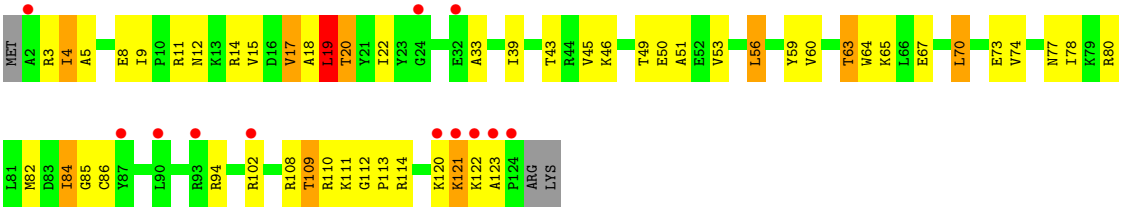
• Molecule 45: 30S ribosomal protein S12

Chain DL:

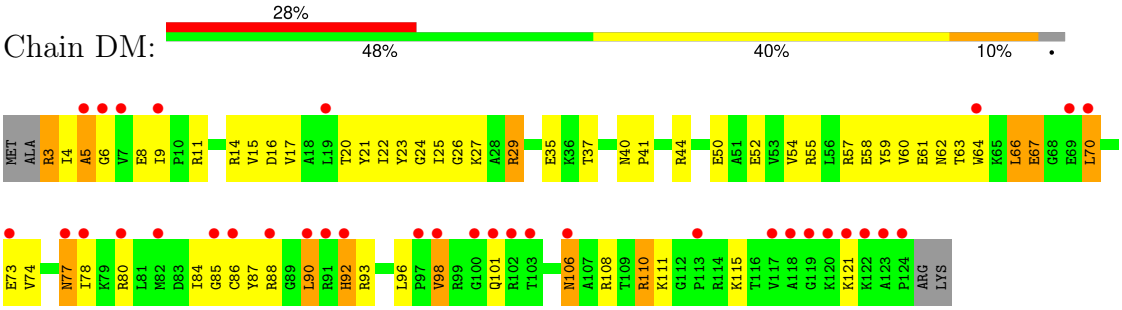


• Molecule 46: 30S ribosomal protein S13

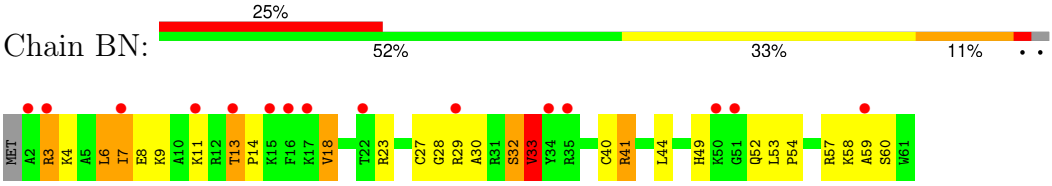
Chain BM:



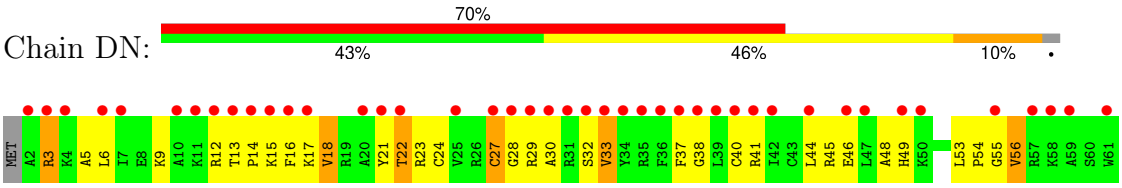
• Molecule 46: 30S ribosomal protein S13



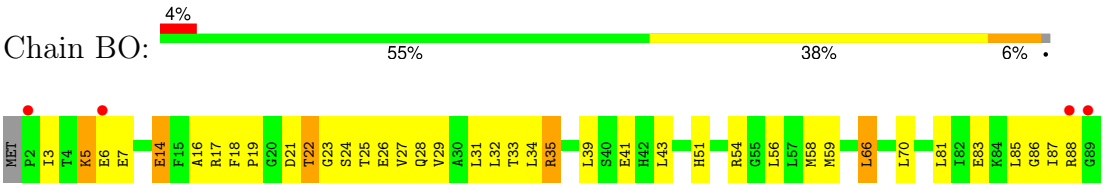
• Molecule 47: 30S ribosomal protein S14 type Z



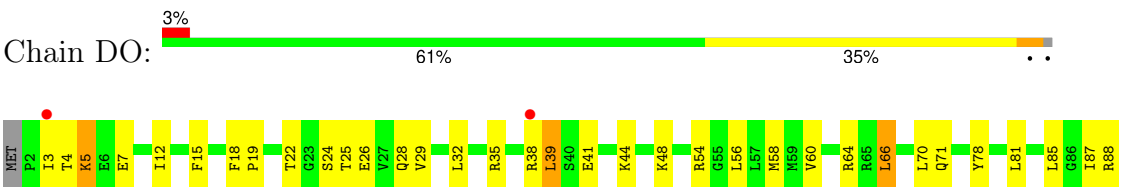
• Molecule 47: 30S ribosomal protein S14 type Z



• Molecule 48: 30S ribosomal protein S15

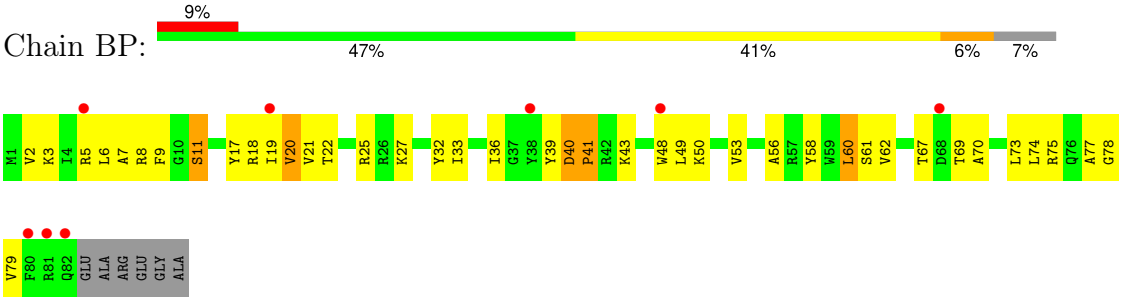


• Molecule 48: 30S ribosomal protein S15



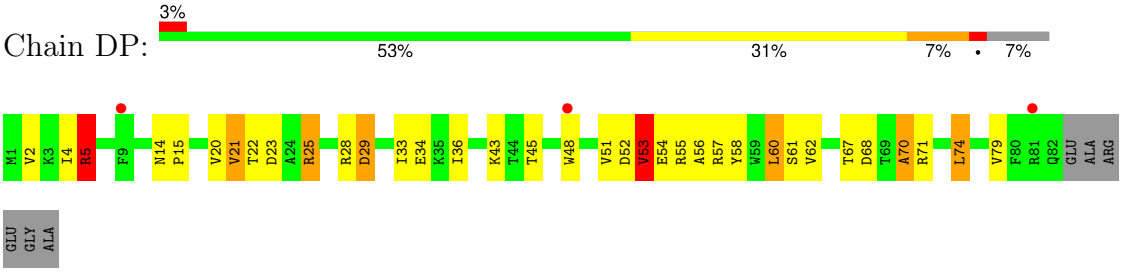
• Molecule 49: 30S ribosomal protein S16

Chain BP:



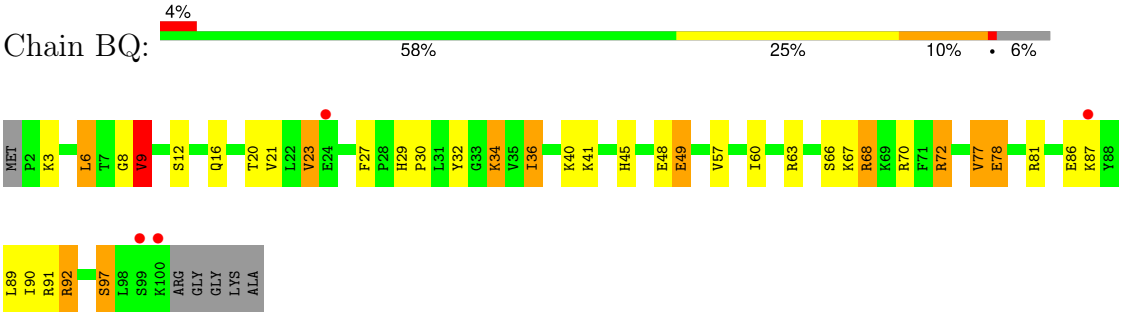
• Molecule 49: 30S ribosomal protein S16

Chain DP:



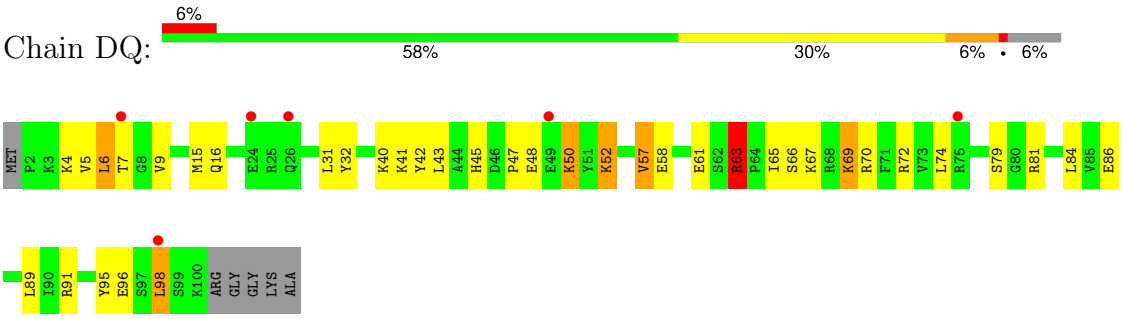
• Molecule 50: 30S ribosomal protein S17

Chain BQ:



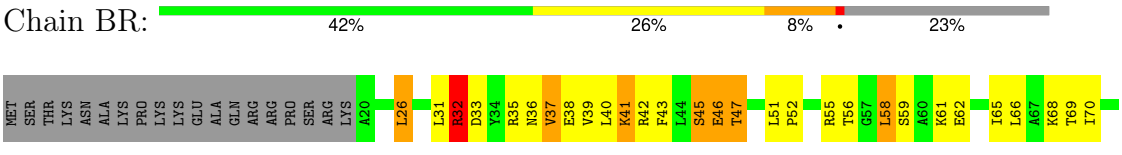
• Molecule 50: 30S ribosomal protein S17

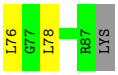
Chain DQ:



• Molecule 51: 30S ribosomal protein S18

Chain BR:



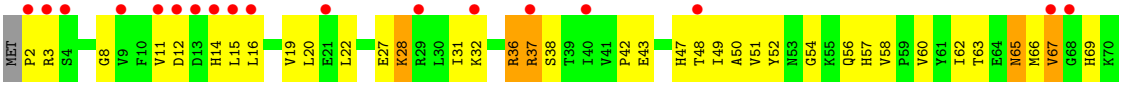


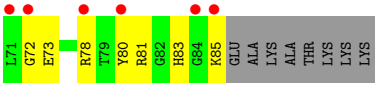
• Molecule 51: 30S ribosomal protein S18

Chain DR:

• Molecule 52: 30S ribosomal protein S19

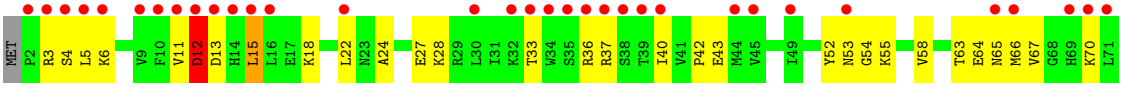
Chain BS:

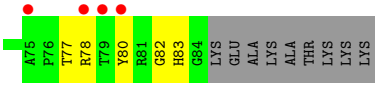




• Molecule 52: 30S ribosomal protein S19

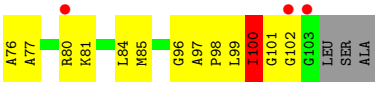
Chain DS:





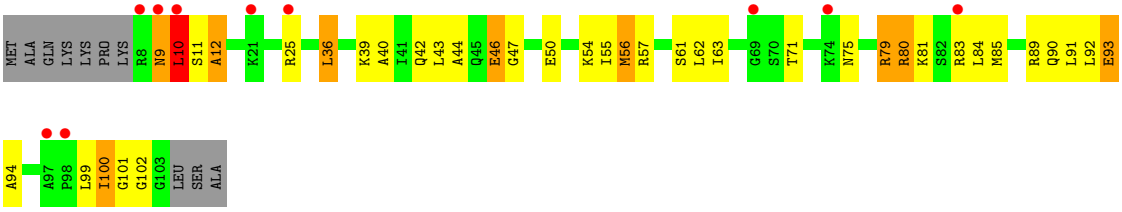
• Molecule 53: 30S ribosomal protein S20

Chain BT:

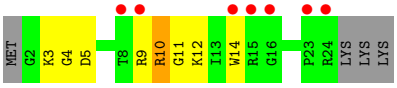


• Molecule 53: 30S ribosomal protein S20

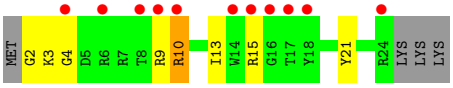
Chain DT:



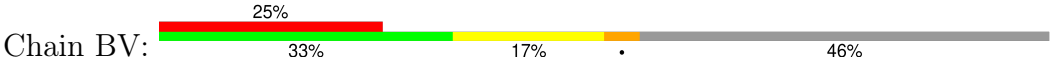
• Molecule 54: 30S ribosomal protein Thx

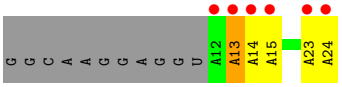


• Molecule 54: 30S ribosomal protein Thx

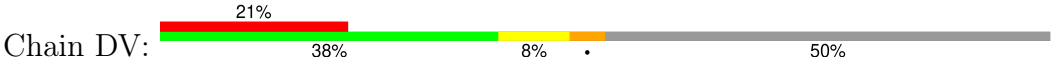


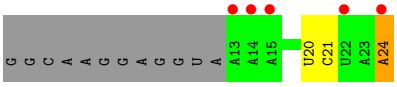
• Molecule 55: mRNA



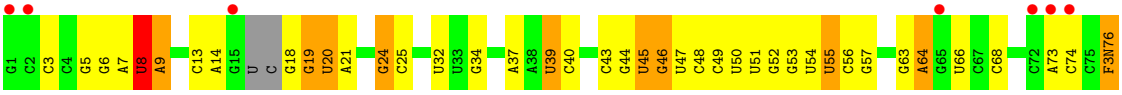


• Molecule 55: mRNA

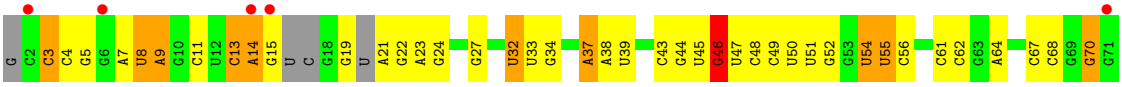




• Molecule 56: A-site tRNA

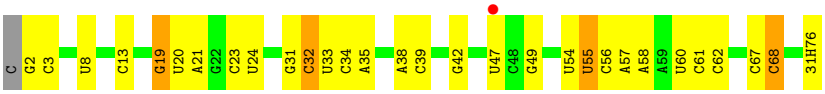


• Molecule 56: A-site tRNA



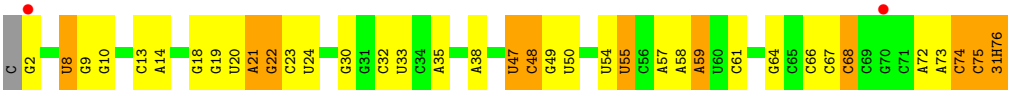
• Molecule 57: P-site tRNA

Chain BX:



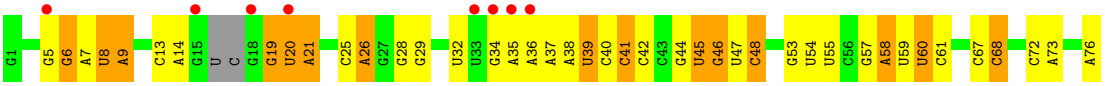
• Molecule 57: P-site tRNA

Chain DX:



• Molecule 58: E-site tRNA

Chain BY:

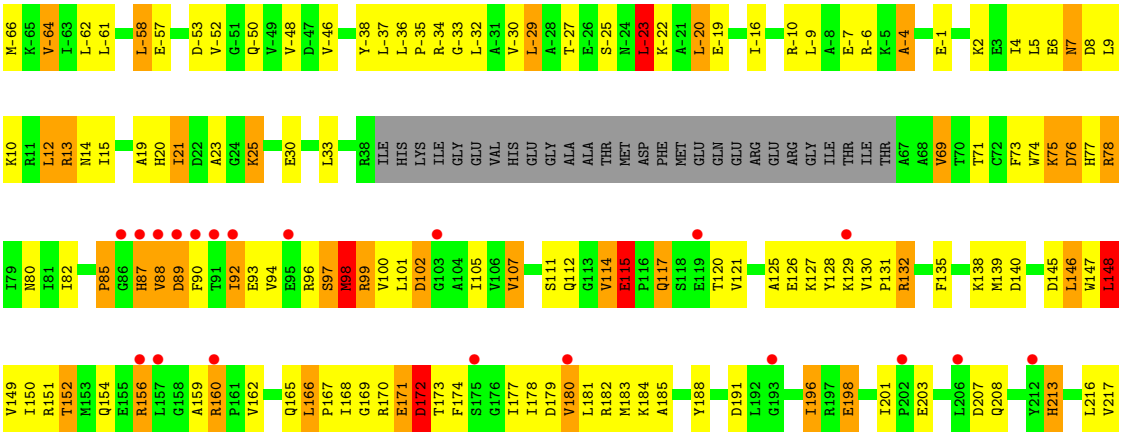


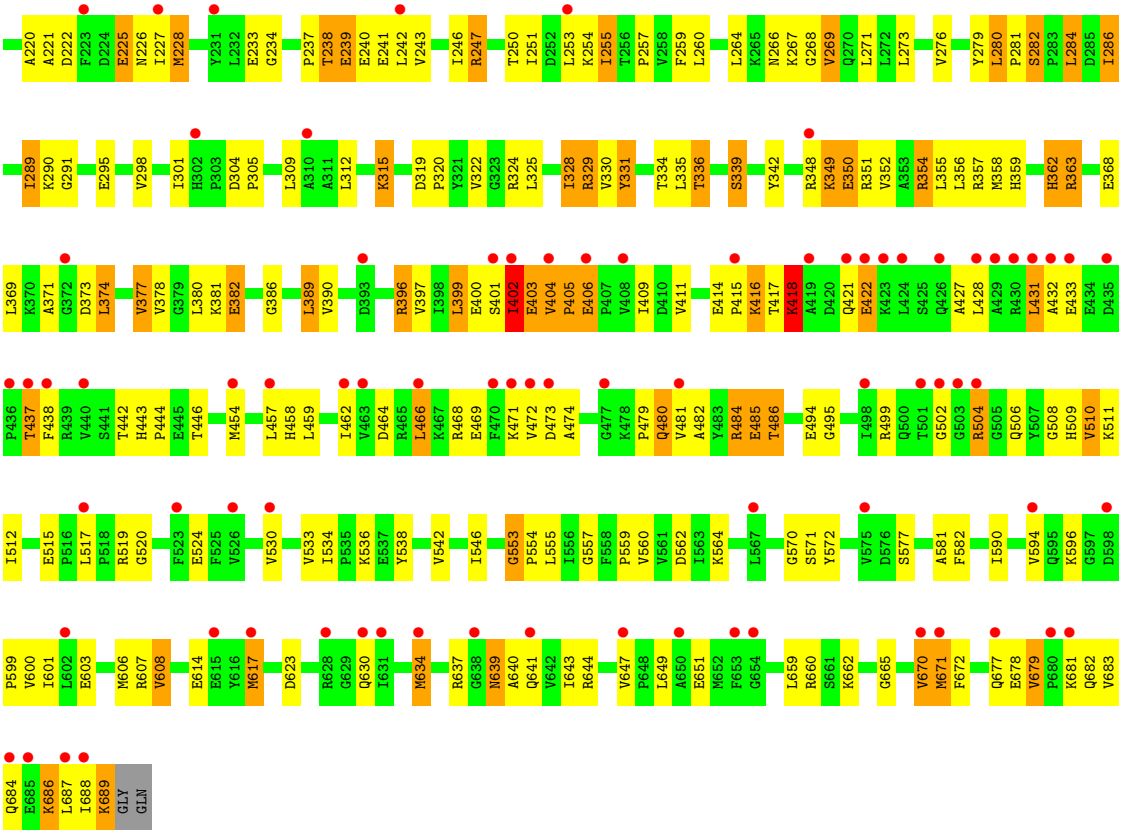
• Molecule 58: E-site tRNA

Chain DY:

• Molecule 59: 50S ribosomal protein L9,Elongation factor G

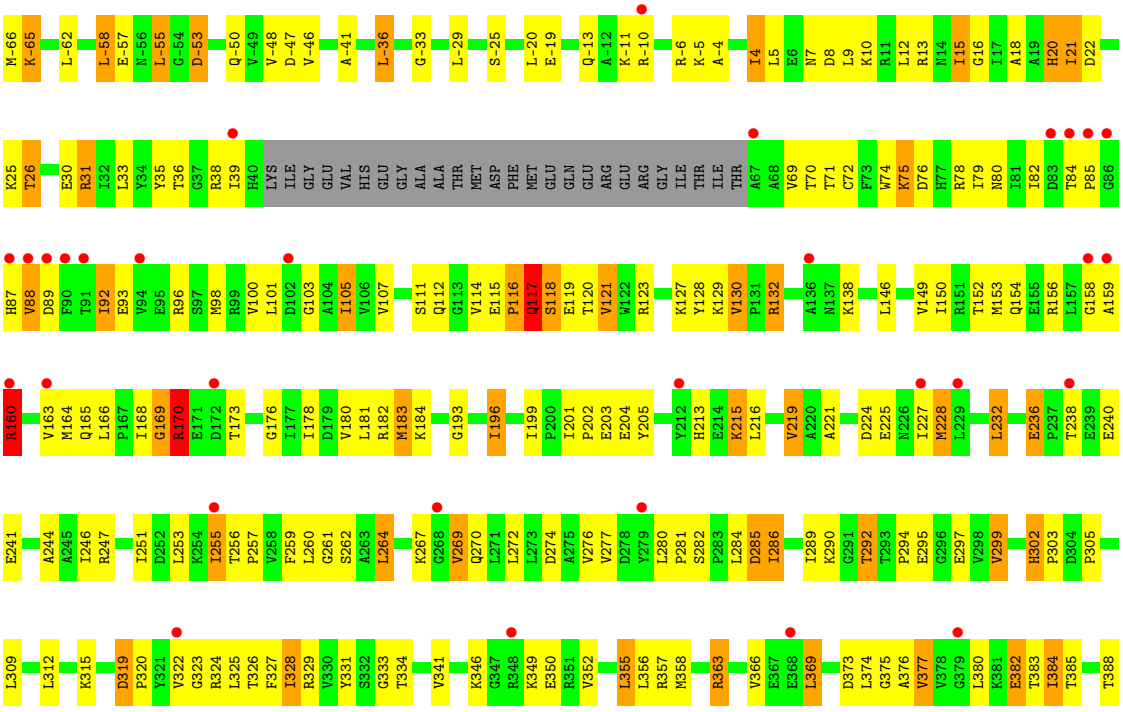
Chain BZ:

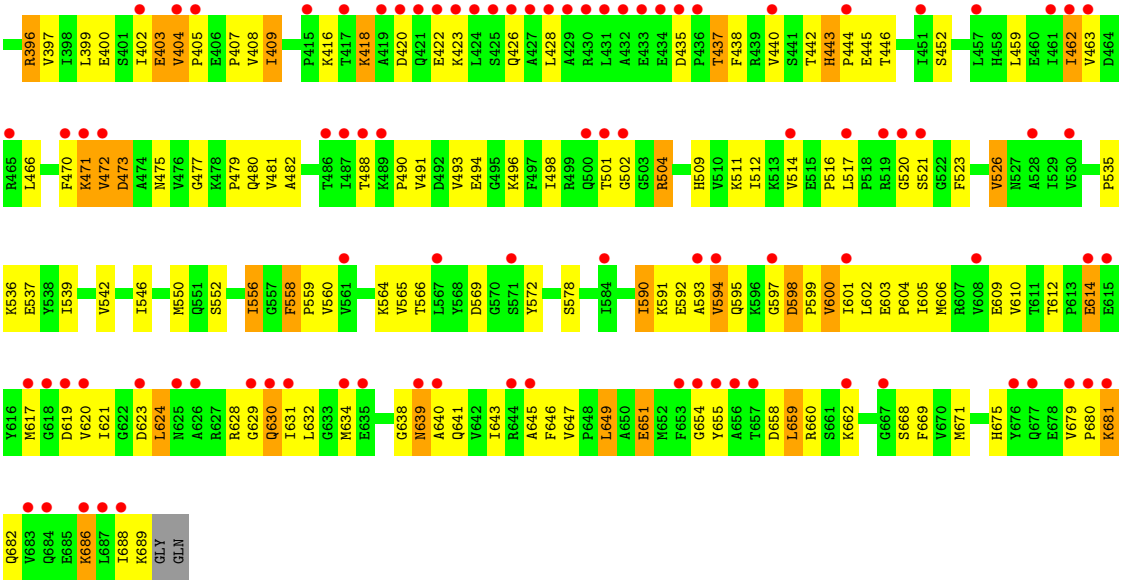




• Molecule 59: 50S ribosomal protein L9,Elongation factor G

Chain DZ:




R396 V397 I398 L399 E400 S401 I402 E403 V404 P405 E406 P407 V408 I409 P415 K416 T417 K418 A419 D420 Q421 E422 K423 L424 S425 Q426 A427 L428 A429 R430 L431 A432 E433 E434 D435 P436 T437 F438 R439 V440 S441 T442 H443 P444 E445 T446 I451 S452 L457 H458 L459 E460 I461 I462 V463 D464
R465 L466 F470 K471 V472 D473 A474 N475 V476 G477 K478 P479 Q480 V481 A482 T486 I487 T488 K489 P490 V491 D492 V493 E494 G495 K496 F497 I498 R499 Q500 T501 G502 G503 R504 H509 V510 K511 I512 K513 V514 E515 P516 L517 P518 R519 G520 S521 G522 F523 V526 N527 A528 I529 V530 P535
K536 E537 Y538 I539 V542 I546 M550 Q551 S552 I556 G557 F558 P559 V560 V561 K564 V565 T566 L567 Y568 D569 G570 S571 Y572 S578 I584 I590 K591 E592 A593 V594 Q595 K596 G597 D598 P599 V600 I601 L602 E603 P604 I605 M606 R607 V608 E609 V610 T611 T612 P613 E614 E615
Y616 M617 G618 D619 V620 I621 G622 D623 L624 N625 A626 R627 R628 G629 Q630 I631 L632 G633 M634 E635 G638 N639 A640 Q641 V642 I643 R644 A645 F646 V647 P648 L649 A650 E651 M652 F653 G654 Y655 A656 T657 D658 L659 R660 S661 K662 G667 S668 F669 V670 M671 H675 Y676 Q677 E678 V679 P680 K681
Q682 V683 Q684 E685 K686 L687 I688 K689 GLY GLN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	209.89Å 449.03Å 622.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.63 – 2.80 49.63 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.2 (49.63-2.80) 99.2 (49.63-2.80)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.85 (at 2.81Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8.2_1309)	Depositor
R, R_{free}	0.202 , 0.252 0.203 , 0.251	Depositor DCC
R_{free} test set	71166 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	54.8	Xtriage
Anisotropy	0.148	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 66.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	313372	wwPDB-VP
Average B, all atoms (Å^2)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.43% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, GDP, 31H, 4SU, 5MU, K, SF4, 7MG, 5MC, MIA, F3N, PSU, ZN

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	0.63	0/69281	0.79	17/108144 (0.0%)
1	CA	0.48	0/69179	0.67	15/107984 (0.0%)
2	AB	0.52	0/2878	0.75	0/4490
2	CB	0.36	0/2878	0.57	0/4490
3	AC	0.42	0/1083	0.97	6/1460 (0.4%)
3	CC	0.42	0/1083	0.97	5/1460 (0.3%)
4	AD	0.96	0/2186	1.25	13/2944 (0.4%)
4	CD	0.82	0/2192	1.15	6/2951 (0.2%)
5	AE	0.99	0/1592	1.31	15/2149 (0.7%)
5	CE	0.80	0/1592	1.14	5/2149 (0.2%)
6	AF	0.92	1/1619 (0.1%)	1.21	8/2193 (0.4%)
6	CF	0.70	0/1615	1.10	7/2188 (0.3%)
7	AG	0.64	0/1450	1.08	6/1959 (0.3%)
7	CG	0.48	0/1449	0.97	5/1958 (0.3%)
8	AH	0.85	0/1356	1.21	11/1834 (0.6%)
8	CH	0.54	0/1356	1.01	5/1834 (0.3%)
9	AK	0.59	0/640	1.37	11/889 (1.2%)
9	CK	0.47	0/640	1.48	11/889 (1.2%)
10	AL	0.46	0/503	0.92	2/673 (0.3%)
10	CL	0.54	0/503	1.06	4/673 (0.6%)
11	AN	0.99	1/1144 (0.1%)	1.27	5/1543 (0.3%)
11	CN	0.71	0/1144	1.12	7/1543 (0.5%)
12	AO	0.94	1/943 (0.1%)	1.19	3/1269 (0.2%)
12	CO	0.82	0/943	1.09	2/1269 (0.2%)
13	AP	0.86	0/1156	1.16	3/1537 (0.2%)
13	CP	0.62	0/1152	1.13	9/1533 (0.6%)
14	AQ	0.94	0/1143	1.18	5/1527 (0.3%)
14	CQ	0.70	0/1143	1.03	3/1527 (0.2%)
15	AR	0.92	0/982	1.13	2/1312 (0.2%)
15	CR	0.76	0/982	1.01	0/1312
16	AS	0.70	0/887	1.10	1/1180 (0.1%)
16	CS	0.58	0/880	1.06	2/1172 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	AT	0.93	0/1105	1.20	7/1477 (0.5%)
17	CT	0.72	0/1097	1.05	4/1468 (0.3%)
18	AU	1.05	0/977	1.18	3/1301 (0.2%)
18	CU	0.73	0/977	0.99	2/1301 (0.2%)
19	AV	0.99	0/782	1.31	4/1049 (0.4%)
19	CV	0.67	0/782	0.97	0/1049
20	AW	1.13	1/897 (0.1%)	1.17	3/1205 (0.2%)
20	CW	0.87	0/897	1.14	2/1205 (0.2%)
21	AX	0.93	0/764	1.13	2/1025 (0.2%)
21	CX	0.77	0/764	1.13	4/1025 (0.4%)
22	AY	0.89	1/819 (0.1%)	1.20	2/1095 (0.2%)
22	CY	0.65	0/819	1.07	2/1095 (0.2%)
23	AZ	0.65	0/1379	1.10	10/1873 (0.5%)
23	CZ	0.49	0/1390	1.02	10/1890 (0.5%)
24	A0	0.84	0/662	1.12	2/881 (0.2%)
24	C0	0.68	0/662	1.08	3/881 (0.3%)
25	A1	0.85	0/762	1.08	1/1014 (0.1%)
25	C1	0.77	0/762	1.03	0/1014
26	A2	0.93	0/590	1.08	3/781 (0.4%)
26	C2	0.64	0/590	0.93	0/781
27	A3	1.00	0/474	1.22	4/635 (0.6%)
27	C3	0.64	0/469	1.06	1/630 (0.2%)
28	A4	0.52	0/571	1.19	5/768 (0.7%)
28	C4	0.48	0/545	1.10	6/737 (0.8%)
29	A5	1.11	0/469	1.35	5/635 (0.8%)
29	C5	0.88	0/469	1.18	0/635
30	A6	0.96	1/460 (0.2%)	1.08	0/613
30	C6	0.73	0/456	1.09	2/608 (0.3%)
31	A7	1.06	1/426 (0.2%)	1.15	1/561 (0.2%)
31	C7	0.88	0/426	1.12	2/561 (0.4%)
32	A8	0.99	0/525	1.22	3/691 (0.4%)
32	C8	0.74	0/525	1.07	0/691
33	A9	0.97	0/310	1.28	0/407
33	C9	0.65	0/310	1.05	1/407 (0.2%)
34	BA	0.39	0/36027	0.60	5/56227 (0.0%)
34	DA	0.35	0/36170	0.56	2/56452 (0.0%)
35	BB	0.51	0/1881	1.07	16/2542 (0.6%)
35	DB	0.46	0/1860	0.99	9/2518 (0.4%)
36	BC	0.51	0/1576	0.97	5/2130 (0.2%)
36	DC	0.46	0/1568	0.93	4/2122 (0.2%)
37	BD	0.60	0/1689	1.05	7/2267 (0.3%)
37	DD	0.59	0/1708	1.03	6/2289 (0.3%)
38	BE	0.64	0/1145	1.08	4/1543 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	DE	0.58	0/1149	1.12	9/1548 (0.6%)
39	BF	0.65	0/825	0.99	2/1118 (0.2%)
39	DF	0.63	0/833	0.92	1/1128 (0.1%)
40	BG	0.53	0/1250	0.97	3/1679 (0.2%)
40	DG	0.48	0/1254	0.93	1/1683 (0.1%)
41	BH	0.64	0/1108	1.06	4/1494 (0.3%)
41	DH	0.52	0/1108	1.02	4/1494 (0.3%)
42	BI	0.53	0/1005	0.96	0/1350
42	DI	0.47	0/997	0.93	1/1343 (0.1%)
43	BJ	0.54	0/722	0.94	0/982
43	DJ	0.48	0/727	1.03	4/988 (0.4%)
44	BK	0.64	0/848	1.05	0/1149
44	DK	0.64	0/848	1.12	6/1149 (0.5%)
45	BL	0.67	0/946	0.99	2/1274 (0.2%)
45	DL	0.63	0/946	0.97	0/1274
46	BM	0.54	0/977	1.10	5/1310 (0.4%)
46	DM	0.47	0/961	0.91	2/1291 (0.2%)
47	BN	0.55	0/501	1.01	3/664 (0.5%)
47	DN	0.46	0/501	0.84	0/664
48	BO	0.62	0/739	1.01	4/985 (0.4%)
48	DO	0.57	0/739	0.96	3/985 (0.3%)
49	BP	0.65	0/697	1.06	5/939 (0.5%)
49	DP	0.65	0/693	0.97	3/935 (0.3%)
50	BQ	0.63	0/836	1.00	3/1117 (0.3%)
50	DQ	0.57	0/836	1.02	3/1117 (0.3%)
51	BR	0.63	0/560	1.05	1/746 (0.1%)
51	DR	0.63	0/560	0.97	2/746 (0.3%)
52	BS	0.47	0/676	0.93	2/911 (0.2%)
52	DS	0.49	0/661	1.03	4/893 (0.4%)
53	BT	0.60	0/730	1.08	2/965 (0.2%)
53	DT	0.64	0/733	1.10	5/969 (0.5%)
54	BU	0.47	0/203	0.91	0/266
54	DU	0.45	0/203	0.91	0/266
55	BV	0.36	0/310	0.47	0/480
55	DV	0.31	0/282	0.43	0/437
56	BW	0.26	0/1577	0.38	0/2454
56	DW	0.25	0/1531	0.38	0/2379
57	BX	0.40	0/1700	0.60	0/2650
57	DX	0.42	2/1700 (0.1%)	0.55	1/2650 (0.0%)
58	BY	0.27	1/1602 (0.1%)	0.44	0/2493
58	DY	0.23	0/1579	0.34	0/2455
59	BZ	0.57	0/5763	1.03	25/7804 (0.3%)
59	DZ	0.56	0/5784	1.00	22/7835 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
All	All	0.57	10/333310 (0.0%)	0.81	478/497173 (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
1	AA	0	1
28	A4	0	1
35	BB	0	1
53	BT	0	1
53	DT	0	1
59	DZ	0	1
All	All	0	6

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	DX	74	C	O3'-P	-8.91	1.47	1.61
30	A6	23	THR	CA-CB	6.13	1.62	1.53
57	DX	8	4SU	O3'-P	6.05	1.62	1.56
12	AO	98	VAL	CA-CB	5.67	1.61	1.54
31	A7	13	ALA	CA-CB	-5.55	1.44	1.53
6	AF	90	PHE	CA-C	-5.38	1.46	1.53
11	AN	5	VAL	CA-CB	5.37	1.58	1.54
20	AW	11	ARG	CA-C	-5.30	1.47	1.53
22	AY	39	VAL	CA-CB	-5.06	1.48	1.54
58	BY	8	4SU	O3'-P	5.00	1.61	1.56

All (478) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	CK	68	LEU	CA-C-N	15.24	138.89	119.84
9	CK	68	LEU	C-N-CA	15.24	138.89	119.84
9	CK	76	GLY	CA-C-N	13.20	136.34	119.84
9	CK	76	GLY	C-N-CA	13.20	136.34	119.84
28	A4	60	GLN	N-CA-C	-11.01	99.86	113.18
46	BM	84	ILE	N-CA-C	9.87	120.69	110.62
9	AK	104	ILE	CA-C-N	9.49	131.70	119.84
9	AK	104	ILE	C-N-CA	9.49	131.70	119.84
9	AK	76	GLY	CA-C-N	9.35	131.52	119.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	AK	76	GLY	C-N-CA	9.35	131.52	119.84
5	AE	73	GLU	CA-C-N	9.12	131.24	119.84
5	AE	73	GLU	C-N-CA	9.12	131.24	119.84
6	AF	89	VAL	CA-C-N	-8.97	109.49	122.67
6	AF	89	VAL	C-N-CA	-8.97	109.49	122.67
59	BZ	280	LEU	CA-C-N	8.90	128.98	119.90
59	BZ	280	LEU	C-N-CA	8.90	128.98	119.90
44	DK	38	ASN	CA-C-N	8.87	128.94	119.89
44	DK	38	ASN	C-N-CA	8.87	128.94	119.89
20	AW	17	VAL	CB-CA-C	-8.54	100.44	112.22
21	CX	10	ALA	CA-C-N	-8.41	109.91	120.51
21	CX	10	ALA	C-N-CA	-8.41	109.91	120.51
1	AA	2014	G	C2'-C3'-O3'	8.36	122.04	109.50
28	A4	40	HIS	CA-C-N	8.31	130.23	119.84
28	A4	40	HIS	C-N-CA	8.31	130.23	119.84
22	CY	31	LEU	CA-C-N	8.30	127.60	118.97
22	CY	31	LEU	C-N-CA	8.30	127.60	118.97
14	AQ	22	LYS	N-CA-C	-8.27	102.20	111.14
1	AA	1150	C	OP1-P-O3'	-8.24	83.27	108.00
4	CD	46	GLN	N-CA-C	-8.23	102.68	114.12
14	CQ	136	ALA	N-CA-C	-8.14	103.14	113.23
4	AD	229	VAL	CB-CA-C	-8.08	99.63	112.16
5	AE	137	HIS	CA-C-N	-8.06	111.14	120.89
5	AE	137	HIS	C-N-CA	-8.06	111.14	120.89
27	A3	40	THR	CA-C-N	-8.02	110.69	119.19
27	A3	40	THR	C-N-CA	-8.02	110.69	119.19
1	CA	1992	G	C2'-C3'-O3'	8.02	121.53	109.50
5	CE	85	ASN	CA-C-N	7.89	128.51	119.99
5	CE	85	ASN	C-N-CA	7.89	128.51	119.99
17	AT	127	ALA	N-CA-C	-7.72	98.40	110.36
1	AA	1150	C	OP2-P-O3'	-7.59	85.23	108.00
46	BM	112	GLY	CA-C-N	7.57	129.30	119.84
46	BM	112	GLY	C-N-CA	7.57	129.30	119.84
17	CT	88	ILE	CB-CA-C	-7.55	103.12	111.35
24	C0	82	ARG	CA-C-N	7.50	129.22	119.84
24	C0	82	ARG	C-N-CA	7.50	129.22	119.84
35	BB	193	ASP	CA-C-N	7.40	129.09	119.84
35	BB	193	ASP	C-N-CA	7.40	129.09	119.84
59	DZ	-4	ALA	N-CA-C	-7.26	105.60	114.75
4	CD	229	VAL	CB-CA-C	-7.26	100.90	112.16
18	AU	9	VAL	N-CA-C	7.24	117.23	110.42
38	DE	69	VAL	CA-C-N	7.23	128.87	119.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	DE	69	VAL	C-N-CA	7.23	128.87	119.84
11	AN	39	ARG	CA-C-N	7.08	126.78	119.56
11	AN	39	ARG	C-N-CA	7.08	126.78	119.56
59	BZ	8	ASP	N-CA-C	-7.07	104.52	113.43
36	DC	125	GLU	N-CA-C	-7.07	103.32	112.23
51	BR	32	ARG	N-CA-C	-7.06	103.15	114.09
43	DJ	52	GLY	CA-C-N	7.03	128.25	120.45
43	DJ	52	GLY	C-N-CA	7.03	128.25	120.45
5	AE	20	ALA	CA-C-N	-7.01	116.75	122.85
5	AE	20	ALA	C-N-CA	-7.01	116.75	122.85
4	AD	56	GLY	N-CA-C	7.00	124.98	115.32
9	AK	128	LEU	CA-C-N	6.98	128.56	119.84
9	AK	128	LEU	C-N-CA	6.98	128.56	119.84
13	AP	47	ASP	CA-C-N	6.97	126.94	119.28
13	AP	47	ASP	C-N-CA	6.97	126.94	119.28
8	AH	127	GLU	CA-C-N	-6.96	112.72	120.45
8	AH	127	GLU	C-N-CA	-6.96	112.72	120.45
1	AA	2701	U	C4'-C3'-O3'	6.94	119.81	109.40
5	CE	137	HIS	N-CA-C	6.94	118.11	110.13
5	AE	31	CYS	CA-C-N	6.92	127.30	119.83
5	AE	31	CYS	C-N-CA	6.92	127.30	119.83
8	AH	13	LYS	N-CA-C	-6.91	99.44	109.59
1	CA	1653	G	P-O3'-C3'	6.91	130.56	120.20
59	DZ	-11	LYS	N-CA-C	-6.89	102.25	111.96
6	CF	24	LEU	CA-C-N	-6.86	113.24	120.03
6	CF	24	LEU	C-N-CA	-6.86	113.24	120.03
53	DT	11	SER	N-CA-C	-6.86	104.91	112.72
35	BB	9	GLU	N-CA-C	6.84	125.37	110.80
9	CK	104	ILE	CA-C-N	6.83	128.38	119.84
9	CK	104	ILE	C-N-CA	6.83	128.38	119.84
17	AT	52	ILE	CB-CA-C	-6.83	102.63	110.41
45	BL	124	LYS	CA-C-N	6.81	128.36	119.84
45	BL	124	LYS	C-N-CA	6.81	128.36	119.84
59	BZ	378	VAL	CB-CA-C	-6.81	101.65	110.98
1	CA	2689	U	C4'-C3'-O3'	6.79	119.59	109.40
4	AD	42	GLY	N-CA-C	-6.78	105.49	115.72
10	CL	98	ARG	N-CA-C	6.76	117.50	108.38
41	DH	119	LEU	N-CA-C	6.76	119.44	109.24
5	AE	8	LYS	CA-C-N	-6.73	114.40	122.35
5	AE	8	LYS	C-N-CA	-6.73	114.40	122.35
4	AD	98	VAL	CA-C-N	6.73	130.21	120.38
4	AD	98	VAL	C-N-CA	6.73	130.21	120.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	AZ	100	VAL	CA-C-N	6.73	128.25	119.84
23	AZ	100	VAL	C-N-CA	6.73	128.25	119.84
59	DZ	319	ASP	CA-C-N	6.73	126.52	119.05
59	DZ	319	ASP	C-N-CA	6.73	126.52	119.05
3	AC	203	GLU	N-CA-C	-6.73	104.64	114.39
23	CZ	14	LYS	CA-C-N	6.72	126.68	119.28
23	CZ	14	LYS	C-N-CA	6.72	126.68	119.28
22	AY	58	GLY	N-CA-C	6.72	123.56	111.34
3	CC	203	GLU	N-CA-C	-6.71	104.65	114.39
4	AD	131	LEU	CA-C-N	-6.69	112.89	119.78
4	AD	131	LEU	C-N-CA	-6.69	112.89	119.78
46	BM	120	LYS	N-CA-C	6.67	119.57	108.96
6	AF	157	VAL	CB-CA-C	-6.65	101.94	111.19
35	DB	193	ASP	CA-C-N	6.64	126.59	119.28
35	DB	193	ASP	C-N-CA	6.64	126.59	119.28
59	DZ	261	GLY	N-CA-C	6.64	119.52	110.69
13	CP	44	GLY	CA-C-N	6.62	133.62	121.70
13	CP	44	GLY	C-N-CA	6.62	133.62	121.70
35	BB	231	GLU	CA-C-N	-6.61	113.83	120.31
35	BB	231	GLU	C-N-CA	-6.61	113.83	120.31
31	C7	6	GLN	CA-C-N	6.58	126.61	119.90
31	C7	6	GLN	C-N-CA	6.58	126.61	119.90
37	DD	38	TYR	CA-C-N	6.58	127.16	120.38
37	DD	38	TYR	C-N-CA	6.58	127.16	120.38
6	CF	9	ILE	N-CA-C	6.55	115.19	107.73
59	DZ	282	SER	N-CA-C	-6.54	102.46	110.31
28	C4	52	THR	N-CA-C	-6.52	107.18	114.62
53	DT	94	ALA	N-CA-C	-6.52	105.08	113.16
59	BZ	115	GLU	CA-C-N	6.49	127.95	119.84
59	BZ	115	GLU	C-N-CA	6.49	127.95	119.84
1	AA	537	G	O4'-C1'-N9	6.48	117.92	108.20
11	CN	128	HIS	CA-C-N	6.47	126.60	119.87
11	CN	128	HIS	C-N-CA	6.47	126.60	119.87
37	BD	19	LEU	N-CA-C	-6.46	99.77	110.17
37	DD	171	GLY	CA-C-N	6.46	127.91	119.84
37	DD	171	GLY	C-N-CA	6.46	127.91	119.84
7	CG	45	GLU	N-CA-C	-6.45	104.67	112.54
3	AC	16	ASP	CA-C-N	6.41	125.64	118.97
3	AC	16	ASP	C-N-CA	6.41	125.64	118.97
12	CO	118	ALA	CA-C-N	6.40	125.90	119.24
12	CO	118	ALA	C-N-CA	6.40	125.90	119.24
41	BH	4	ASP	CA-C-N	6.39	126.15	119.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	BH	4	ASP	C-N-CA	6.39	126.15	119.05
10	CL	112	MET	CA-C-N	-6.39	115.20	121.65
10	CL	112	MET	C-N-CA	-6.39	115.20	121.65
10	AL	98	ARG	N-CA-C	6.34	117.49	108.74
3	CC	16	ASP	CA-C-N	6.33	125.55	118.97
3	CC	16	ASP	C-N-CA	6.33	125.55	118.97
5	CE	73	GLU	CA-C-N	6.33	127.75	119.84
5	CE	73	GLU	C-N-CA	6.33	127.75	119.84
11	AN	97	ARG	N-CA-C	-6.31	105.71	113.41
22	AY	38	ILE	CB-CA-C	-6.31	102.33	110.98
50	BQ	9	VAL	CB-CA-C	-6.31	101.80	111.08
35	BB	128	GLU	N-CA-C	-6.31	104.89	112.59
33	C9	4	ARG	N-CA-C	6.31	116.89	108.38
1	AA	1821	C	O3'-P-O5'	-6.29	94.56	104.00
16	CS	37	ALA	N-CA-C	6.29	117.90	107.20
1	AA	2045	G	O5'-P-OP1	-6.29	89.13	108.00
1	AA	2641	A	N9-C1'-C2'	6.26	123.39	114.00
59	BZ	213	HIS	N-CA-C	-6.25	104.36	112.68
36	DC	29	TYR	N-CA-C	-6.25	105.67	113.55
49	DP	70	ALA	N-CA-C	-6.23	106.65	114.56
19	AV	38	LEU	N-CA-C	-6.21	106.33	114.04
1	AA	1255	A	C4'-C3'-O3'	6.21	118.72	109.40
20	CW	13	SER	CA-C-N	6.18	127.57	119.84
20	CW	13	SER	C-N-CA	6.18	127.57	119.84
38	BE	67	VAL	N-CA-C	6.18	117.59	108.45
6	AF	58	ALA	N-CA-C	6.17	120.53	113.19
38	DE	48	ALA	N-CA-C	6.17	113.68	108.13
53	BT	11	SER	N-CA-C	-6.17	104.93	112.88
4	AD	105	ILE	CA-C-N	-6.15	113.17	121.66
4	AD	105	ILE	C-N-CA	-6.15	113.17	121.66
48	BO	18	PHE	CA-C-N	6.14	127.52	119.84
48	BO	18	PHE	C-N-CA	6.14	127.52	119.84
1	CA	752	A	C2'-C3'-O3'	6.14	118.71	109.50
40	BG	13	GLN	CA-C-N	6.11	126.12	119.89
40	BG	13	GLN	C-N-CA	6.11	126.12	119.89
59	DZ	118	SER	N-CA-C	-6.09	103.80	111.11
39	BF	6	VAL	N-CA-C	6.06	117.11	108.93
7	AG	31	VAL	CA-C-N	6.05	127.41	119.84
7	AG	31	VAL	C-N-CA	6.05	127.41	119.84
14	CQ	28	ALA	N-CA-C	6.04	121.96	113.56
30	C6	40	CYS	CA-C-N	-6.03	113.60	120.89
30	C6	40	CYS	C-N-CA	-6.03	113.60	120.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	AZ	67	LEU	CA-C-N	6.02	129.30	120.46
23	AZ	67	LEU	C-N-CA	6.02	129.30	120.46
59	DZ	169	GLY	N-CA-C	6.01	120.82	113.79
4	AD	220	HIS	CA-C-N	-5.99	115.38	122.93
4	AD	220	HIS	C-N-CA	-5.99	115.38	122.93
5	AE	47	VAL	CB-CA-C	-5.99	101.77	110.63
59	BZ	480	GLN	N-CA-C	-5.97	103.38	112.99
23	AZ	129	SER	CA-C-N	5.97	125.65	119.56
23	AZ	129	SER	C-N-CA	5.97	125.65	119.56
14	AQ	96	VAL	CB-CA-C	-5.97	104.10	111.08
28	A4	52	THR	N-CA-C	-5.97	103.37	111.55
15	AR	84	ALA	CA-C-N	-5.94	112.74	119.28
15	AR	84	ALA	C-N-CA	-5.94	112.74	119.28
11	CN	39	ARG	CA-C-N	5.94	127.27	119.84
11	CN	39	ARG	C-N-CA	5.94	127.27	119.84
35	DB	51	LEU	N-CA-C	-5.93	104.76	112.23
29	A5	26	THR	CB-CA-C	5.92	116.45	109.47
28	C4	68	ARG	N-CA-C	5.92	121.13	111.37
50	DQ	63	ARG	CA-C-N	5.91	127.23	119.84
50	DQ	63	ARG	C-N-CA	5.91	127.23	119.84
17	AT	53	ARG	CB-CA-C	-5.91	101.32	110.78
23	CZ	107	THR	CA-C-N	5.91	125.93	119.90
23	CZ	107	THR	C-N-CA	5.91	125.93	119.90
36	DC	155	GLY	N-CA-C	5.90	119.22	110.60
59	DZ	160	ARG	N-CA-C	5.89	122.83	109.81
18	AU	41	ALA	N-CA-C	-5.89	104.78	111.14
40	BG	78	ARG	N-CA-C	5.88	118.06	108.76
59	BZ	269	VAL	N-CA-C	-5.88	105.11	110.82
35	BB	14	GLY	N-CA-C	-5.87	107.63	115.32
8	AH	115	VAL	N-CA-C	5.86	116.31	107.75
17	CT	48	ILE	CB-CA-C	-5.85	103.54	111.15
1	AA	455	A	C5'-C4'-C3'	-5.85	107.22	116.00
24	C0	44	ARG	N-CA-C	-5.85	106.30	113.50
8	AH	3	ARG	N-CA-C	5.85	118.75	108.75
36	BC	4	LYS	N-CA-C	5.84	118.71	110.23
59	BZ	639	ASN	N-CA-C	5.84	117.75	110.91
35	BB	172	ILE	CB-CA-C	-5.84	104.51	111.81
51	DR	51	LEU	CA-C-N	5.83	125.84	119.89
51	DR	51	LEU	C-N-CA	5.83	125.84	119.89
49	BP	40	ASP	CA-C-N	5.83	127.13	119.84
49	BP	40	ASP	C-N-CA	5.83	127.13	119.84
52	BS	67	VAL	N-CA-C	5.82	116.47	110.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
59	BZ	-4	ALA	N-CA-C	-5.82	103.75	112.54
7	AG	52	ILE	N-CA-C	5.82	112.44	106.21
23	AZ	86	VAL	CB-CA-C	-5.82	101.86	110.82
4	CD	271	ILE	CB-CA-C	-5.81	104.43	112.04
17	AT	121	ILE	CB-CA-C	-5.80	104.21	112.22
6	AF	40	GLN	N-CA-C	-5.77	104.99	111.28
34	BA	913	A	C2'-C3'-O3'	5.77	118.16	109.50
32	A8	29	LYS	N-CA-C	5.77	117.22	110.41
9	CK	85	ASP	CA-C-N	5.77	127.05	119.84
9	CK	85	ASP	C-N-CA	5.77	127.05	119.84
19	AV	99	ILE	CB-CA-C	-5.76	103.18	111.19
38	DE	95	ALA	CA-C-N	5.76	127.04	119.84
38	DE	95	ALA	C-N-CA	5.76	127.04	119.84
59	BZ	117	GLN	N-CA-C	-5.75	104.93	111.14
6	AF	89	VAL	N-CA-C	5.75	117.27	111.00
32	A8	33	ASN	N-CA-C	5.74	120.28	113.28
4	AD	106	ILE	N-CA-CB	5.73	116.78	110.53
11	CN	104	LYS	N-CA-C	-5.73	105.03	111.28
1	CA	1210	A	P-O3'-C3'	5.72	128.78	120.20
13	CP	12	ALA	N-CA-C	-5.72	105.19	111.82
1	CA	2689	U	P-O3'-C3'	5.72	128.78	120.20
53	BT	101	GLY	N-CA-C	5.71	120.88	110.71
59	DZ	299	VAL	N-CA-C	5.71	116.09	108.27
48	DO	18	PHE	CA-C-N	5.71	126.97	119.84
48	DO	18	PHE	C-N-CA	5.71	126.97	119.84
24	A0	10	THR	N-CA-C	5.70	119.26	110.42
48	BO	23	GLY	N-CA-C	5.70	124.02	113.76
49	DP	71	ARG	N-CA-C	-5.70	105.82	112.89
4	CD	244	ARG	CA-C-N	-5.70	114.51	120.38
4	CD	244	ARG	C-N-CA	-5.70	114.51	120.38
47	BN	33	VAL	N-CA-C	5.69	116.06	107.80
52	DS	15	LEU	N-CA-C	-5.69	106.97	114.31
52	BS	36	ARG	N-CA-C	-5.69	106.38	113.38
39	BF	60	PHE	N-CA-C	5.68	118.66	107.98
6	CF	183	VAL	N-CA-C	5.68	116.45	110.72
29	A5	6	VAL	CA-C-N	-5.67	114.09	119.76
29	A5	6	VAL	C-N-CA	-5.67	114.09	119.76
59	DZ	269	VAL	N-CA-C	-5.67	106.93	111.81
21	CX	7	VAL	N-CA-C	5.67	115.86	110.53
9	CK	128	LEU	CA-C-N	5.67	126.16	120.04
9	CK	128	LEU	C-N-CA	5.67	126.16	120.04
59	BZ	148	LEU	N-CA-C	-5.66	105.48	112.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	BB	218	ALA	N-CA-C	-5.64	106.08	113.12
26	A2	56	GLN	N-CA-C	-5.63	105.22	111.36
38	DE	113	ALA	N-CA-C	-5.63	106.25	113.23
1	AA	1255	A	P-O3'-C3'	5.63	128.64	120.20
35	BB	12	GLU	N-CA-C	-5.63	106.58	113.50
59	DZ	111	SER	N-CA-C	-5.62	106.42	113.28
36	BC	182	ILE	CB-CA-C	-5.61	104.53	111.32
23	AZ	115	GLY	N-CA-C	5.60	119.28	111.10
36	BC	19	GLU	N-CA-C	-5.60	105.21	113.61
1	CA	512	G	O4'-C1'-N9	5.60	116.60	108.20
21	AX	23	GLU	N-CA-C	-5.60	106.03	112.92
59	DZ	443	HIS	CA-C-N	5.60	125.70	119.32
59	DZ	443	HIS	C-N-CA	5.60	125.70	119.32
46	BM	109	THR	N-CA-C	-5.60	106.45	113.28
1	AA	1157	A	O4'-C1'-N9	5.60	116.89	108.50
23	CZ	155	LEU	N-CA-C	5.59	117.13	110.19
13	CP	62	LEU	CA-C-N	5.59	125.35	119.76
13	CP	62	LEU	C-N-CA	5.59	125.35	119.76
59	BZ	159	ALA	N-CA-C	5.58	118.09	110.55
1	CA	752	A	P-O3'-C3'	5.58	128.57	120.20
14	AQ	12	GLN	N-CA-C	5.58	117.88	109.23
13	CP	132	LYS	N-CA-C	-5.58	105.30	111.71
36	BC	194	GLY	N-CA-C	5.57	118.03	111.63
11	CN	78	TYR	CA-C-N	-5.57	114.19	119.76
11	CN	78	TYR	C-N-CA	-5.57	114.19	119.76
8	CH	16	SER	N-CA-C	5.56	117.58	108.52
7	CG	31	VAL	CA-C-N	5.55	126.78	119.84
7	CG	31	VAL	C-N-CA	5.55	126.78	119.84
44	DK	120	ARG	CA-C-N	5.55	125.50	119.78
44	DK	120	ARG	C-N-CA	5.55	125.50	119.78
8	AH	9	ILE	CB-CA-C	-5.55	104.49	111.04
38	BE	113	ALA	N-CA-C	-5.54	106.60	113.19
8	CH	17	VAL	CB-CA-C	-5.53	105.59	112.45
35	DB	25	ASN	CA-C-N	5.53	125.23	119.82
35	DB	25	ASN	C-N-CA	5.53	125.23	119.82
44	DK	114	VAL	CA-C-O	5.52	122.81	119.94
27	C3	56	VAL	CB-CA-C	-5.51	102.28	110.33
28	C4	39	CYS	N-CA-C	5.51	118.81	112.97
52	DS	82	GLY	N-CA-C	5.51	120.01	111.08
9	AK	68	LEU	CA-C-N	5.51	126.73	119.84
9	AK	68	LEU	C-N-CA	5.51	126.73	119.84
50	DQ	57	VAL	N-CA-C	5.50	116.84	108.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	CA	1210	A	C4'-C3'-O3'	5.50	117.66	109.40
59	BZ	-23	LEU	N-CA-C	-5.50	106.07	112.89
1	CA	195	A	P-O3'-C3'	5.50	128.44	120.20
46	DM	9	ILE	CA-C-N	5.49	126.71	119.84
46	DM	9	ILE	C-N-CA	5.49	126.71	119.84
19	AV	35	LEU	CA-C-N	5.49	125.39	119.85
19	AV	35	LEU	C-N-CA	5.49	125.39	119.85
5	AE	75	VAL	N-CA-CB	-5.46	105.55	112.60
34	DA	1442	G	P-O3'-C3'	5.46	126.25	119.70
41	DH	4	ASP	CA-C-N	5.46	125.11	119.05
41	DH	4	ASP	C-N-CA	5.46	125.11	119.05
35	BB	127	ILE	N-CA-C	5.46	115.91	107.78
6	CF	48	THR	CB-CA-C	-5.45	101.35	110.56
26	A2	8	LYS	N-CA-C	-5.44	105.25	111.07
36	DC	5	ILE	N-CA-C	5.43	116.41	108.53
6	CF	157	VAL	N-CA-C	5.43	115.41	107.37
18	CU	29	SER	N-CA-C	-5.43	107.30	114.31
13	CP	73	GLY	N-CA-C	5.43	121.42	112.84
13	CP	55	ARG	N-CA-C	-5.42	103.23	110.55
7	AG	88	ILE	N-CA-C	5.42	117.31	112.17
34	BA	1067	A	C2'-C3'-O3'	5.42	117.62	109.50
1	AA	1821	C	P-O3'-C3'	5.41	128.31	120.20
14	AQ	31	ASP	N-CA-C	-5.41	107.34	114.04
14	CQ	131	ILE	CB-CA-C	-5.39	103.68	111.34
6	CF	132	VAL	N-CA-C	5.39	115.35	108.12
8	AH	28	GLY	CA-C-N	5.38	125.71	119.47
8	AH	28	GLY	C-N-CA	5.38	125.71	119.47
47	BN	13	THR	CA-C-N	5.38	125.68	119.92
47	BN	13	THR	C-N-CA	5.38	125.68	119.92
59	BZ	553	GLY	CA-C-N	5.38	126.57	119.84
59	BZ	553	GLY	C-N-CA	5.38	126.57	119.84
37	DD	58	LEU	N-CA-C	-5.38	105.10	110.97
27	A3	8	LEU	CA-C-N	-5.38	116.12	122.36
27	A3	8	LEU	C-N-CA	-5.38	116.12	122.36
1	CA	271(M)	G	OP1-P-O3'	5.38	117.03	105.20
10	CL	130	SER	N-CA-C	-5.38	106.31	112.92
59	DZ	10	LYS	N-CA-C	-5.38	106.68	113.18
9	AK	44	LEU	N-CA-C	-5.37	106.10	113.30
40	DG	79	ARG	N-CA-C	5.37	122.24	110.80
42	DI	23	ASN	N-CA-C	5.36	118.03	111.82
18	AU	50	ARG	N-CA-C	-5.35	105.35	111.07
53	DT	75	ASN	N-CA-C	5.35	117.86	111.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
59	BZ	608	VAL	N-CA-C	5.33	115.54	107.75
8	CH	28	GLY	CA-C-N	5.33	125.39	119.32
8	CH	28	GLY	C-N-CA	5.33	125.39	119.32
8	AH	92	ILE	N-CA-C	5.32	115.95	110.36
35	BB	182	ILE	CA-C-N	5.32	126.49	119.84
35	BB	182	ILE	C-N-CA	5.32	126.49	119.84
59	BZ	98	MET	N-CA-C	5.32	122.12	110.80
59	BZ	403	GLU	N-CA-C	5.32	115.56	108.38
49	BP	70	ALA	N-CA-C	-5.31	107.17	113.97
1	AA	2220	A	O3'-P-O5'	-5.31	96.04	104.00
12	AO	81	ASP	CA-C-N	-5.31	115.68	123.00
12	AO	81	ASP	C-N-CA	-5.31	115.68	123.00
32	A8	61	LEU	N-CA-C	-5.30	106.81	113.28
23	CZ	102	LEU	N-CA-C	5.29	117.22	108.13
1	AA	2298	A	N9-C1'-C2'	5.28	121.92	114.00
37	BD	39	PRO	CA-C-N	5.28	125.25	120.03
37	BD	39	PRO	C-N-CA	5.28	125.25	120.03
35	BB	23	ARG	N-CA-C	-5.27	104.28	111.56
1	CA	752	A	C4'-C3'-O3'	5.27	117.30	109.40
26	A2	19	VAL	CB-CA-C	-5.27	105.18	112.24
23	CZ	67	LEU	CA-C-N	5.27	126.42	119.84
23	CZ	67	LEU	C-N-CA	5.27	126.42	119.84
35	DB	23	ARG	N-CA-C	-5.26	103.77	111.30
50	BQ	23	VAL	CB-CA-C	-5.26	104.47	110.73
5	AE	168	MET	N-CA-C	5.26	118.31	109.95
9	AK	10	LEU	N-CA-C	-5.25	107.89	114.56
34	BA	913	A	P-O3'-C3'	5.25	128.08	120.20
38	BE	35	GLY	N-CA-C	5.25	118.20	110.80
36	BC	202	ILE	N-CA-C	5.25	115.41	107.80
35	BB	123	ALA	N-CA-C	-5.25	106.65	113.16
38	BE	48	ALA	N-CA-C	5.25	112.94	108.22
59	BZ	166	LEU	CA-C-N	5.24	126.06	120.13
59	BZ	166	LEU	C-N-CA	5.24	126.06	120.13
9	CK	89	ALA	N-CA-C	-5.24	106.65	112.57
9	AK	89	ALA	N-CA-C	-5.23	106.29	113.30
3	AC	68	GLY	N-CA-C	5.23	125.58	113.18
59	DZ	132	ARG	N-CA-C	5.23	117.90	108.48
4	AD	271	ILE	N-CA-C	-5.23	107.31	111.81
24	A0	13	GLY	N-CA-C	5.23	124.07	115.34
37	BD	108	LEU	N-CA-C	-5.23	106.49	112.92
3	CC	68	GLY	N-CA-C	5.22	125.56	113.18
37	DD	88	VAL	N-CA-C	5.22	115.14	107.15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	CC	201	LYS	N-CA-C	-5.22	102.88	110.08
11	AN	5	VAL	CA-C-N	5.22	124.98	119.76
11	AN	5	VAL	C-N-CA	5.22	124.98	119.76
21	CX	54	VAL	N-CA-C	5.21	115.98	108.48
23	CZ	122	ARG	N-CA-C	-5.21	105.61	111.28
34	BA	687	A	C2'-C3'-O3'	5.21	117.31	109.50
3	AC	201	LYS	N-CA-C	-5.20	102.91	110.08
23	AZ	98	MET	N-CA-C	5.20	116.19	108.60
29	A5	12	SER	N-CA-C	5.20	117.00	110.24
44	DK	53	SER	N-CA-C	-5.18	106.91	113.18
7	CG	141	PHE	CA-C-N	5.18	124.80	119.05
7	CG	141	PHE	C-N-CA	5.18	124.80	119.05
35	DB	230	VAL	N-CA-C	5.16	115.00	107.88
38	DE	92	LYS	CA-C-N	5.16	125.32	119.90
38	DE	92	LYS	C-N-CA	5.16	125.32	119.90
1	CA	1653	G	C2'-C3'-O3'	5.16	117.23	109.50
3	AC	46	ALA	CA-C-O	5.15	120.93	117.94
6	AF	154	VAL	N-CA-C	5.14	115.26	107.75
10	AL	85	GLU	N-CA-C	-5.14	107.55	113.88
29	A5	27	PRO	O-C-N	5.14	123.67	121.31
38	DE	18	ARG	N-CA-C	-5.14	101.47	109.24
41	DH	112	LEU	N-CA-C	5.14	117.72	108.48
1	CA	1790	C	O3'-P-O5'	-5.13	96.30	104.00
49	BP	11	SER	N-CA-C	5.13	114.92	108.45
1	CA	856	C	C2'-C3'-O3'	5.13	121.40	113.70
8	AH	41	MET	CA-C-N	-5.13	115.94	122.77
8	AH	41	MET	C-N-CA	-5.13	115.94	122.77
59	BZ	601	ILE	N-CA-C	5.13	115.73	107.73
17	CT	19	LEU	CA-C-N	5.13	125.60	120.52
17	CT	19	LEU	C-N-CA	5.13	125.60	120.52
35	DB	129	GLU	N-CA-C	-5.13	106.71	113.12
53	DT	101	GLY	N-CA-C	5.13	119.84	110.71
31	A7	47	ARG	N-CA-C	5.12	119.58	113.23
16	AS	87	PHE	N-CA-C	5.12	116.65	108.41
18	CU	50	ARG	N-CA-C	-5.12	105.59	111.07
37	BD	188	LEU	CA-C-N	5.12	125.03	119.76
37	BD	188	LEU	C-N-CA	5.12	125.03	119.76
28	C4	59	PHE	N-CA-C	5.11	115.89	107.20
57	DX	74	C	O3'-P-O5'	5.11	111.67	104.00
59	DZ	-36	LEU	CA-C-N	-5.11	114.78	120.45
59	DZ	-36	LEU	C-N-CA	-5.11	114.78	120.45
8	CH	4	ILE	N-CA-C	5.10	116.03	111.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	DJ	96	ILE	N-CA-C	5.10	116.06	108.46
28	A4	65	ASP	N-CA-C	-5.09	107.35	113.21
35	BB	17	PHE	N-CA-C	5.09	121.65	110.80
4	CD	147	LEU	N-CA-C	-5.09	107.61	113.88
34	DA	115	G	C2'-C3'-O3'	5.09	117.14	109.50
35	DB	188	ALA	N-CA-C	5.09	116.71	108.26
20	AW	94	ASP	CA-C-N	-5.09	116.31	123.13
20	AW	94	ASP	C-N-CA	-5.09	116.31	123.13
50	BQ	8	GLY	N-CA-C	5.08	119.00	110.56
49	BP	77	ALA	N-CA-C	-5.08	106.83	112.57
6	AF	53	THR	N-CA-CB	-5.07	102.71	110.42
41	BH	134	ILE	CB-CA-C	-5.07	105.21	111.70
41	BH	103	VAL	CB-CA-C	-5.07	105.15	111.08
48	BO	22	THR	N-CA-C	-5.07	103.46	110.35
39	DF	60	PHE	N-CA-C	5.07	117.65	107.41
7	AG	121	ASN	CA-C-N	5.06	125.14	119.87
7	AG	121	ASN	C-N-CA	5.06	125.14	119.87
28	C4	40	HIS	CA-C-N	5.06	124.50	119.24
28	C4	40	HIS	C-N-CA	5.06	124.50	119.24
43	DJ	18	ALA	N-CA-C	-5.06	106.79	113.12
59	DZ	639	ASN	N-CA-C	5.06	118.11	111.28
14	AQ	35	VAL	N-CA-C	5.06	115.59	108.36
17	AT	80	SER	CA-C-N	5.06	124.67	119.56
17	AT	80	SER	C-N-CA	5.06	124.67	119.56
25	A1	7	ILE	CB-CA-C	-5.05	105.83	111.80
13	CP	44	GLY	CA-C-O	-5.05	116.17	122.74
13	AP	145	PRO	CB-CA-C	-5.05	107.62	111.87
59	BZ	149	VAL	N-CA-C	-5.05	105.78	110.53
59	BZ	677	GLN	N-CA-C	5.05	116.48	108.96
23	CZ	86	VAL	N-CA-C	5.05	115.98	108.46
1	AA	1397	C	OP1-P-O3'	5.05	123.14	108.00
48	DO	66	LEU	N-CA-C	-5.05	105.86	111.36
34	BA	1201	A	P-O3'-C3'	5.04	127.77	120.20
59	DZ	558	PHE	CA-C-N	5.04	126.14	119.84
59	DZ	558	PHE	C-N-CA	5.04	126.14	119.84
12	AO	22	ILE	N-CA-C	5.04	118.56	113.47
52	DS	58	VAL	CA-C-N	5.04	126.14	119.84
52	DS	58	VAL	C-N-CA	5.04	126.14	119.84
21	AX	69	TYR	N-CA-C	5.03	116.80	108.20
17	AT	12	SER	N-CA-C	5.02	117.49	111.71
59	DZ	323	GLY	N-CA-C	5.02	116.63	111.56
16	CS	65	VAL	CB-CA-C	-5.02	105.55	111.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	990	A	C6-C5-N7	-5.01	117.25	132.30
49	DP	5	ARG	N-CA-C	5.01	114.77	108.45
53	DT	12	ALA	N-CA-C	-5.01	105.52	111.69
23	AZ	12	GLY	N-CA-C	5.01	119.96	114.40
37	BD	44	GLY	N-CA-C	5.00	118.74	112.73
5	AE	30	PRO	CA-C-N	-5.00	116.39	122.64
5	AE	30	PRO	C-N-CA	-5.00	116.39	122.64

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
28	A4	59	PHE	Peptide
1	AA	537	G	Sidechain
35	BB	8	LYS	Peptide
53	BT	9	ASN	Peptide
53	DT	9	ASN	Peptide
59	DZ	159	ALA	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	61861	0	31186	662	2
1	CA	61771	0	31146	787	0
2	AB	2573	0	1306	18	0
2	CB	2573	0	1306	26	0
3	AC	1063	0	1091	144	5
3	CC	1063	0	1089	158	12
4	AD	2136	0	2218	57	0
4	CD	2142	0	2229	66	0
5	AE	1559	0	1618	50	0
5	CE	1559	0	1618	45	0
6	AF	1584	0	1625	40	0
6	CF	1580	0	1619	51	0
7	AG	1425	0	1443	52	0
7	CG	1424	0	1434	44	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	AH	1330	0	1407	25	0
8	CH	1330	0	1407	42	0
9	AK	641	0	309	11	0
9	CK	641	0	309	13	0
10	AL	498	0	521	18	0
10	CL	498	0	521	21	0
11	AN	1117	0	1184	26	0
11	CN	1117	0	1184	21	0
12	AO	933	0	996	27	0
12	CO	933	0	996	24	0
13	AP	1139	0	1223	35	0
13	CP	1135	0	1212	49	0
14	AQ	1122	0	1179	37	0
14	CQ	1122	0	1179	40	0
15	AR	968	0	1033	19	0
15	CR	968	0	1033	29	0
16	AS	877	0	938	21	0
16	CS	870	0	923	35	0
17	AT	1091	0	1151	33	0
17	CT	1083	0	1136	28	0
18	AU	959	0	1019	25	0
18	CU	959	0	1019	30	0
19	AV	771	0	830	13	0
19	CV	771	0	830	20	0
20	AW	886	0	940	15	0
20	CW	886	0	940	20	0
21	AX	750	0	814	20	0
21	CX	750	0	814	19	0
22	AY	806	0	881	27	0
22	CY	806	0	882	38	0
23	AZ	1349	0	1355	39	0
23	CZ	1360	0	1363	43	0
24	A0	653	0	674	20	0
24	C0	653	0	674	20	0
25	A1	755	0	826	20	0
25	C1	755	0	826	22	0
26	A2	588	0	643	10	0
26	C2	588	0	643	14	0
27	A3	469	0	518	6	0
27	C3	464	0	514	8	0
28	A4	558	0	545	25	0
28	C4	532	0	506	20	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	A5	455	0	465	7	0
29	C5	455	0	465	11	0
30	A6	453	0	473	14	0
30	C6	449	0	469	13	0
31	A7	418	0	467	10	0
31	C7	418	0	467	10	0
32	A8	517	0	582	23	0
32	C8	517	0	582	19	0
33	A9	307	0	335	8	0
33	C9	307	0	335	11	0
34	BA	32185	0	16245	439	0
34	DA	32312	0	16308	512	1
35	BB	1846	0	1867	83	0
35	DB	1825	0	1828	104	0
36	BC	1552	0	1546	54	0
36	DC	1544	0	1524	68	0
37	BD	1659	0	1676	61	0
37	DD	1678	0	1718	54	0
38	BE	1129	0	1185	44	0
38	DE	1133	0	1191	43	0
39	BF	812	0	804	19	0
39	DF	820	0	814	27	0
40	BG	1231	0	1238	22	0
40	DG	1235	0	1249	32	0
41	BH	1088	0	1126	40	0
41	DH	1088	0	1126	38	0
42	BI	986	0	995	40	0
42	DI	978	0	966	41	0
43	BJ	709	0	650	34	0
43	DJ	714	0	672	34	0
44	BK	833	0	836	24	0
44	DK	833	0	836	18	0
45	BL	930	0	980	10	0
45	DL	930	0	980	30	0
46	BM	966	0	1024	36	0
46	DM	950	0	988	41	0
47	BN	492	0	529	22	0
47	DN	492	0	531	34	0
48	BO	728	0	760	20	0
48	DO	728	0	760	14	0
49	BP	681	0	697	28	0
49	DP	677	0	686	22	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
50	BQ	823	0	891	26	0
50	DQ	823	0	891	22	0
51	BR	555	0	618	17	0
51	DR	555	0	618	21	0
52	BS	661	0	675	39	0
52	DS	646	0	644	28	0
53	BT	728	0	798	28	0
53	DT	731	0	807	22	0
54	BU	199	0	208	7	0
54	DU	199	0	208	5	0
55	BV	277	0	140	4	0
55	DV	252	0	130	3	0
56	BW	1599	0	830	25	0
56	DW	1552	0	794	22	0
57	BX	1635	0	838	14	0
57	DX	1635	0	839	25	0
58	BY	1581	0	805	22	0
58	DY	1561	0	796	16	0
59	BZ	5663	0	5746	260	12
59	DZ	5682	0	5766	201	6
60	A0	5	0	0	0	0
60	A1	2	0	0	0	0
60	A2	1	0	0	0	0
60	A4	1	0	0	0	0
60	A5	3	0	0	0	0
60	A6	2	0	0	0	0
60	A7	6	0	0	0	0
60	A8	2	0	0	0	0
60	A9	1	0	0	0	0
60	AA	817	0	0	0	0
60	AB	23	0	0	0	0
60	AD	11	0	0	0	0
60	AE	5	0	0	0	0
60	AF	8	0	0	0	0
60	AG	3	0	0	0	0
60	AH	1	0	0	0	0
60	AN	3	0	0	0	0
60	AO	1	0	0	0	0
60	AP	3	0	0	0	0
60	AQ	3	0	0	0	0
60	AR	2	0	0	0	0
60	AU	4	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	AV	4	0	0	0	0
60	AW	4	0	0	0	0
60	AX	1	0	0	0	0
60	AY	1	0	0	0	0
60	AZ	1	0	0	0	0
60	BA	213	0	0	0	0
60	BB	1	0	0	0	0
60	BD	1	0	0	0	0
60	BE	1	0	0	0	0
60	BF	1	0	0	0	0
60	BK	1	0	0	0	0
60	BL	2	0	0	0	0
60	BM	1	0	0	0	0
60	BN	2	0	0	0	0
60	BT	1	0	0	0	0
60	BV	1	0	0	0	0
60	BW	2	0	0	0	0
60	BX	15	0	0	0	0
60	BY	2	0	0	0	0
60	BZ	1	0	0	0	0
60	C0	2	0	0	0	0
60	C3	1	0	0	0	0
60	C5	1	0	0	0	0
60	C7	1	0	0	0	0
60	C8	1	0	0	0	0
60	CA	664	0	0	0	0
60	CB	13	0	0	0	0
60	CD	4	0	0	0	0
60	CE	6	0	0	0	0
60	CF	6	0	0	0	0
60	CG	1	0	0	0	0
60	CN	1	0	0	0	0
60	CO	2	0	0	0	0
60	CP	1	0	0	0	0
60	CQ	4	0	0	0	0
60	CR	2	0	0	0	0
60	CU	1	0	0	0	0
60	CV	2	0	0	0	0
60	CY	1	0	0	0	0
60	DA	168	0	0	0	0
60	DD	1	0	0	0	0
60	DE	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	DF	1	0	0	0	0
60	DJ	1	0	0	0	0
60	DK	2	0	0	0	0
60	DT	1	0	0	0	0
60	DW	1	0	0	0	0
60	DX	1	0	0	0	0
60	DZ	1	0	0	0	0
61	AA	1	0	0	0	0
62	A4	1	0	0	0	0
62	A5	1	0	0	0	0
62	A6	1	0	0	0	0
62	A9	1	0	0	0	0
62	AY	1	0	0	0	0
62	BN	1	0	0	0	0
62	C4	1	0	0	0	0
62	C5	1	0	0	0	0
62	C6	1	0	0	0	0
62	C9	1	0	0	0	0
62	CY	1	0	0	0	0
62	DN	1	0	0	0	0
63	BD	8	0	0	1	0
63	DD	8	0	0	1	0
64	BZ	28	0	12	7	0
64	DZ	28	0	12	7	0
65	A0	6	0	0	0	0
65	A1	1	0	0	0	0
65	A3	1	0	0	0	0
65	A5	3	0	0	0	0
65	A6	2	0	0	0	0
65	A7	4	0	0	1	0
65	A8	10	0	0	1	0
65	AA	1408	0	0	48	0
65	AB	36	0	0	1	0
65	AD	15	0	0	1	0
65	AE	19	0	0	1	0
65	AF	7	0	0	0	0
65	AG	3	0	0	0	0
65	AH	1	0	0	0	0
65	AN	2	0	0	0	0
65	AO	1	0	0	0	0
65	AP	15	0	0	2	0
65	AQ	4	0	0	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
65	AR	2	0	0	2	0
65	AS	1	0	0	0	0
65	AT	2	0	0	0	0
65	AU	5	0	0	0	0
65	AV	2	0	0	0	0
65	AW	2	0	0	0	0
65	AX	3	0	0	0	0
65	AZ	1	0	0	0	0
65	BA	212	0	0	13	0
65	BD	2	0	0	0	0
65	BE	2	0	0	0	0
65	BL	1	0	0	0	0
65	BM	1	0	0	0	0
65	BV	2	0	0	0	0
65	BW	3	0	0	0	0
65	BX	8	0	0	0	0
65	BY	1	0	0	0	0
65	BZ	2	0	0	0	0
65	C0	6	0	0	1	0
65	C1	2	0	0	0	0
65	C3	2	0	0	0	0
65	C6	1	0	0	1	0
65	C7	1	0	0	0	0
65	C8	3	0	0	0	0
65	CA	985	0	0	52	0
65	CB	9	0	0	1	0
65	CD	14	0	0	0	0
65	CE	13	0	0	1	0
65	CF	7	0	0	0	0
65	CN	2	0	0	0	0
65	CP	10	0	0	1	0
65	CQ	1	0	0	0	0
65	CR	1	0	0	0	0
65	CT	3	0	0	0	0
65	CU	2	0	0	0	0
65	CV	1	0	0	0	0
65	CY	1	0	0	0	0
65	DA	155	0	0	6	0
65	DE	4	0	0	0	0
65	DJ	1	0	0	0	0
65	DK	2	0	0	0	0
65	DL	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
65	DW	2	0	0	0	0
65	DX	1	0	0	0	0
All	All	313372	0	210866	5452	19

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 (5452) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:1860:G:H5'	3:CC:206:LYS:CD	1.27	1.64
1:CA:1860:G:H5"	3:CC:206:LYS:CG	1.28	1.64
1:AA:1891:G:C5'	3:AC:206:LYS:HD2	1.35	1.54
1:CA:1860:G:C5'	3:CC:206:LYS:HD2	1.25	1.53
1:CA:1860:G:C5'	3:CC:206:LYS:CG	1.84	1.50
1:CA:1860:G:C5'	3:CC:206:LYS:CD	1.76	1.45
1:CA:1053:C:H42	1:CA:1107:G:N2	1.04	1.41
1:CA:1053:C:N4	1:CA:1107:G:H22	1.16	1.38
1:CA:1860:G:C4'	3:CC:206:LYS:HD2	1.53	1.35
1:CA:1860:G:H4'	3:CC:206:LYS:CD	1.59	1.32
1:AA:1891:G:C5'	3:AC:206:LYS:CD	2.09	1.31
1:AA:1891:G:C4'	3:AC:206:LYS:HD2	1.58	1.31
1:AA:1891:G:H4'	3:AC:206:LYS:CD	1.60	1.29
1:CA:1860:G:C4'	3:CC:206:LYS:CD	2.06	1.29
1:AA:1891:G:H5"	3:AC:206:LYS:CG	1.68	1.22
1:AA:1891:G:H5'	3:AC:206:LYS:HD2	1.20	1.09
1:CA:1798:U:H5'	4:CD:259:THR:HG22	1.34	1.09
1:AA:1891:G:H5"	3:AC:206:LYS:HG2	1.36	1.06
1:AA:1891:G:O3'	3:AC:206:LYS:HG3	1.54	1.05
1:AA:2198:A:HO2'	3:AC:45:HIS:CD2	1.74	1.04
1:CA:1860:G:C4'	3:CC:206:LYS:HG3	1.87	1.02
1:CA:2132:U:N3	3:CC:6:LYS:HE3	1.74	1.02
1:CA:1860:G:C4'	3:CC:206:LYS:CG	2.32	1.02
1:AA:1249:A:H2	1:AA:1287:A:H62	1.06	1.02
1:CA:1860:G:H5'	3:CC:206:LYS:CE	1.90	1.01
1:CA:1053:C:N4	1:CA:1107:G:N2	1.87	1.00
1:AA:9:U:H3	1:AA:2641:A:H2	1.08	0.99
21:AX:31:HIS:HD2	21:AX:33:LYS:H	1.07	0.99
59:BZ:99:ARG:HB3	59:BZ:99:ARG:HH11	1.26	0.99
1:AA:1829:U:H5'	4:AD:259:THR:HG22	1.43	0.98
1:CA:1860:G:H4'	3:CC:206:LYS:HD3	1.42	0.98

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:2198:A:O2'	3:AC:45:HIS:CD2	2.17	0.98
1:CA:1860:G:H5"	3:CC:206:LYS:HG3	1.38	0.98
1:AA:1891:G:H5"	3:AC:206:LYS:CD	1.86	0.96
1:AA:1405:A:H61	1:AA:1418:U:H3	1.10	0.96
59:BZ:13:ARG:HH12	59:BZ:247:ARG:HH22	1.11	0.96
21:CX:35:THR:HG22	21:CX:38:GLU:H	1.30	0.95
1:AA:535:C:OP1	65:AA:3901:HOH:O	1.83	0.95
1:CA:1204:A:H2	1:CA:1241:A:H62	1.14	0.95
1:AA:1891:G:C4'	3:AC:206:LYS:CD	2.26	0.95
59:DZ:119:GLU:OE1	59:DZ:156:ARG:NH1	2.00	0.94
34:BA:160:A:N6	34:BA:345:C:OP2	2.01	0.94
35:BB:16:HIS:HB2	35:BB:204:ASN:HB3	1.49	0.94
13:AP:39:LYS:NZ	65:AP:301:HOH:O	2.00	0.94
1:AA:1736:A:H62	1:AA:1745:A:H2	1.13	0.94
1:AA:1891:G:C5'	3:AC:206:LYS:CG	2.42	0.93
1:CA:1689:A:H62	1:CA:1698:A:H2	1.04	0.93
1:AA:1090:G:O2'	1:AA:1157:A:N6	2.01	0.93
34:DA:1086:U:H3	34:DA:1099:G:H22	1.16	0.92
1:CA:397:G:N7	65:CA:3706:HOH:O	2.03	0.92
1:CA:1860:G:H5"	3:CC:206:LYS:HG2	0.94	0.92
34:BA:1158:C:H5	34:BA:1181:G:H1	1.19	0.90
1:CA:1021:A:H62	1:CA:1141:U:H3	1.15	0.90
1:AA:2511:C:OP1	65:AA:3902:HOH:O	1.87	0.89
22:CY:102:CYS:SG	22:CY:103:GLY:N	2.42	0.89
20:AW:12:ILE:HD13	20:AW:17:VAL:HG22	1.55	0.89
59:BZ:78:ARG:HH11	59:BZ:78:ARG:HG3	1.38	0.89
23:AZ:29:TYR:HB3	23:AZ:34:ASN:HD22	1.37	0.89
34:BA:975:A:H4'	34:BA:976:G:H5"	1.56	0.88
34:BA:964:A:OP1	65:BA:1901:HOH:O	1.88	0.88
3:CC:31:LYS:NZ	3:CC:181:PHE:O	2.06	0.88
17:CT:55:ASN:H	17:CT:59:THR:HG22	1.36	0.87
34:BA:937:A:OP2	65:BA:1902:HOH:O	1.92	0.87
3:AC:31:LYS:NZ	3:AC:181:PHE:O	2.06	0.87
6:CF:185:ASP:HA	6:CF:188:ARG:HD3	1.57	0.87
35:DB:185:ILE:HG22	35:DB:199:TYR:HB2	1.55	0.86
3:AC:52:PRO:HG2	3:AC:53:ARG:HD3	1.57	0.86
1:CA:2714:G:OP2	65:CA:3701:HOH:O	1.91	0.86
34:DA:975:A:H4'	34:DA:976:G:H5"	1.58	0.86
34:DA:376:G:H5"	49:DP:5:ARG:HD3	1.58	0.86
3:CC:52:PRO:HG2	3:CC:53:ARG:HD3	1.57	0.86
24:C0:10:THR:HG22	24:C0:12:ASN:H	1.40	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1716:A:OP2	65:AA:3903:HOH:O	1.94	0.85
1:AA:2201:C:O4'	3:AC:169:THR:HG22	1.76	0.85
22:AY:54:LYS:HA	22:AY:56:PRO:HD3	1.58	0.85
44:BK:79:SER:HA	44:BK:104:GLN:HB2	1.59	0.85
13:CP:100:LEU:HD12	13:CP:112:LEU:HD11	1.57	0.84
18:AU:108:GLU:OE2	18:AU:112:ARG:NH1	2.10	0.84
59:BZ:169:GLY:HA3	59:BZ:174:PHE:HA	1.59	0.84
34:BA:1502:A:H2	34:BA:1505:G:H1	1.24	0.84
43:BJ:35:SER:HB3	43:BJ:73:ASP:HB2	1.58	0.84
1:AA:1356:G:OP2	31:A7:9:ARG:NH1	2.10	0.84
1:AA:1891:G:H4'	3:AC:206:LYS:HD3	1.56	0.84
59:BZ:405:PRO:HD2	59:BZ:406:GLU:HG2	1.60	0.83
34:DA:1166:G:N2	34:DA:1170:A:OP2	2.09	0.83
34:BA:538:G:H5"	45:BL:114:LYS:HB2	1.60	0.83
34:BA:664:G:H22	34:BA:741:G:H1	1.24	0.83
1:CA:1603:A:OP1	65:CA:3702:HOH:O	1.95	0.83
12:AO:2:ILE:HD12	12:AO:6:THR:HG21	1.59	0.83
1:CA:2178:C:O2'	3:CC:169:THR:HB	1.76	0.83
34:DA:656:C:O2'	48:DO:28:GLN:NE2	2.12	0.83
1:AA:1094:A:OP2	1:AA:1155:C:N4	2.12	0.82
1:AA:2297:C:OP2	30:A6:6:ARG:NH1	2.12	0.82
14:AQ:111:GLU:OE1	14:AQ:133:ARG:NH2	2.13	0.82
34:DA:922:G:H4'	38:DE:20:GLN:HA	1.59	0.82
13:CP:39:LYS:HB2	13:CP:45:LEU:HG	1.61	0.82
3:AC:54:ARG:NH2	3:AC:56:ASP:HB3	1.95	0.82
1:CA:1860:G:H4'	3:CC:206:LYS:CG	2.03	0.82
1:CA:2206:G:H3'	1:CA:2207:G:C8	2.15	0.82
8:CH:98:LEU:HD22	8:CH:125:VAL:HG23	1.61	0.82
53:DT:56:MET:HE1	53:DT:85:MET:HG2	1.61	0.81
1:AA:1100:A:H62	1:AA:1151:U:H3	1.29	0.81
1:AA:2128:G:H1	1:AA:2205:C:H42	1.27	0.81
43:DJ:49:VAL:HG23	47:DN:41:ARG:HB2	1.61	0.81
5:AE:179:GLU:HB3	5:AE:181:LEU:HD22	1.60	0.81
34:BA:1129:C:H5"	42:BI:16:ARG:HH12	1.46	0.81
34:DA:653:A:OP1	41:DH:56:LYS:NZ	2.13	0.81
38:DE:122:GLU:O	38:DE:126:ARG:NH1	2.14	0.81
59:BZ:97:SER:O	59:BZ:99:ARG:N	2.12	0.81
45:DL:24:VAL:HG11	45:DL:27:LEU:HD22	1.62	0.81
35:BB:69:LEU:HB3	35:BB:162:ILE:HG22	1.60	0.81
3:CC:54:ARG:NH2	3:CC:56:ASP:HB3	1.95	0.81
53:DT:10:LEU:HB3	53:DT:12:ALA:H	1.45	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:A0:11:ARG:O	24:A0:14:ARG:NH2	2.14	0.80
1:CA:1019:U:H3	1:CA:1142(A):A:H62	1.27	0.80
59:DZ:358:MET:HE1	59:DZ:363:ARG:NH1	1.97	0.80
35:BB:111:ARG:HG2	35:BB:111:ARG:HH11	1.46	0.80
1:AA:2299:A:H62	1:AA:2356:U:H3	1.27	0.80
59:BZ:357:ARG:NH1	59:BZ:373:ASP:OD1	2.15	0.79
40:BG:111:ARG:NH1	40:BG:113:GLU:OE2	2.15	0.79
34:DA:664:G:H22	34:DA:741:G:H1	1.25	0.79
59:DZ:358:MET:HE1	59:DZ:363:ARG:HH12	1.48	0.79
1:AA:1219:A:H1'	1:AA:1220:U:H5"	1.62	0.79
7:CG:80:PHE:O	7:CG:82:LEU:N	2.15	0.79
34:BA:376:G:H5"	49:BP:5:ARG:HG2	1.64	0.79
36:BC:37:GLN:NE2	47:BN:52:GLN:OE1	2.16	0.79
1:CA:2132:U:C4	3:CC:6:LYS:HE3	2.18	0.79
34:BA:656:C:O2'	48:BO:28:GLN:NE2	2.15	0.79
38:DE:74:GLY:HA3	38:DE:116:THR:HG22	1.64	0.79
41:DH:51:VAL:HG11	41:DH:60:ARG:HH11	1.46	0.79
1:CA:529:A:N6	1:CA:2041:U:O2	2.15	0.79
24:C0:11:ARG:O	24:C0:14:ARG:NH2	2.16	0.79
59:BZ:380:LEU:HD21	59:BZ:389:LEU:HD21	1.64	0.79
17:AT:55:ASN:H	17:AT:59:THR:HG22	1.45	0.79
1:AA:1891:G:C4'	3:AC:206:LYS:CG	2.61	0.79
59:BZ:363:ARG:HG2	59:BZ:363:ARG:HH11	1.46	0.79
1:CA:1860:G:C3'	3:CC:206:LYS:HG3	2.12	0.79
1:CA:2287:A:H62	1:CA:2344:U:H3	1.30	0.79
34:DA:115:G:OP1	65:DA:1801:HOH:O	2.01	0.79
34:DA:1320:C:N3	52:DS:36:ARG:NH2	2.31	0.78
59:BZ:480:GLN:O	59:BZ:482:ALA:N	2.17	0.78
1:CA:1860:G:C5'	3:CC:206:LYS:HG2	1.77	0.78
28:C4:36:CYS:SG	28:C4:37:SER:N	2.55	0.78
4:AD:69:ARG:NH2	4:AD:128:GLY:O	2.16	0.78
22:AY:92:ASN:H	22:AY:92:ASN:HD22	1.29	0.78
58:DY:7:A:H61	58:DY:66:U:H3	1.30	0.78
35:BB:115:LEU:HD13	35:BB:145:LEU:HB3	1.65	0.78
1:CA:880:G:H22	1:CA:898:C:H1'	1.46	0.78
1:CA:2296:U:OP2	16:CS:9:ARG:NH2	2.17	0.78
59:BZ:169:GLY:O	59:BZ:173:THR:OG1	2.02	0.78
1:CA:1817:G:OP1	4:CD:88:ARG:NH2	2.16	0.78
36:BC:58:GLU:HB3	43:BJ:92:THR:HG21	1.65	0.78
1:CA:631:A:OP1	13:CP:65:ARG:NH1	2.16	0.78
24:C0:5:LYS:NZ	57:DX:2:G:OP1	2.17	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:BI:17:VAL:HG21	42:BI:81:ILE:HG22	1.65	0.77
4:CD:148:GLU:HB2	4:CD:151:LYS:HD2	1.66	0.77
14:AQ:21:THR:HG21	14:AQ:101:ARG:HD3	1.64	0.77
1:CA:528:A:O2'	1:CA:529:A:H5"	1.83	0.77
1:AA:1100:A:N6	1:AA:1151:U:H3	1.81	0.77
35:BB:150:SER:O	35:BB:153:ARG:NH1	2.17	0.77
34:DA:344:A:H5"	34:DA:345:C:H5	1.48	0.77
36:DC:70:VAL:HG22	36:DC:72:LYS:H	1.49	0.77
3:AC:20:VAL:O	3:AC:21:TYR:HB2	1.83	0.77
21:AX:31:HIS:CD2	21:AX:33:LYS:H	1.98	0.77
22:AY:92:ASN:HB2	22:AY:94:LYS:H	1.48	0.77
34:DA:48:C:OP2	65:DA:1801:HOH:O	2.03	0.77
39:DF:87:ARG:HH11	39:DF:87:ARG:HG3	1.49	0.77
19:AV:98:GLU:OE2	19:AV:100:ARG:NH1	2.17	0.77
23:AZ:117:LEU:HD11	23:AZ:144:LEU:HD22	1.66	0.77
56:BW:5:G:H2'	56:BW:6:G:H8	1.50	0.77
59:BZ:329:ARG:HH11	59:BZ:331:TYR:HE1	1.33	0.77
3:AC:27:ALA:O	3:AC:30:VAL:HG22	1.85	0.77
15:AR:33:ARG:NH1	15:AR:115:GLU:OE2	2.16	0.77
36:DC:179:ARG:NH1	36:DC:206:GLU:OE1	2.17	0.77
1:AA:1007:G:OP1	65:AA:3905:HOH:O	2.03	0.76
53:BT:10:LEU:HB3	53:BT:12:ALA:H	1.50	0.76
1:CA:1155:A:H5"	18:CU:55:ARG:HH11	1.50	0.76
3:CC:20:VAL:O	3:CC:21:TYR:HB2	1.83	0.76
1:AA:992:G:OP2	65:AA:3906:HOH:O	2.03	0.76
3:AC:24:ASP:O	3:AC:28:ARG:HG3	1.85	0.76
59:BZ:78:ARG:HH11	59:BZ:78:ARG:CG	1.96	0.76
1:CA:1031:G:H21	33:C9:36:GLN:HE22	1.31	0.76
15:AR:67:LEU:HD13	15:AR:76:VAL:HG21	1.67	0.76
3:CC:24:ASP:O	3:CC:28:ARG:HG3	1.85	0.76
1:AA:1829:U:OP2	4:AD:274:ARG:NH2	2.19	0.76
59:BZ:148:LEU:O	59:BZ:152:THR:OG1	2.04	0.76
34:DA:1224:G:O2'	34:DA:1322:C:OP1	2.04	0.76
59:DZ:247:ARG:NH1	59:DZ:251:ILE:HD11	2.00	0.76
1:AA:1740:U:O2'	4:AD:14:ARG:NH2	2.18	0.76
1:CA:1310:G:OP2	31:C7:9:ARG:NH1	2.19	0.76
1:AA:1016:C:OP2	65:AA:3907:HOH:O	2.03	0.76
1:AA:2658:C:OP2	1:AA:2745:G:O2'	2.02	0.76
56:BW:50:U:H3	56:BW:64:A:H61	1.33	0.76
1:CA:827:U:OP1	65:CA:3703:HOH:O	2.02	0.76
1:CA:1039:G:O6	1:CA:1116:C:N4	2.19	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:DA:1103:C:OP1	35:DB:96:ARG:NH2	2.18	0.76
1:CA:271(R):G:H5"	25:C1:97:LEU:HD21	1.66	0.76
3:CC:27:ALA:O	3:CC:30:VAL:HG22	1.85	0.76
56:DW:76:F3N:H5'	56:DW:76:F3N:H8	1.66	0.76
59:DZ:165:GLN:HE21	59:DZ:260:LEU:H	1.33	0.76
1:CA:878:A:N6	1:CA:899:A:O2'	2.18	0.76
1:AA:1891:G:C3'	3:AC:206:LYS:HG3	2.16	0.76
6:AF:195:ASP:HB3	6:AF:198:ALA:H	1.50	0.75
1:CA:731:C:OP2	65:CA:3704:HOH:O	2.02	0.75
1:AA:894:U:OP2	65:AA:3904:HOH:O	2.02	0.75
56:BW:19:G:H1	56:BW:56:C:H42	1.33	0.75
1:CA:301:G:OP2	22:CY:84:ARG:NH2	2.18	0.75
59:BZ:373:ASP:OD2	59:BZ:374:LEU:N	2.18	0.75
1:CA:614(B):G:H2'	6:CF:44:ARG:HH11	1.51	0.75
4:CD:96:HIS:HD2	4:CD:102:LYS:HG2	1.52	0.75
1:AA:2227:G:H5'	1:AA:2228:G:N7	2.02	0.75
59:DZ:129:LYS:HD3	59:DZ:521:SER:HB2	1.67	0.75
1:AA:927:G:H2'	1:AA:928:G:H8	1.52	0.75
34:DA:677:U:H3	34:DA:713:G:H22	1.35	0.75
34:DA:838:G:H1	34:DA:848:C:H42	1.34	0.75
15:AR:3:HIS:NE2	65:AR:5101:HOH:O	2.20	0.75
4:CD:125:ILE:HB	39:DF:81:ILE:HD11	1.68	0.75
20:CW:34:ASN:OD1	20:CW:37:ARG:NH2	2.18	0.75
1:CA:1024:G:OP2	65:CA:3705:HOH:O	2.03	0.75
1:CA:2138:C:H42	1:CA:2153:G:H1	1.35	0.75
34:BA:504:C:OP1	65:BA:1903:HOH:O	2.04	0.74
34:DA:1255:G:OP1	43:DJ:45:ARG:NH2	2.19	0.74
1:CA:370:G:N7	65:CA:3731:HOH:O	2.20	0.74
15:CR:55:ALA:HB2	15:CR:79:LEU:HD13	1.69	0.74
1:AA:1151:U:H2'	1:AA:1152:G:C8	2.22	0.74
1:AA:2122:G:H1	1:AA:2211:U:H3	1.33	0.74
37:BD:49:ARG:HE	37:BD:49:ARG:H	1.35	0.74
59:DZ:116:PRO:O	59:DZ:118:SER:N	2.21	0.74
1:CA:2099:U:H3	1:CA:2190:G:H1	1.35	0.74
34:DA:619:U:N3	37:DD:134:ASP:OD1	2.21	0.74
59:DZ:-66:MET:N	59:DZ:-46:VAL:O	2.19	0.74
59:DZ:203:GLU:N	59:DZ:203:GLU:OE2	2.20	0.74
3:CC:48:LEU:HB3	3:CC:50:ILE:HD12	1.70	0.74
1:AA:354:A:HO2'	1:AA:355:A:H8	1.36	0.74
46:DM:58:GLU:O	46:DM:62:ASN:ND2	2.20	0.74
1:AA:427:G:N7	65:AA:3930:HOH:O	2.19	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:DA:992:U:H3	34:DA:1044:A:H62	1.36	0.74
34:DA:953:G:H5'	34:DA:965:A:H61	1.51	0.74
1:CA:1860:G:O3'	3:CC:206:LYS:HG3	1.88	0.74
44:DK:92:GLU:OE2	51:DR:87:ARG:NH1	2.21	0.74
34:BA:165:C:H2'	34:BA:166:G:C8	2.23	0.74
1:AA:1405:A:N6	1:AA:1418:U:H3	1.84	0.73
43:DJ:29:ARG:HB2	43:DJ:84:GLN:HE22	1.53	0.73
1:CA:2646:C:OP2	1:CA:2732:G:O2'	2.06	0.73
59:DZ:21:ILE:HD11	59:DZ:117:GLN:HE22	1.51	0.73
34:BA:560:U:OP2	65:BA:1904:HOH:O	2.07	0.73
1:CA:1842:G:O2'	4:CD:253:GLN:NE2	2.21	0.73
13:CP:38:GLN:O	13:CP:40:SER:N	2.22	0.73
1:AA:2825:C:H5'	29:A5:29:THR:HG21	1.68	0.73
1:CA:517:C:OP1	29:C5:16:ARG:NH2	2.22	0.73
35:BB:16:HIS:O	35:BB:18:GLY:N	2.21	0.73
59:DZ:363:ARG:HG2	59:DZ:363:ARG:HH11	1.53	0.73
34:BA:1305:G:N2	34:BA:1331:G:H1'	2.02	0.73
59:BZ:13:ARG:HH12	59:BZ:247:ARG:NH2	1.84	0.73
1:CA:2176:A:O2'	3:CC:45:HIS:CD2	2.41	0.73
1:AA:1873:G:O2'	4:AD:253:GLN:NE2	2.22	0.73
5:AE:127:ASP:OD2	65:AE:401:HOH:O	2.07	0.73
20:AW:4:LYS:HE2	20:AW:6:ILE:HD11	1.70	0.73
59:BZ:437:THR:HG22	59:BZ:454:MET:HE3	1.70	0.73
34:DA:1075:C:OP1	35:DB:179:LYS:NZ	2.22	0.73
37:BD:178:VAL:O	37:BD:180:GLY:N	2.21	0.73
1:CA:2177:C:O2	3:CC:173:HIS:CE1	2.42	0.73
23:CZ:45:ASP:OD2	23:CZ:49:ARG:NH1	2.22	0.73
1:AA:1055:A:OP2	11:AN:37:LYS:NZ	2.22	0.73
35:BB:7:VAL:HG11	35:BB:221:LEU:HD23	1.70	0.73
34:DA:137:C:H42	34:DA:226:G:H1	1.37	0.73
34:DA:1030(A):G:N2	34:DA:1030(D):A:OP2	2.20	0.73
41:DH:29:SER:HB3	41:DH:32:LYS:HG3	1.70	0.73
1:AA:2324:U:H5'	7:AG:88:ILE:HD11	1.71	0.73
1:AA:2859:U:O4	17:AT:23:ARG:NH2	2.21	0.73
12:AO:97:ARG:NH1	34:BA:339:C:OP2	2.20	0.73
7:CG:38:VAL:HG22	7:CG:93:THR:HG23	1.71	0.73
15:CR:33:ARG:NH2	29:C5:57:VAL:O	2.22	0.73
6:AF:185:ASP:HA	6:AF:188:ARG:HD3	1.71	0.72
34:BA:166:G:H2'	34:BA:167:G:H8	1.53	0.72
34:BA:505:G:N7	65:BA:1913:HOH:O	2.22	0.72
34:BA:558:G:OP1	65:BA:1906:HOH:O	2.07	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:C4:61:ARG:HG3	52:DS:42:PRO:HG3	1.71	0.72
38:DE:100:VAL:O	38:DE:107:ARG:NH2	2.22	0.72
1:AA:1001:G:OP2	14:AQ:14:ARG:NH2	2.22	0.72
34:BA:1030(C):G:N7	34:BA:1031:G:N2	2.37	0.72
49:BP:53:VAL:HG13	49:BP:79:VAL:HG22	1.70	0.72
56:DW:11:C:H42	56:DW:24:G:H1	1.36	0.72
1:AA:1065:U:H3	1:AA:1188:A:H62	1.35	0.72
1:CA:2357:U:OP1	24:C0:20:ARG:NH1	2.22	0.72
42:DI:16:ARG:HB2	42:DI:64:THR:HG23	1.70	0.72
36:BC:40:ARG:NH2	36:BC:55:VAL:O	2.22	0.72
35:DB:178:ARG:HH22	41:DH:68:ARG:HH22	1.35	0.72
1:AA:831:A:OP2	65:AA:3910:HOH:O	2.08	0.72
1:CA:991:C:OP2	65:CA:3710:HOH:O	2.08	0.72
1:CA:2046:G:H5'	29:C5:19:ARG:HA	1.70	0.72
34:BA:167:G:H2'	34:BA:168:G:H8	1.55	0.72
42:BI:128:ARG:NH2	57:BX:33:U:OP2	2.21	0.72
59:BZ:102:ASP:OD2	59:BZ:329:ARG:NH2	2.22	0.72
1:AA:1657:C:OP1	65:AA:3909:HOH:O	2.07	0.72
34:BA:1054:C:OP2	65:BA:1905:HOH:O	2.07	0.72
38:DE:88:LYS:HB3	38:DE:123:LEU:HB2	1.71	0.72
34:DA:1065:U:OP2	34:DA:1190:G:N2	2.22	0.72
35:DB:69:LEU:HB3	35:DB:162:ILE:HG22	1.70	0.72
1:AA:467:U:O2	6:AF:46:ARG:NH2	2.23	0.72
20:AW:2:GLU:OE2	20:AW:72:LYS:HE2	1.90	0.72
50:DQ:66:SER:O	50:DQ:70:ARG:NH1	2.23	0.72
59:BZ:13:ARG:NH1	59:BZ:247:ARG:HH22	1.86	0.72
59:BZ:363:ARG:HG2	59:BZ:363:ARG:NH1	2.01	0.72
1:CA:2445:G:OP1	6:CF:74:ARG:NH2	2.23	0.72
12:CO:63:VAL:HG12	12:CO:106:LEU:HD11	1.72	0.72
34:DA:1239:A:H4'	34:DA:1240:U:H5'	1.70	0.72
1:AA:1189:A:OP1	11:AN:25:ARG:NH2	2.23	0.71
42:BI:40:LEU:O	42:BI:42:ARG:N	2.23	0.71
1:AA:1151:U:H2'	1:AA:1152:G:H8	1.51	0.71
3:AC:48:LEU:HB3	3:AC:50:ILE:HD12	1.70	0.71
17:AT:60:THR:HG22	17:AT:77:PRO:HA	1.70	0.71
1:CA:1622:G:OP2	65:CA:3711:HOH:O	2.08	0.71
48:DO:5:LYS:H	48:DO:5:LYS:HD3	1.55	0.71
1:AA:2337:G:OP2	65:AA:3908:HOH:O	2.06	0.71
1:CA:641:C:O2'	1:CA:2350:C:OP1	2.04	0.71
1:CA:1754:C:OP1	17:CT:96:ARG:NH1	2.22	0.71
6:CF:53:THR:HG22	6:CF:56:GLU:HG3	1.71	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:DD:187:ARG:NH2	37:DD:193:ASP:OD2	2.23	0.71
59:DZ:82:ILE:HD12	59:DZ:101:LEU:HB3	1.72	0.71
59:DZ:466:LEU:HG	59:DZ:472:VAL:HG21	1.71	0.71
14:AQ:14:ARG:HG2	14:AQ:41:TRP:HH2	1.55	0.71
45:DL:32:PHE:HB3	45:DL:84:LEU:HD11	1.72	0.71
1:AA:1891:G:C4'	3:AC:206:LYS:HG3	2.20	0.71
1:CA:775:G:N3	65:CA:3738:HOH:O	2.23	0.71
1:AA:2291:G:N7	24:A0:14:ARG:NH1	2.37	0.71
34:BA:1226:C:O2'	46:BM:111:LYS:NZ	2.23	0.71
1:CA:740:U:OP2	65:CA:3708:HOH:O	2.07	0.71
1:CA:2124:G:H4'	3:CC:175:PRO:HG3	1.72	0.71
34:BA:255:G:H1'	50:BQ:16:GLN:HE21	1.54	0.71
59:BZ:396:ARG:HG3	59:BZ:396:ARG:HH21	1.56	0.71
1:CA:971:C:OP2	65:CA:3707:HOH:O	2.07	0.71
8:CH:107:VAL:HG11	8:CH:162:ILE:HD11	1.70	0.71
34:DA:1238:A:OP2	65:DA:1802:HOH:O	2.07	0.71
3:AC:51:ASP:HB3	3:AC:57:GLN:OE1	1.91	0.71
23:AZ:98:MET:HE2	23:AZ:100:VAL:HG22	1.72	0.71
41:BH:10:LEU:HD22	41:BH:83:ILE:HD11	1.72	0.71
3:CC:51:ASP:HB3	3:CC:57:GLN:OE1	1.91	0.71
59:DZ:225:GLU:HA	59:DZ:228:MET:HB3	1.72	0.71
48:DO:39:LEU:HD13	48:DO:56:LEU:HB2	1.73	0.71
59:DZ:466:LEU:HA	59:DZ:470:PHE:HD2	1.56	0.71
19:AV:40:LEU:HB2	19:AV:46:VAL:HG13	1.72	0.71
1:CA:2823:A:OP1	5:CE:159:HIS:NE2	2.21	0.71
1:AA:1391:C:OP2	65:AA:3912:HOH:O	2.08	0.70
3:AC:55:SER:O	3:AC:57:GLN:N	2.22	0.70
34:BA:427:U:OP1	37:BD:13:ARG:NH2	2.23	0.70
59:BZ:87:HIS:O	59:BZ:89:ASP:N	2.24	0.70
1:CA:2022:U:OP1	65:CA:3709:HOH:O	2.07	0.70
47:DN:21:TYR:OH	47:DN:23:ARG:NH2	2.24	0.70
59:DZ:169:GLY:H	59:DZ:170:ARG:HH12	1.39	0.70
36:BC:150:LYS:HG3	36:BC:169:ALA:HB2	1.73	0.70
52:BS:32:LYS:HA	52:BS:50:ALA:HB3	1.72	0.70
59:BZ:114:VAL:CG1	59:BZ:156:ARG:HH12	2.05	0.70
38:BE:43:LEU:HD21	38:BE:132:ALA:HB1	1.73	0.70
38:BE:100:VAL:O	38:BE:107:ARG:NH2	2.24	0.70
1:AA:1891:G:H4'	3:AC:206:LYS:CG	2.21	0.70
34:BA:953:G:H5'	34:BA:965:A:H61	1.56	0.70
3:CC:55:SER:O	3:CC:57:GLN:N	2.22	0.70
31:A7:24:THR:HG22	31:A7:27:GLY:H	1.56	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:CG:101:ILE:HG22	7:CG:105:LYS:HE2	1.73	0.70
1:AA:325:G:OP2	22:AY:84:ARG:NH2	2.24	0.70
36:BC:181:ASN:HD22	36:BC:204:LEU:HB2	1.57	0.70
1:CA:1026:U:OP1	65:CA:3705:HOH:O	2.09	0.70
1:CA:1860:G:H5'	3:CC:206:LYS:HD2	0.85	0.70
10:CL:99:ILE:HG23	10:CL:103:GLN:HB2	1.74	0.70
38:DE:75:THR:OG1	38:DE:117:ASP:O	2.07	0.70
59:BZ:329:ARG:NH1	59:BZ:331:TYR:HE1	1.89	0.70
59:BZ:546:ILE:HG23	59:BZ:590:ILE:HG13	1.73	0.70
15:CR:67:LEU:HD13	15:CR:76:VAL:HG21	1.73	0.70
17:CT:54:ARG:HA	17:CT:59:THR:HB	1.72	0.70
1:AA:2442:A:OP1	65:AA:3911:HOH:O	2.08	0.70
1:CA:1108:U:C5	1:CA:1109:C:C5	2.79	0.70
44:BK:19:ALA:HB3	44:BK:82:VAL:HG22	1.73	0.70
41:DH:119:LEU:HD13	41:DH:123:GLU:HG2	1.74	0.70
1:AA:2299:A:H2	1:AA:2358:A:H62	1.40	0.70
1:AA:2459:G:OP2	65:AA:3913:HOH:O	2.08	0.70
42:BI:23:ASN:HD22	42:BI:25:LYS:HG2	1.57	0.70
59:BZ:165:GLN:HE21	59:BZ:259:PHE:HB3	1.56	0.70
38:DE:80:ILE:HD13	41:DH:104:ARG:HH21	1.56	0.69
46:DM:37:THR:O	46:DM:55:ARG:NH1	2.24	0.69
37:BD:15:GLU:HG3	37:BD:63:LYS:HD3	1.74	0.69
39:BF:28:ARG:O	39:BF:32:ASN:ND2	2.24	0.69
3:CC:25:GLU:HA	3:CC:28:ARG:HD2	1.74	0.69
7:CG:64:THR:HB	7:CG:94:LEU:HD21	1.74	0.69
3:AC:57:GLN:HG3	3:AC:57:GLN:O	1.93	0.69
1:CA:1528:A:OP2	65:CA:3713:HOH:O	2.09	0.69
1:CA:1762:A:N1	65:CA:3744:HOH:O	2.25	0.69
7:CG:64:THR:HG21	7:CG:92:VAL:HG11	1.74	0.69
34:DA:254:G:OP1	50:DQ:66:SER:OG	2.10	0.69
10:CL:106:GLU:HA	10:CL:109:LYS:HD3	1.74	0.69
32:C8:10:ALA:HB3	32:C8:62:LEU:HD21	1.73	0.69
1:AA:2801:C:OP1	5:AE:61:ARG:NH2	2.25	0.69
3:AC:183:PRO:HG2	3:AC:184:GLU:OE2	1.92	0.69
34:BA:356:A:N3	34:BA:368:U:O2'	2.24	0.69
34:BA:1086:U:H3	34:BA:1099:G:H22	1.38	0.69
1:CA:1419:A:OP2	65:CA:3712:HOH:O	2.09	0.69
35:DB:120:ALA:O	35:DB:122:PHE:N	2.25	0.69
1:AA:1221:G:H1'	1:AA:1222:A:H5'	1.75	0.69
1:AA:1324:A:OP1	15:AR:36:THR:HG23	1.91	0.69
29:A5:16:ARG:HG3	29:A5:17:ASP:N	2.08	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:BI:3:GLN:OE1	42:BI:20:ARG:NH2	2.21	0.69
59:BZ:227:ILE:HG23	59:BZ:237:PRO:HG2	1.74	0.69
3:CC:15:VAL:O	3:CC:16:ASP:HB3	1.92	0.69
17:CT:65:LYS:HE2	17:CT:67:SER:HB2	1.75	0.69
43:DJ:30:SER:O	43:DJ:81:THR:OG1	2.10	0.69
1:AA:483:A:H5"	65:AA:4069:HOH:O	1.93	0.69
3:AC:15:VAL:O	3:AC:16:ASP:HB3	1.92	0.69
9:AK:73:GLY:O	9:AK:75:GLN:N	2.24	0.69
1:AA:671:A:H2'	1:AA:672:G:O4'	1.93	0.69
22:AY:102:CYS:SG	22:AY:103:GLY:N	2.66	0.69
1:CA:526:A:OP1	65:CA:3714:HOH:O	2.10	0.69
3:CC:46:ALA:HB3	3:CC:172:ILE:CG2	2.23	0.69
3:CC:46:ALA:HB3	3:CC:172:ILE:HG22	1.75	0.69
34:DA:353:A:H8	34:DA:353:A:H5'	1.57	0.69
1:AA:553:A:C8	1:AA:553:A:H3'	2.28	0.68
3:AC:46:ALA:HB3	3:AC:172:ILE:HG22	1.75	0.68
3:CC:183:PRO:HG2	3:CC:184:GLU:OE2	1.93	0.68
4:CD:276:LYS:H	4:CD:276:LYS:HD3	1.58	0.68
34:DA:1060:C:C5	36:DC:2:GLY:HA3	2.28	0.68
59:DZ:26:THR:OG1	64:DZ:702:GDP:O1B	2.10	0.68
1:AA:2146:G:H1	1:AA:2196:C:H42	1.41	0.68
46:BM:17:VAL:O	46:BM:20:THR:OG1	2.09	0.68
1:CA:1061:U:H4'	1:CA:1070:A:H1'	1.75	0.68
44:DK:99:GLN:HG2	44:DK:105:VAL:HG21	1.74	0.68
1:AA:2200:C:O2'	3:AC:169:THR:HB	1.93	0.68
3:AC:25:GLU:HA	3:AC:28:ARG:HD2	1.75	0.68
17:AT:54:ARG:HA	17:AT:59:THR:HB	1.76	0.68
59:BZ:87:HIS:HB3	59:BZ:90:PHE:HB3	1.75	0.68
37:DD:150:GLU:HA	37:DD:153:ARG:HE	1.59	0.68
1:AA:932:C:H3'	1:AA:933:C:H5"	1.75	0.68
34:BA:1255:G:O2'	34:BA:1258:G:O2'	2.10	0.68
44:DK:98:LEU:O	44:DK:101:SER:OG	2.06	0.68
3:CC:30:VAL:HG23	3:CC:31:LYS:H	1.58	0.68
34:DA:117:G:OP2	65:DA:1803:HOH:O	2.11	0.68
34:DA:1060:C:H5	36:DC:2:GLY:HA3	1.58	0.68
46:DM:14:ARG:HG3	46:DM:44:ARG:HH11	1.58	0.68
56:DW:27:G:H1	56:DW:43:C:H42	1.40	0.68
2:CB:76:G:N7	65:CB:3101:HOH:O	2.25	0.68
28:C4:44:THR:O	28:C4:46:GLN:N	2.26	0.68
34:DA:983:A:N1	34:DA:1222:G:N2	2.41	0.68
1:AA:2007:G:OP2	65:AA:3916:HOH:O	2.11	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:DA:976:G:H5'	34:DA:1358:U:O2'	1.94	0.68
1:AA:139:A:H8	1:AA:1454:C:HO2'	1.42	0.68
22:AY:102:CYS:SG	22:AY:104:GLY:N	2.63	0.68
41:BH:114:THR:OG1	41:BH:117:GLY:O	2.11	0.68
5:CE:97:LYS:N	5:CE:100:GLU:OE1	2.24	0.68
16:CS:5:THR:N	16:CS:8:GLU:OE1	2.26	0.68
34:DA:1004:A:H62	34:DA:1037:C:H2'	1.59	0.68
34:DA:1255:G:P	43:DJ:45:ARG:HH22	2.16	0.68
1:AA:2586:G:OP1	65:AA:3915:HOH:O	2.11	0.68
3:AC:30:VAL:HG23	3:AC:31:LYS:H	1.58	0.68
35:BB:60:ASP:OD1	35:BB:64:ARG:NH2	2.26	0.68
58:BY:60:U:H5"	58:BY:61:C:H5	1.56	0.68
1:CA:299:A:H5"	22:CY:86:ARG:HH21	1.59	0.68
1:CA:307:G:H21	1:CA:330:A:H62	1.42	0.68
1:CA:1604:C:OP2	65:CA:3715:HOH:O	2.11	0.68
5:CE:12:THR:HG21	17:CT:11:GLU:OE2	1.92	0.68
56:BW:5:G:H2'	56:BW:6:G:C8	2.30	0.68
3:CC:30:VAL:HG23	3:CC:31:LYS:N	2.09	0.68
1:AA:1114:G:N2	1:AA:1141:A:O3'	2.27	0.67
3:AC:30:VAL:HG23	3:AC:31:LYS:N	2.09	0.67
59:BZ:114:VAL:HG23	59:BZ:152:THR:HB	1.75	0.67
42:DI:99:LEU:HB3	42:DI:101:PHE:CE1	2.29	0.67
47:DN:23:ARG:HH11	47:DN:30:ALA:HB2	1.58	0.67
1:AA:2457:G:OP1	6:AF:74:ARG:NH2	2.27	0.67
3:AC:46:ALA:HB3	3:AC:172:ILE:CG2	2.23	0.67
4:AD:206:LEU:HD22	4:AD:211:ARG:HG2	1.75	0.67
26:A2:9:GLN:HE22	26:A2:56:GLN:HB3	1.58	0.67
1:CA:813:U:H2'	1:CA:814:C:C6	2.30	0.67
1:CA:882:G:H2'	1:CA:883:G:H8	1.59	0.67
1:CA:2611:U:C4	29:C5:3:LYS:HG2	2.30	0.67
12:CO:64:ARG:HG2	12:CO:79:PHE:CG	2.29	0.67
23:CZ:150:LEU:H	23:CZ:172:ALA:HB3	1.59	0.67
1:AA:1431:G:O2'	1:AA:1442:U:O2	2.10	0.67
37:BD:178:VAL:HG12	37:BD:179:GLU:H	1.58	0.67
42:BI:43:ALA:O	42:BI:45:ALA:N	2.28	0.67
3:CC:176:VAL:HG11	3:CC:190:ILE:HD13	1.76	0.67
34:DA:1502:A:H2	34:DA:1505:G:H1	1.38	0.67
46:DM:25:ILE:HG23	46:DM:29:ARG:HB3	1.75	0.67
1:AA:399:G:OP2	25:A1:69:LYS:NZ	2.24	0.67
1:AA:626:A:H4'	1:AA:627:G:H5'	1.76	0.67
1:AA:2227:G:H3'	1:AA:2228:G:C8	2.30	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:BE:110:LEU:HD13	38:BE:118:ILE:HD13	1.77	0.67
6:CF:101:LEU:O	6:CF:106:ARG:NH1	2.26	0.67
8:CH:9:ILE:HB	8:CH:50:VAL:HB	1.74	0.67
34:DA:1305:G:N2	34:DA:1331:G:H1'	2.09	0.67
38:DE:102:ALA:HB1	38:DE:106:PRO:HG2	1.75	0.67
48:DO:41:GLU:HA	48:DO:44:LYS:HD2	1.75	0.67
9:AK:26:LEU:HA	9:AK:84:GLU:HA	1.74	0.67
34:BA:353:A:H5'	34:BA:353:A:H8	1.60	0.67
37:BD:111:ALA:HB2	37:BD:120:LEU:HD12	1.75	0.67
1:CA:1430:C:H2'	1:CA:1431:U:C6	2.30	0.67
1:CA:1547:C:H2'	1:CA:1548:C:H6	1.60	0.67
1:CA:2070:G:OP2	65:CA:3716:HOH:O	2.12	0.67
34:DA:1316:G:OP1	47:DN:17:LYS:NZ	2.25	0.67
51:DR:56:THR:HB	51:DR:58:LEU:HD23	1.77	0.67
36:BC:50:ALA:HB1	36:BC:70:VAL:HG21	1.74	0.67
1:CA:1057:A:O2'	1:CA:1058:G:OP1	2.09	0.67
36:DC:52:LEU:HD23	36:DC:55:VAL:HG23	1.75	0.67
1:AA:2772:G:N7	65:AA:3952:HOH:O	2.27	0.67
1:CA:2114:A:N1	1:CA:2171:A:N6	2.40	0.67
26:C2:1:MET:N	26:C2:52:ASP:OD1	2.23	0.67
28:C4:16:CYS:SG	28:C4:17:GLY:N	2.67	0.67
34:DA:920:U:H2'	34:DA:921:U:C6	2.29	0.67
43:DJ:17:ASP:OD1	43:DJ:70:ARG:NH1	2.26	0.67
1:AA:2396:G:OP2	24:A0:55:ARG:NH1	2.26	0.67
2:AB:7:G:OP2	65:AB:3101:HOH:O	2.11	0.67
44:BK:18:ARG:NH1	44:BK:20:TYR:OH	2.27	0.67
1:CA:2104:G:H1	1:CA:2185:C:H42	1.42	0.67
42:BI:128:ARG:NH1	57:BX:35:A:OP2	2.27	0.67
1:CA:1022:G:N7	11:CN:66:LYS:HE2	2.10	0.67
34:DA:560:U:O2'	34:DA:561:U:OP2	2.13	0.67
59:DZ:494:GLU:HG2	59:DZ:511:LYS:HG2	1.75	0.67
37:BD:187:ARG:NH1	37:BD:190:ASP:OD1	2.28	0.67
44:BK:34:ASP:HB3	44:BK:40:ILE:HD11	1.75	0.67
45:BL:53:ARG:HG3	45:BL:93:LEU:HD21	1.76	0.67
59:BZ:20:HIS:ND1	59:BZ:115:GLU:HB3	2.09	0.67
1:CA:2177:C:O2	3:CC:173:HIS:HE1	1.78	0.67
1:CA:2286:A:H4'	1:CA:2287:A:O4'	1.95	0.67
1:AA:925:A:H61	1:AA:945:A:H1'	1.59	0.66
3:AC:42:VAL:HG13	3:AC:43:GLU:N	2.10	0.66
9:AK:70:GLU:O	9:AK:72:ASP:N	2.28	0.66
1:CA:1970:A:OP1	65:CA:3717:HOH:O	2.12	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:CC:57:GLN:O	3:CC:57:GLN:HG3	1.93	0.66
34:DA:959:A:HO2'	34:DA:984:C:HO2'	1.43	0.66
3:AC:31:LYS:NZ	3:AC:180:SER:O	2.28	0.66
40:BG:111:ARG:NH2	40:BG:126:ASP:OD2	2.28	0.66
59:DZ:329:ARG:HD3	59:DZ:331:TYR:CZ	2.31	0.66
1:AA:237:G:OP1	65:AA:3917:HOH:O	2.13	0.66
34:BA:1303:C:OP1	65:BA:1908:HOH:O	2.14	0.66
37:BD:107:ARG:HH22	37:BD:194:LEU:HD11	1.59	0.66
9:CK:73:GLY:O	9:CK:75:GLN:N	2.21	0.66
1:AA:1249:A:H2	1:AA:1287:A:N6	1.88	0.66
1:CA:2590:A:OP2	4:CD:238:GLY:HA2	1.94	0.66
4:CD:8:PRO:HB3	4:CD:14:ARG:HB2	1.76	0.66
10:AL:106:GLU:HA	10:AL:109:LYS:HD3	1.77	0.66
34:BA:1069:C:OP2	65:BA:1907:HOH:O	2.13	0.66
56:BW:51:U:H2'	56:BW:52:G:H8	1.60	0.66
35:DB:52:GLU:O	35:DB:56:ARG:HG2	1.96	0.66
57:DX:73:A:H5"	57:DX:74:C:H5'	1.76	0.66
22:AY:15:VAL:HG21	22:AY:42:VAL:HG11	1.78	0.66
34:BA:1221:G:OP1	34:BA:1320:C:N4	2.23	0.66
3:CC:63:VAL:O	3:CC:161:ARG:HA	1.96	0.66
42:DI:28:VAL:HG22	42:DI:63:ILE:HB	1.76	0.66
43:DJ:38:ILE:HD11	43:DJ:71:LEU:HD23	1.78	0.66
59:DZ:181:LEU:HD12	59:DZ:216:LEU:HD21	1.78	0.66
1:AA:1711:A:OP1	65:AA:3918:HOH:O	2.13	0.66
34:DA:1054:C:C4	56:DW:34:G:H1'	2.29	0.66
37:BD:22:LYS:HB2	63:BD:501:SF4:S4	2.36	0.66
36:DC:59:ARG:HG3	36:DC:64:VAL:HG13	1.77	0.66
3:AC:176:VAL:HG11	3:AC:190:ILE:HD13	1.76	0.66
34:BA:166:G:H2'	34:BA:167:G:C8	2.30	0.66
34:BA:1348:U:H4'	42:BI:120:ARG:HD2	1.77	0.66
1:CA:833:U:O2	13:CP:55:ARG:NH2	2.29	0.66
1:CA:855:G:O2'	24:C0:27:GLU:OE2	2.14	0.66
1:CA:1341:U:OP2	1:CA:1394:U:O2'	2.11	0.66
3:CC:42:VAL:HG13	3:CC:43:GLU:N	2.10	0.66
3:CC:65:LEU:HB3	3:CC:189:ASN:ND2	2.11	0.66
35:DB:201:ILE:HG21	35:DB:214:ILE:HG21	1.78	0.66
34:BA:193:C:H2'	34:BA:194:C:H6	1.61	0.66
34:DA:1239:A:H62	34:DA:1299:A:H62	1.41	0.66
1:AA:1079:U:OP1	33:A9:9:ARG:NH2	2.29	0.65
3:AC:65:LEU:HB3	3:AC:189:ASN:ND2	2.11	0.65
20:AW:18:ARG:NH1	20:AW:76:VAL:O	2.29	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:DZ:264:LEU:HB2	64:DZ:702:GDP:C6	2.31	0.65
1:CA:1332:G:OP1	65:CA:3720:HOH:O	2.14	0.65
17:CT:56:GLY:O	17:CT:59:THR:HG23	1.96	0.65
18:CU:76:TYR:OH	18:CU:92:ARG:NH1	2.28	0.65
1:CA:300:A:P	22:CY:86:ARG:HH22	2.19	0.65
1:CA:1604:C:OP2	65:CA:3702:HOH:O	2.15	0.65
6:CF:192:LEU:HD13	6:CF:194:MET:HE2	1.77	0.65
34:DA:222:U:H2'	34:DA:223:U:C6	2.30	0.65
3:AC:41:THR:O	3:AC:42:VAL:HB	1.94	0.65
3:AC:63:VAL:O	3:AC:161:ARG:HA	1.95	0.65
7:AG:179:PRO:HB2	28:A4:42:PHE:HE1	1.61	0.65
1:CA:1315:C:OP2	65:CA:3720:HOH:O	2.15	0.65
28:C4:40:HIS:HB3	28:C4:43:TYR:HB2	1.78	0.65
34:DA:266:G:H5"	34:DA:268:C:H41	1.62	0.65
7:AG:137:GLU:HG2	7:AG:152:LEU:HD13	1.78	0.65
17:AT:16:ARG:NH2	17:AT:83:ILE:O	2.29	0.65
3:CC:206:LYS:NZ	3:CC:206:LYS:HB3	2.12	0.65
42:DI:43:ALA:HA	42:DI:74:ILE:HD13	1.77	0.65
13:AP:50:ARG:HD3	32:A8:7:HIS:CD2	2.32	0.65
34:BA:200:G:H1	34:BA:217:C:H42	1.43	0.65
34:BA:1304:G:OP2	65:BA:1908:HOH:O	2.15	0.65
35:BB:195:ASP:O	41:BH:68:ARG:NH2	2.30	0.65
59:BZ:191:ASP:O	59:BZ:266:ASN:ND2	2.22	0.65
1:CA:2327:A:H2'	1:CA:2328:A:C8	2.31	0.65
3:CC:41:THR:O	3:CC:42:VAL:HB	1.94	0.65
35:DB:91:PRO:HG3	35:DB:155:LEU:HD23	1.79	0.65
35:DB:162:ILE:HD11	35:DB:184:VAL:HG22	1.78	0.65
34:BA:642:A:N3	41:BH:113:SER:OG	2.30	0.65
1:CA:1495:A:H2'	1:CA:1496:A:C8	2.32	0.65
1:AA:1087:C:H42	1:AA:1160:G:H1	1.45	0.65
1:AA:2138:G:N2	1:AA:2184:G:OP1	2.26	0.65
20:AW:14:PRO:HG2	20:AW:78:GLU:HG2	1.77	0.65
42:BI:42:ARG:NH1	42:BI:71:SER:OG	2.29	0.65
59:BZ:160:ARG:HD2	59:BZ:160:ARG:H	1.61	0.65
34:DA:1000:U:H3	34:DA:1041:A:H61	1.44	0.65
35:DB:100:GLY:O	35:DB:104:ASN:N	2.25	0.65
37:DD:127:THR:HB	37:DD:132:ARG:HA	1.79	0.65
1:AA:2199:C:O2	3:AC:173:HIS:CE1	2.50	0.65
16:AS:3:ARG:C	16:AS:3:ARG:HD3	2.22	0.65
19:CV:21:ARG:HG2	19:CV:91:TYR:CD2	2.31	0.65
34:DA:403:C:OP1	37:DD:137:SER:OG	2.14	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:DN:22:THR:HB	47:DN:33:VAL:HB	1.79	0.65
1:AA:2776:G:OP2	65:AA:3919:HOH:O	2.13	0.65
23:AZ:53:ILE:HG22	23:AZ:71:VAL:HG12	1.79	0.65
34:BA:1369:C:H2'	34:BA:1370:G:C8	2.31	0.65
1:CA:816:C:OP2	65:CA:3719:HOH:O	2.13	0.65
59:DZ:610:VAL:HG13	59:DZ:659:LEU:HD11	1.78	0.65
1:AA:1891:G:H5'	3:AC:206:LYS:CD	2.00	0.64
53:BT:56:MET:HE1	53:BT:85:MET:HA	1.78	0.64
20:CW:65:LEU:HD12	20:CW:68:ARG:HE	1.62	0.64
3:AC:206:LYS:HB3	3:AC:206:LYS:NZ	2.12	0.64
34:DA:1129:C:H2'	34:DA:1139:G:N7	2.11	0.64
37:DD:61:LYS:NZ	37:DD:207:TYR:OH	2.31	0.64
50:DQ:15:MET:HE1	50:DQ:43:LEU:HD13	1.79	0.64
56:DW:3:C:O2	56:DW:70:G:N2	2.17	0.64
1:AA:1219:A:H4'	1:AA:1220:U:OP1	1.97	0.64
7:AG:41:GLN:NE2	7:AG:154:GLY:O	2.30	0.64
41:BH:73:ASP:OD2	41:BH:75:ARG:NH1	2.31	0.64
30:A6:44:ARG:HB3	30:A6:44:ARG:NH1	2.12	0.64
57:BX:61:C:H2'	57:BX:62:C:H6	1.62	0.64
1:CA:848:G:H2'	1:CA:849:A:C8	2.33	0.64
30:C6:13:CYS:SG	30:C6:47:THR:HG21	2.37	0.64
41:DH:86:ILE:HG21	41:DH:133:LEU:HD13	1.78	0.64
3:AC:69:LEU:O	3:AC:178:LYS:HG3	1.98	0.64
34:BA:1318:A:H1'	52:BS:37:ARG:HH21	1.61	0.64
1:CA:1082:U:H4'	10:CL:117:THR:HB	1.78	0.64
23:CZ:117:LEU:HD12	23:CZ:174:VAL:HG22	1.80	0.64
1:AA:2460:A:OP1	65:AA:3902:HOH:O	2.14	0.64
1:AA:2601:A:OP1	65:AA:3910:HOH:O	2.14	0.64
3:AC:68:GLY:N	3:AC:189:ASN:HD21	1.96	0.64
1:CA:1800:C:OP2	4:CD:183:ARG:NH2	2.29	0.64
34:DA:396:G:OP1	59:DZ:349:LYS:NZ	2.31	0.64
42:DI:8:GLY:N	42:DI:15:ALA:O	2.27	0.64
1:AA:630:U:OP1	6:AF:102:PRO:HA	1.98	0.64
36:BC:52:LEU:HD23	36:BC:53:ALA:H	1.63	0.64
1:CA:1250:G:N7	13:CP:18:ARG:NH2	2.45	0.64
10:CL:81:ALA:HB1	10:CL:99:ILE:HD11	1.79	0.64
12:CO:35:VAL:HG23	12:CO:65:THR:HG23	1.78	0.64
34:DA:189(F):U:O2	50:DQ:63:ARG:NH2	2.30	0.64
37:DD:18:LYS:NZ	37:DD:31:CYS:SG	2.71	0.64
1:AA:9:U:N3	1:AA:2641:A:H2	1.89	0.64
1:AA:239:G:OP2	32:A8:13:ARG:NH2	2.31	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:AY:92:ASN:HB2	22:AY:94:LYS:N	2.12	0.64
23:AZ:157:LEU:HD21	23:AZ:163:LEU:HD13	1.79	0.64
36:BC:114:PRO:O	36:BC:118:GLN:NE2	2.31	0.64
1:CA:528:A:C2	1:CA:2043:C:H4'	2.33	0.64
19:CV:62:LEU:HD23	19:CV:93:GLU:HG2	1.80	0.64
35:DB:204:ASN:OD1	35:DB:205:ASP:N	2.31	0.64
59:DZ:170:ARG:N	59:DZ:170:ARG:HH11	1.96	0.64
7:AG:41:GLN:HB3	7:AG:43:LEU:HD22	1.79	0.64
34:BA:1158:C:H5	34:BA:1181:G:N1	1.95	0.64
34:BA:1182:G:H4'	34:BA:1183:A:H5'	1.80	0.64
45:BL:7:ILE:HA	45:BL:10:LEU:HD12	1.80	0.64
46:BM:59:TYR:O	46:BM:63:THR:OG1	2.15	0.64
1:CA:2424:C:O2	1:CA:2429:G:O2'	2.14	0.64
3:CC:69:LEU:O	3:CC:178:LYS:HG3	1.97	0.64
35:BB:54:THR:HG21	35:BB:201:ILE:HD11	1.79	0.64
58:BY:8:4SU:H4'	58:BY:48:C:H4'	1.80	0.64
1:CA:2723:C:H5"	15:CR:1:MET:HE2	1.78	0.64
1:AA:791:G:OP1	65:AA:3920:HOH:O	2.15	0.63
4:AD:122:ASP:OD1	4:AD:122:ASP:N	2.24	0.63
7:AG:48:GLU:HA	7:AG:51:ARG:HE	1.62	0.63
1:CA:2243:U:H2'	1:CA:2244:U:C6	2.33	0.63
15:CR:21:TYR:OH	15:CR:43:GLU:HG2	1.98	0.63
3:AC:29:LEU:O	3:AC:32:GLU:N	2.32	0.63
8:AH:90:LYS:HD3	8:AH:159:GLU:HG2	1.79	0.63
13:AP:125:VAL:HG21	13:AP:138:LEU:HD21	1.80	0.63
34:BA:600:C:H2'	34:BA:601:C:C6	2.33	0.63
59:BZ:82:ILE:HD12	59:BZ:101:LEU:HD23	1.80	0.63
1:CA:2136:C:O2'	1:CA:2137:C:O5'	2.13	0.63
3:CC:31:LYS:NZ	3:CC:180:SER:O	2.28	0.63
11:CN:123:TYR:OH	11:CN:130:HIS:NE2	2.31	0.63
34:DA:986:A:O2'	52:DS:55:LYS:O	2.16	0.63
50:DQ:81:ARG:HB3	50:DQ:84:LEU:HD12	1.80	0.63
59:DZ:363:ARG:HH11	59:DZ:363:ARG:CG	2.09	0.63
3:AC:44:VAL:CG2	3:AC:176:VAL:HG21	2.28	0.63
30:A6:13:CYS:SG	30:A6:47:THR:HG21	2.39	0.63
12:CO:25:LEU:HD12	12:CO:38:VAL:HG12	1.80	0.63
35:DB:213:LEU:HD22	35:DB:214:ILE:HD13	1.80	0.63
59:DZ:-53:ASP:H	59:DZ:-50:GLN:NE2	1.97	0.63
59:DZ:117:GLN:O	59:DZ:121:VAL:N	2.30	0.63
3:AC:7:ARG:O	3:AC:11:LEU:HD23	1.99	0.63
14:AQ:10:ARG:HG2	14:AQ:11:LYS:HG3	1.80	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:BS:63:THR:OG1	52:BS:65:ASN:ND2	2.32	0.63
3:CC:7:ARG:O	3:CC:11:LEU:HD23	1.99	0.63
11:AN:46:VAL:HG23	11:AN:48:MET:HG2	1.80	0.63
59:BZ:73:PHE:CE2	59:BZ:78:ARG:NH1	2.67	0.63
49:DP:5:ARG:HB3	49:DP:67:THR:HG23	1.80	0.63
58:DY:12:U:H3	58:DY:23:A:H61	1.45	0.63
34:BA:421:U:OP2	34:BA:422:C:N4	2.30	0.63
59:BZ:184:LYS:HD2	59:BZ:198:GLU:OE2	1.98	0.63
34:DA:1130:A:O2'	42:DI:3:GLN:OE1	2.17	0.63
42:DI:99:LEU:HB3	42:DI:101:PHE:HE1	1.62	0.63
1:CA:1143:A:OP1	11:CN:25:ARG:NH2	2.31	0.63
1:CA:1860:G:C5'	3:CC:206:LYS:HG3	1.88	0.63
3:CC:68:GLY:N	3:CC:189:ASN:HD21	1.96	0.63
20:CW:18:ARG:NH1	20:CW:76:VAL:O	2.31	0.63
34:DA:986:A:H1'	52:DS:55:LYS:HA	1.81	0.63
34:DA:1118:C:OP1	42:DI:104:ARG:NH1	2.32	0.63
49:DP:52:ASP:O	49:DP:54:GLU:N	2.32	0.63
1:AA:1218:G:O2'	1:AA:1219:A:O4'	2.16	0.63
3:AC:6:LYS:HG3	3:AC:7:ARG:N	2.14	0.63
4:AD:71:ASP:OD2	4:AD:103:ARG:NH2	2.32	0.63
1:CA:96:G:H4'	26:C2:48:HIS:CD2	2.33	0.63
15:CR:56:LYS:NZ	15:CR:90:ARG:O	2.32	0.63
17:CT:39:ARG:NH2	34:DA:345:C:OP2	2.32	0.63
1:AA:990:A:OP2	65:AA:3921:HOH:O	2.16	0.63
34:BA:992:U:O2	34:BA:1043:C:N4	2.32	0.63
34:BA:1525:G:OP1	44:BK:120:ARG:NH2	2.32	0.63
53:BT:9:ASN:HB3	53:BT:10:LEU:HD12	1.80	0.63
59:BZ:78:ARG:HG3	59:BZ:78:ARG:NH1	2.07	0.63
59:BZ:127:LYS:HG3	59:BZ:520:GLY:HA3	1.81	0.63
3:CC:6:LYS:HG3	3:CC:7:ARG:N	2.14	0.63
3:CC:44:VAL:CG2	3:CC:176:VAL:HG21	2.28	0.63
37:DD:103:ASN:OD1	37:DD:114:ARG:NE	2.28	0.63
39:DF:23:LYS:HG2	39:DF:61:LEU:HD21	1.81	0.63
43:DJ:5:ARG:N	43:DJ:73:ASP:OD1	2.32	0.63
1:AA:2045:G:H5'	1:AA:2629:C:H4'	1.79	0.62
1:AA:2152:U:H4'	1:AA:2155:G:H4'	1.81	0.62
34:BA:972:C:O2'	43:BJ:55:LYS:O	2.16	0.62
38:BE:68:GLU:HG2	38:BE:70:PRO:HD3	1.81	0.62
59:BZ:238:THR:HG23	59:BZ:241:GLU:HB2	1.80	0.62
1:CA:636:G:HO2'	1:CA:638:G:HO2'	1.46	0.62
1:CA:2176:A:H2'	1:CA:2177:C:C6	2.34	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:CC:29:LEU:O	3:CC:32:GLU:N	2.31	0.62
42:DI:128:ARG:NH2	57:DX:33:U:OP2	2.32	0.62
57:DX:9:G:O2'	57:DX:10:G:N7	2.24	0.62
1:AA:1199:C:OP1	18:AU:92:ARG:NH1	2.32	0.62
50:BQ:45:HIS:HB3	50:BQ:72:ARG:HB3	1.82	0.62
6:CF:185:ASP:OD1	6:CF:188:ARG:NH1	2.31	0.62
1:AA:1480:A:H61	1:AA:1605:A:H62	1.47	0.62
3:AC:68:GLY:H	3:AC:189:ASN:HD21	1.47	0.62
35:BB:17:PHE:HB2	35:BB:44:LEU:HD21	1.81	0.62
35:BB:155:LEU:HD21	35:BB:159:PRO:HD3	1.82	0.62
1:CA:2785:C:OP1	5:CE:41:LYS:NZ	2.32	0.62
1:AA:1501:U:OP1	15:AR:77:ARG:NH1	2.32	0.62
21:AX:57:LEU:HD21	21:AX:78:LYS:HE2	1.80	0.62
34:BA:598:U:H4'	41:BH:94:TYR:CD2	2.34	0.62
36:BC:19:GLU:HB3	36:BC:40:ARG:HH22	1.65	0.62
1:CA:731:C:OP1	65:CA:3722:HOH:O	2.16	0.62
1:CA:2206:G:H3'	1:CA:2207:G:N7	2.15	0.62
1:CA:2839:G:H5'	15:CR:46:GLY:HA2	1.81	0.62
6:CF:155:LEU:HD23	6:CF:186:ILE:HG13	1.81	0.62
1:AA:611:U:H2'	1:AA:612:C:C6	2.35	0.62
1:CA:1798:U:OP2	4:CD:274:ARG:NH2	2.32	0.62
34:DA:406:G:H5'	37:DD:5:ILE:HD11	1.82	0.62
34:DA:1133:G:H2'	34:DA:1134:G:H8	1.63	0.62
34:DA:1228:C:OP1	46:DM:115:LYS:N	2.30	0.62
36:DC:58:GLU:HB3	43:DJ:92:THR:HG21	1.82	0.62
36:DC:65:ALA:HA	36:DC:100:ALA:HB3	1.81	0.62
34:BA:153:C:H42	34:BA:168:G:H1	1.48	0.62
48:BO:17:ARG:HG3	48:BO:17:ARG:HH11	1.64	0.62
1:CA:2788:C:O2'	1:CA:2809:A:N3	2.30	0.62
34:DA:958:A:N6	52:DS:77:THR:O	2.32	0.62
1:AA:927:G:H2'	1:AA:928:G:C8	2.34	0.62
56:BW:63:G:H2'	56:BW:64:A:O4'	2.00	0.62
34:DA:1318:A:H1'	52:DS:37:ARG:HD3	1.80	0.62
35:DB:16:HIS:CG	35:DB:17:PHE:H	2.17	0.62
39:DF:67:MET:HE1	39:DF:75:LEU:HD12	1.80	0.62
1:AA:798:A:H5'	20:AW:90:ARG:HA	1.82	0.62
1:AA:957:A:H2'	14:AQ:9:TYR:OH	2.00	0.62
1:AA:1154:U:O2'	1:AA:1155:C:H6	1.82	0.62
13:AP:59:LEU:HD11	32:A8:10:ALA:HB2	1.81	0.62
3:CC:53:ARG:HD3	3:CC:53:ARG:H	1.65	0.62
30:C6:6:ARG:NH1	30:C6:26:ASN:HB2	2.14	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:DA:1073:U:H2'	34:DA:1074:G:H8	1.65	0.62
34:BA:255:G:H1'	50:BQ:16:GLN:NE2	2.15	0.62
42:BI:99:LEU:HB3	42:BI:101:PHE:HE1	1.64	0.62
6:CF:101:LEU:HD12	6:CF:102:PRO:HD2	1.82	0.62
34:DA:523:A:H61	45:DL:92:ASP:HB2	1.64	0.62
1:AA:202:A:H2'	1:AA:203:G:O4'	2.00	0.62
1:AA:1154:U:HO2'	1:AA:1155:C:H6	1.48	0.62
3:AC:53:ARG:HD3	3:AC:53:ARG:H	1.65	0.62
13:AP:1:MET:HE2	13:AP:6:LEU:HD23	1.82	0.62
34:BA:1062:U:H2'	34:BA:1063:C:C6	2.35	0.62
1:CA:993:G:OP1	18:CU:50:ARG:NH2	2.32	0.62
3:CC:11:LEU:HD12	3:CC:33:LEU:HA	1.82	0.62
1:AA:1405:A:N1	1:AA:1418:U:O4	2.33	0.61
1:AA:1529:G:O6	1:AA:1553:A:N6	2.33	0.61
6:AF:28:ILE:O	6:AF:30:PRO:HD3	1.99	0.61
19:AV:49:THR:HG22	19:AV:49:THR:O	2.00	0.61
34:BA:877:C:H5"	41:BH:88:LYS:HD3	1.82	0.61
59:BZ:319:ASP:OD1	59:BZ:363:ARG:NH2	2.33	0.61
1:CA:2328:A:H2'	1:CA:2329:G:C8	2.35	0.61
1:CA:2805:G:H2'	1:CA:2807:G:C8	2.35	0.61
34:DA:460:G:O6	34:DA:470:C:H5"	2.00	0.61
34:DA:991:U:H4'	34:DA:992:U:OP1	1.99	0.61
19:AV:76:LYS:HB2	19:AV:81:TYR:HB3	1.82	0.61
1:CA:2355:C:H1'	24:C0:39:ARG:HH21	1.63	0.61
19:CV:98:GLU:OE1	19:CV:100:ARG:NH1	2.33	0.61
35:DB:13:ALA:N	35:DB:14:GLY:HA3	2.15	0.61
7:AG:110:ALA:HB1	7:AG:140:ILE:HG23	1.82	0.61
34:BA:1123:A:H61	34:BA:1149:C:H42	1.49	0.61
59:BZ:328:ILE:O	59:BZ:374:LEU:HB2	2.00	0.61
1:CA:1109:C:H2'	1:CA:1110:G:C8	2.35	0.61
34:DA:1010:G:N2	34:DA:1020:U:O2	2.34	0.61
38:DE:139:LEU:C	38:DE:141:GLN:H	2.08	0.61
14:AQ:12:GLN:HG2	14:AQ:73:PRO:HD2	1.83	0.61
49:BP:75:ARG:O	49:BP:78:GLY:N	2.27	0.61
1:CA:2238:G:N7	65:CA:3760:HOH:O	2.31	0.61
14:CQ:85:LYS:HG2	24:C0:7:LEU:HB3	1.82	0.61
34:DA:1002:G:C4	34:DA:1003:G:H8	2.18	0.61
34:DA:1302:U:OP2	46:DM:21:TYR:OH	2.10	0.61
34:BA:266:G:H5"	34:BA:268:C:H41	1.65	0.61
1:CA:1876:A:H2'	1:CA:1877:A:C8	2.35	0.61
5:CE:59:VAL:HG21	5:CE:74:PRO:HB3	1.82	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:DZ:129:LYS:HZ1	59:DZ:517:LEU:HG	1.66	0.61
1:AA:1834:A:H4'	4:AD:259:THR:HG23	1.83	0.61
4:AD:71:ASP:HB3	4:AD:103:ARG:HH22	1.66	0.61
28:A4:10:VAL:HG21	28:A4:29:PRO:HG3	1.81	0.61
1:CA:1081:U:OP1	10:CL:125:ARG:NH1	2.33	0.61
4:CD:142:VAL:HG13	4:CD:191:ALA:HB1	1.81	0.61
14:CQ:138:ASP:OD2	23:CZ:81:ARG:NH1	2.34	0.61
59:DZ:659:LEU:HD12	59:DZ:669:PHE:HD1	1.66	0.61
7:AG:161:THR:HG22	7:AG:163:ALA:H	1.65	0.61
28:A4:44:THR:O	28:A4:46:GLN:N	2.34	0.61
36:BC:134:ILE:HG23	36:BC:151:VAL:HB	1.83	0.61
34:DA:1022:G:H2'	34:DA:1023:G:H8	1.64	0.61
34:DA:1062:U:H2'	34:DA:1063:C:C6	2.35	0.61
42:DI:8:GLY:HA2	42:DI:79:LEU:HD23	1.83	0.61
58:DY:51:U:H3	58:DY:63:G:H1	1.46	0.61
1:AA:354:A:H2	1:AA:1255:A:HO2'	1.49	0.61
1:AA:625:G:O2'	1:AA:702:A:N6	2.34	0.61
1:AA:1604:C:OP2	1:AA:1605:A:O2'	2.19	0.61
23:AZ:72:ARG:NH2	23:AZ:97:GLU:O	2.33	0.61
30:A6:44:ARG:HB3	30:A6:44:ARG:HH11	1.66	0.61
59:BZ:509:HIS:HB3	59:BZ:571:SER:H	1.66	0.61
1:CA:300:A:OP2	22:CY:86:ARG:NH2	2.34	0.61
34:DA:1312:G:H5'	52:DS:5:LEU:HD11	1.81	0.61
1:AA:542:C:OP1	29:A5:16:ARG:NH2	2.30	0.61
5:AE:117:MET:SD	5:AE:136:ARG:HB3	2.41	0.61
36:DC:125:GLU:HG3	36:DC:190:ARG:O	2.01	0.61
42:DI:3:GLN:HG2	42:DI:20:ARG:HE	1.64	0.61
1:AA:2348:A:H61	24:A0:43:THR:CG2	2.14	0.61
7:AG:41:GLN:HE22	7:AG:153:ARG:HB3	1.66	0.61
34:BA:1255:G:OP1	43:BJ:45:ARG:NH2	2.33	0.61
35:BB:100:GLY:O	35:BB:104:ASN:N	2.27	0.61
43:BJ:40:LEU:HB2	43:BJ:69:ASN:HB2	1.83	0.61
56:BW:9:A:N3	56:BW:45:U:H2'	2.16	0.61
1:CA:1816:G:O6	4:CD:35:LYS:NZ	2.23	0.61
1:CA:2169:A:H2'	1:CA:2170:A:C8	2.36	0.61
42:DI:51:ARG:HG2	42:DI:56:LEU:HD21	1.83	0.61
1:AA:2348:A:H61	24:A0:43:THR:HG21	1.65	0.60
13:CP:138:LEU:HD23	13:CP:145:PRO:HG3	1.82	0.60
35:DB:103:THR:HA	35:DB:180:LEU:HD11	1.83	0.60
58:DY:33:U:H2'	58:DY:35:A:OP2	2.01	0.60
59:DZ:491:VAL:HG21	59:DZ:597:GLY:HA3	1.83	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:AX:35:THR:HG22	21:AX:38:GLU:HB2	1.83	0.60
34:BA:742:G:OP2	48:BO:35:ARG:NH2	2.32	0.60
56:BW:51:U:H2'	56:BW:52:G:C8	2.35	0.60
1:CA:289:A:H2'	1:CA:290:G:O4'	2.01	0.60
6:CF:34:TRP:CZ2	13:CP:8:PRO:HG3	2.35	0.60
34:DA:427:U:OP1	37:DD:13:ARG:NH2	2.34	0.60
34:DA:630:G:H2'	34:DA:631:G:H8	1.65	0.60
34:DA:924:C:O2'	34:DA:1502:A:N6	2.35	0.60
34:DA:962:C:O2'	65:DA:1804:HOH:O	2.15	0.60
49:DP:51:VAL:HG12	49:DP:53:VAL:H	1.66	0.60
1:AA:1093:G:N2	1:AA:1156:G:O2'	2.33	0.60
1:AA:2130:C:H2'	1:AA:2131:U:H6	1.66	0.60
1:AA:2303:U:H2'	1:AA:2304:C:C6	2.36	0.60
1:AA:2331:G:H22	16:AS:3:ARG:NE	1.99	0.60
1:CA:1493:C:N4	1:CA:2206:G:O2'	2.34	0.60
1:CA:2875:C:OP1	17:CT:3:ARG:NH2	2.35	0.60
30:C6:8:LYS:HD3	32:C8:34:TRP:CD2	2.36	0.60
34:DA:1055:A:N3	36:DC:156:ARG:NH1	2.49	0.60
41:DH:49:GLU:OE2	41:DH:62:TYR:OH	2.15	0.60
1:AA:232:U:OP1	32:A8:6:THR:OG1	2.16	0.60
11:AN:42:TRP:CH2	11:AN:44:PRO:HB3	2.36	0.60
34:BA:524:G:H2'	34:BA:525:C:C6	2.36	0.60
35:BB:200:ILE:HB	35:BB:202:PRO:HD3	1.82	0.60
36:BC:19:GLU:HB3	36:BC:40:ARG:NH2	2.16	0.60
58:BY:67:C:H2'	58:BY:68:C:C6	2.36	0.60
59:BZ:-64:VAL:HG12	59:BZ:-29:LEU:HA	1.82	0.60
7:CG:15:VAL:HA	7:CG:175:LEU:HD23	1.83	0.60
34:DA:986:A:N3	52:DS:52:TYR:OH	2.33	0.60
36:DC:8:ILE:HD13	36:DC:184:TYR:HB3	1.82	0.60
1:AA:2044:U:O2'	1:AA:2629:C:H5'	2.02	0.60
3:AC:194:ILE:HD11	3:AC:227:PRO:CB	2.32	0.60
34:BA:410:G:OP1	37:BD:30:LYS:NZ	2.24	0.60
59:BZ:20:HIS:HA	59:BZ:117:GLN:HB2	1.81	0.60
1:CA:271(M):G:H4'	1:CA:271(N):U:OP1	2.01	0.60
1:CA:400:G:N7	65:CA:3767:HOH:O	2.32	0.60
28:C4:59:PHE:HA	28:C4:61:ARG:N	2.17	0.60
1:AA:553:A:H3'	1:AA:553:A:H8	1.66	0.60
1:AA:2262:G:OP1	14:AQ:85:LYS:HE3	2.01	0.60
1:AA:2585:C:H3'	65:AA:3915:HOH:O	2.00	0.60
3:AC:214:TYR:CE2	3:AC:224:ARG:HG2	2.36	0.60
5:AE:105:THR:OG1	5:AE:199:ARG:NH2	2.35	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:CD:146:GLU:HB2	4:CD:189:CYS:HB3	1.84	0.60
8:CH:101:ARG:HH22	8:CH:122:THR:HG23	1.67	0.60
34:DA:630:G:H2'	34:DA:631:G:C8	2.37	0.60
42:DI:23:ASN:HD22	42:DI:23:ASN:H	1.49	0.60
59:DZ:363:ARG:NH1	59:DZ:363:ARG:HG2	2.11	0.60
1:AA:1766:G:H3'	1:AA:1767:A:H5"	1.81	0.60
1:AA:2697:G:H5'	12:AO:68:GLU:OE1	2.02	0.60
13:AP:39:LYS:HD2	13:AP:45:LEU:HD11	1.82	0.60
41:BH:112:LEU:HA	41:BH:134:ILE:HG12	1.81	0.60
59:BZ:12:LEU:HD12	59:BZ:78:ARG:HD2	1.83	0.60
59:BZ:99:ARG:HH11	59:BZ:99:ARG:CB	2.09	0.60
20:CW:88:ARG:NH1	20:CW:94:ASP:OD2	2.34	0.60
34:DA:390:C:O3'	49:DP:28:ARG:NH2	2.34	0.60
34:DA:982:U:O2	34:DA:1222:G:N1	2.31	0.60
34:DA:1189:C:OP1	43:DJ:51:ARG:NH2	2.34	0.60
51:DR:58:LEU:HD12	51:DR:62:GLU:HB3	1.84	0.60
1:AA:2504:U:H2'	1:AA:2505:U:C6	2.37	0.60
35:BB:187:LEU:HA	35:BB:201:ILE:HB	1.82	0.60
57:BX:61:C:H2'	57:BX:62:C:C6	2.36	0.60
1:CA:1021:A:C8	1:CA:1021:A:H3'	2.37	0.60
3:CC:68:GLY:H	3:CC:189:ASN:HD21	1.47	0.60
3:CC:214:TYR:CE2	3:CC:224:ARG:HG2	2.36	0.60
5:CE:56:PRO:HG3	5:CE:74:PRO:HG2	1.84	0.60
14:CQ:26:TYR:CE1	14:CQ:28:ALA:HB2	2.37	0.60
25:C1:72:GLU:OE1	25:C1:76:ARG:NH2	2.35	0.60
35:DB:74:LYS:HD2	35:DB:165:VAL:HG11	1.84	0.60
59:DZ:13:ARG:NE	59:DZ:280:LEU:O	2.30	0.60
1:AA:1312:G:O5'	20:AW:15:ARG:NH2	2.35	0.60
1:AA:2075:G:OP1	5:AE:144:ARG:HG2	2.02	0.60
3:AC:11:LEU:HD12	3:AC:33:LEU:HA	1.82	0.60
16:AS:14:VAL:O	16:AS:18:ILE:HG12	2.01	0.60
18:AU:76:TYR:CE1	18:AU:80:ILE:HG13	2.36	0.60
34:BA:1251:A:H2'	34:BA:1252:A:C8	2.37	0.60
34:DA:975:A:N6	43:DJ:60:ARG:HH12	2.00	0.60
34:DA:1347:G:HO2'	34:DA:1373:G:H1	1.50	0.60
38:DE:81:GLU:HG2	38:DE:90:VAL:HG13	1.82	0.60
41:DH:37:ARG:HH21	41:DH:38:ILE:HD11	1.66	0.60
45:DL:83:VAL:HG23	45:DL:107:ALA:HB2	1.82	0.60
36:BC:43:LEU:HD22	36:BC:47:LEU:HD11	1.83	0.60
59:BZ:276:VAL:HG13	59:BZ:280:LEU:HD12	1.82	0.60
4:CD:17:THR:O	4:CD:211:ARG:NH2	2.34	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:DI:53:VAL:O	42:DI:55:ALA:N	2.34	0.60
1:AA:1093:G:HO2'	1:AA:1156:G:H1	1.50	0.59
7:AG:3:LEU:HD12	7:AG:5:VAL:HG12	1.84	0.59
34:BA:1305:G:H22	34:BA:1331:G:H1'	1.65	0.59
36:BC:6:HIS:HD2	36:BC:8:ILE:H	1.50	0.59
1:CA:793:A:O2'	65:CA:3721:HOH:O	2.14	0.59
1:CA:1153:C:OP1	18:CU:92:ARG:NH1	2.35	0.59
4:CD:131:LEU:HB2	4:CD:136:ILE:HD11	1.83	0.59
34:DA:1003:G:N2	34:DA:1025:U:O4	2.35	0.59
55:DV:20:U:H2'	55:DV:21:C:H6	1.67	0.59
59:DZ:35:TYR:HE2	59:DZ:269:VAL:HB	1.66	0.59
59:DZ:438:PHE:HE2	59:DZ:440:VAL:HG23	1.65	0.59
1:AA:2008:A:OP1	65:AA:3922:HOH:O	2.16	0.59
47:BN:4:LYS:HA	47:BN:7:ILE:HG23	1.83	0.59
1:CA:854:G:O6	65:CA:3718:HOH:O	2.13	0.59
1:CA:918:A:N3	2:CB:80:U:O2'	2.32	0.59
4:CD:96:HIS:CD2	4:CD:102:LYS:HG2	2.34	0.59
13:CP:85:LEU:HA	13:CP:88:LEU:HD12	1.84	0.59
23:CZ:19:ARG:NH1	23:CZ:84:GLU:O	2.35	0.59
34:DA:664:G:N2	34:DA:741:G:H1	1.99	0.59
34:DA:878:G:H5'	41:DH:89:PRO:HG2	1.82	0.59
34:DA:1118:C:H2'	34:DA:1119:C:H6	1.66	0.59
1:AA:2201:C:O4'	3:AC:169:THR:CG2	2.48	0.59
10:AL:77:LEU:HD21	10:AL:111:LYS:HD2	1.84	0.59
14:AQ:56:ARG:NH1	56:BW:52:G:H4'	2.17	0.59
34:BA:193:C:H2'	34:BA:194:C:C6	2.36	0.59
34:BA:555:C:H2'	34:BA:556:C:C6	2.37	0.59
36:BC:53:ALA:HB2	36:BC:115:LEU:HD13	1.84	0.59
59:BZ:179:ASP:N	59:BZ:184:LYS:O	2.29	0.59
1:CA:2273:A:O2'	1:CA:2274:A:H5'	2.02	0.59
1:CA:2781:A:H5"	1:CA:2782:G:H5'	1.84	0.59
5:CE:78:LEU:O	5:CE:79:ARG:HG2	2.01	0.59
7:CG:113:ARG:NH1	7:CG:139:LEU:O	2.34	0.59
34:DA:920:U:H2'	34:DA:921:U:H6	1.67	0.59
34:DA:1073:U:H2'	34:DA:1074:G:C8	2.37	0.59
39:DF:2:ARG:NE	39:DF:69:GLU:HG2	2.17	0.59
1:AA:2255:U:H2'	1:AA:2256:U:C6	2.37	0.59
8:AH:164:TYR:HB2	8:AH:167:GLU:HB2	1.83	0.59
10:AL:77:LEU:HD12	10:AL:107:ILE:HG23	1.85	0.59
12:AO:35:VAL:HG21	12:AO:69:ILE:HD13	1.84	0.59
34:BA:1240:U:OP2	40:BG:116:ALA:N	2.27	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:323:G:HO2'	1:CA:1205:U:H3	1.48	0.59
1:CA:908:C:OP2	14:CQ:22:LYS:NZ	2.35	0.59
1:CA:1053:C:C4	1:CA:1107:G:N2	2.68	0.59
1:CA:1589:C:H2'	1:CA:1590:U:C6	2.37	0.59
1:CA:2132:U:C2	3:CC:6:LYS:HE3	2.37	0.59
1:CA:2485:G:H5"	14:CQ:46:GLN:HE21	1.67	0.59
3:CC:194:ILE:HD11	3:CC:227:PRO:CB	2.32	0.59
14:CQ:110:THR:HG23	14:CQ:113:GLN:HB2	1.83	0.59
23:CZ:108:PRO:HG2	23:CZ:117:LEU:HD13	1.85	0.59
34:DA:1030:C:H42	34:DA:1031:G:H1	1.50	0.59
34:DA:1123:A:H4'	43:DJ:37:PRO:HD2	1.85	0.59
35:DB:189:ASP:OD1	35:DB:189:ASP:N	2.27	0.59
49:DP:43:LYS:HG2	49:DP:48:TRP:CG	2.38	0.59
59:DZ:407:PRO:HB3	59:DZ:452:SER:HB3	1.85	0.59
1:AA:1338:U:H2'	1:AA:1339:C:C6	2.37	0.59
8:AH:88:LEU:HD13	8:AH:130:ARG:HG2	1.84	0.59
42:BI:3:GLN:HG3	42:BI:20:ARG:HE	1.67	0.59
1:CA:1108:U:H6	1:CA:1108:U:O5'	1.85	0.59
1:CA:2166:G:H3'	1:CA:2167:U:H5"	1.84	0.59
44:DK:22:HIS:HB3	44:DK:29:ILE:HB	1.85	0.59
1:AA:331:G:H21	1:AA:354:A:H62	1.50	0.59
1:AA:2013:U:H2'	1:AA:2014:G:H5"	1.84	0.59
8:AH:41:MET:HE2	8:AH:65:HIS:HA	1.84	0.59
34:BA:736:C:H2'	34:BA:737:A:C8	2.37	0.59
35:BB:178:ARG:NH2	41:BH:74:PRO:HB3	2.18	0.59
37:BD:60:GLU:OE1	37:BD:198:VAL:HA	2.01	0.59
34:BA:103:C:P	53:BT:17:ARG:HH21	2.25	0.59
1:CA:2148:G:H2'	1:CA:2149:G:C8	2.37	0.59
1:CA:2165:G:H22	1:CA:2172:U:H5	1.51	0.59
1:CA:2320:A:H2'	1:CA:2320:A:N3	2.17	0.59
3:CC:41:THR:HG22	3:CC:42:VAL:N	2.17	0.59
35:DB:16:HIS:O	35:DB:18:GLY:N	2.36	0.59
35:DB:98:LEU:HB2	35:DB:101:MET:HE3	1.83	0.59
37:DD:13:ARG:NH1	37:DD:38:TYR:O	2.36	0.59
49:DP:43:LYS:HG2	49:DP:48:TRP:CD2	2.37	0.59
7:AG:109:VAL:C	7:AG:112:PRO:HD2	2.28	0.59
34:BA:1326:C:OP1	54:BU:12:LYS:NZ	2.23	0.59
35:BB:201:ILE:HG21	35:BB:214:ILE:HG21	1.83	0.59
36:BC:13:GLY:HA3	47:BN:57:ARG:HH21	1.66	0.59
59:BZ:20:HIS:ND1	59:BZ:117:GLN:HG2	2.18	0.59
1:CA:214:G:O2'	1:CA:216:A:O2'	2.19	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:1792:G:O2'	1:CA:1830:C:OP1	2.20	0.59
1:CA:2139:C:H42	1:CA:2152:G:H1	1.51	0.59
27:C3:8:LEU:HD13	27:C3:31:LEU:HD23	1.84	0.59
41:DH:73:ASP:OD1	41:DH:75:ARG:NH1	2.36	0.59
42:DI:14:VAL:HG23	42:DI:66:ARG:HB3	1.83	0.59
1:AA:1159:U:H2'	1:AA:1160:G:C8	2.38	0.59
26:A2:1:MET:HE2	26:A2:6:VAL:HG22	1.85	0.59
41:BH:51:VAL:HG21	41:BH:60:ARG:HH11	1.67	0.59
1:CA:309:G:N3	1:CA:329:G:O2'	2.35	0.59
23:CZ:70:LEU:HD11	23:CZ:98:MET:HE3	1.84	0.59
53:DT:9:ASN:O	53:DT:10:LEU:HB2	2.02	0.59
1:AA:1775:C:H5'	1:AA:1776:G:OP2	2.03	0.59
36:BC:3:ASN:OD1	36:BC:3:ASN:N	2.36	0.59
42:BI:110:GLU:OE2	42:BI:113:LYS:NZ	2.35	0.59
59:BZ:146:LEU:HD12	59:BZ:167:PRO:HD3	1.85	0.59
1:CA:1108:U:C5	1:CA:1109:C:C4	2.91	0.59
18:CU:86:ALA:HB2	18:CU:116:ALA:HB2	1.84	0.59
34:DA:1330:U:H4'	46:DM:23:TYR:CE1	2.37	0.59
1:AA:278:G:H2'	1:AA:279:G:H5"	1.85	0.58
1:AA:1154:U:H1'	1:AA:1155:C:OP1	2.03	0.58
3:AC:214:TYR:CZ	3:AC:224:ARG:HG2	2.37	0.58
4:AD:52:ARG:NH2	65:AD:401:HOH:O	2.29	0.58
43:BJ:38:ILE:HD11	43:BJ:71:LEU:HD23	1.84	0.58
1:CA:90:U:H1'	1:CA:92:A:C8	2.38	0.58
1:CA:2183:C:H2'	1:CA:2184:G:H8	1.68	0.58
12:CO:120:GLU:OE1	17:CT:67:SER:OG	2.21	0.58
16:CS:10:ARG:O	16:CS:14:VAL:HG13	2.03	0.58
34:DA:839:U:H5"	34:DA:840:C:H5	1.68	0.58
34:DA:1202:G:O4'	47:DN:29:ARG:NH1	2.34	0.58
59:DZ:74:TRP:O	59:DZ:76:ASP:N	2.36	0.58
1:AA:1688:A:H2'	1:AA:1689:G:O4'	2.03	0.58
3:AC:41:THR:HG22	3:AC:42:VAL:N	2.17	0.58
25:A1:3:LYS:HB2	25:A1:61:ARG:NH1	2.18	0.58
34:BA:1125:U:H4'	43:BJ:5:ARG:NH2	2.18	0.58
50:BQ:66:SER:O	50:BQ:70:ARG:NH1	2.36	0.58
56:BW:7:A:H61	56:BW:66:U:H3	1.49	0.58
59:BZ:138:LYS:HG2	64:BZ:702:GDP:C6	2.38	0.58
1:CA:307:G:N1	1:CA:310:A:OP2	2.32	0.58
3:CC:214:TYR:CZ	3:CC:224:ARG:HG2	2.37	0.58
14:CQ:16:ARG:HG2	14:CQ:16:ARG:HH11	1.68	0.58
28:C4:34:GLU:HG2	46:DM:3:ARG:HB3	1.84	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:DB:71:VAL:HG22	35:DB:164:VAL:HA	1.84	0.58
39:DF:35:ALA:HA	39:DF:67:MET:HB3	1.84	0.58
58:DY:50:U:H3	58:DY:64:A:H61	1.51	0.58
59:DZ:346:LYS:HZ3	59:DZ:384:ILE:HG23	1.68	0.58
1:AA:1232:G:H5"	19:AV:81:TYR:CE1	2.37	0.58
14:AQ:2:LEU:HD22	65:AQ:3102:HOH:O	2.02	0.58
34:BA:653:A:OP1	41:BH:56:LYS:NZ	2.36	0.58
46:BM:11:ARG:HB2	46:BM:46:LYS:HB3	1.84	0.58
59:BZ:289:ILE:HD11	59:BZ:331:TYR:HB3	1.85	0.58
1:CA:208:C:H2'	1:CA:209:C:C6	2.39	0.58
1:CA:657:U:H2'	1:CA:658:C:C6	2.38	0.58
8:CH:64:LEU:HD23	8:CH:67:LEU:HD23	1.86	0.58
34:DA:1022:G:H2'	34:DA:1023:G:C8	2.38	0.58
37:DD:173:TRP:HB2	37:DD:187:ARG:O	2.02	0.58
39:DF:8:ILE:HD11	39:DF:79:LEU:HD13	1.85	0.58
47:DN:9:LYS:HG3	47:DN:12:ARG:HD3	1.85	0.58
9:AK:74:LEU:O	9:AK:76:GLY:N	2.35	0.58
12:AO:2:ILE:HG13	12:AO:8:LEU:HD11	1.86	0.58
34:BA:1325:C:H2'	34:BA:1326:C:H6	1.69	0.58
51:BR:56:THR:HB	51:BR:58:LEU:HD23	1.85	0.58
1:CA:244:A:C2	1:CA:255:A:C4	2.92	0.58
1:CA:1427:A:H4'	1:CA:1428:C:O5'	2.02	0.58
48:DO:29:VAL:HG11	48:DO:81:LEU:HD21	1.85	0.58
11:AN:128:HIS:O	11:AN:131:GLN:NE2	2.37	0.58
34:BA:347:G:H2'	34:BA:348:G:O4'	2.03	0.58
34:BA:974:A:OP2	47:BN:29:ARG:NH2	2.36	0.58
34:BA:1191:A:H5"	36:BC:4:LYS:HZ2	1.68	0.58
46:BM:84:ILE:HG13	46:BM:86:CYS:H	1.67	0.58
59:BZ:247:ARG:O	59:BZ:251:ILE:HG13	2.04	0.58
20:CW:64:MET:HE3	20:CW:109:GLU:HG3	1.85	0.58
34:DA:1052:U:H5"	34:DA:1053:G:OP2	2.03	0.58
42:DI:9:ARG:HG2	42:DI:14:VAL:HG12	1.84	0.58
42:DI:80:GLY:HA2	42:DI:83:ARG:HB2	1.84	0.58
1:AA:1898:A:H2'	1:AA:1899:A:C8	2.37	0.58
34:BA:957:U:O2'	34:BA:959:A:N7	2.30	0.58
39:BF:44:GLY:O	39:BF:60:PHE:N	2.30	0.58
47:BN:23:ARG:NH1	47:BN:30:ALA:HB2	2.19	0.58
55:BV:14:A:N1	58:BY:34:G:N1	2.51	0.58
59:BZ:217:VAL:HA	59:BZ:220:ALA:HB3	1.86	0.58
6:CF:126:VAL:HG21	6:CF:129:PHE:CZ	2.39	0.58
34:DA:1220:G:N2	52:DS:54:GLY:O	2.36	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:DZ:4:ILE:HG22	59:DZ:5:LEU:HD23	1.86	0.58
4:AD:221:VAL:HG22	4:AD:226:MET:HE2	1.85	0.58
34:BA:149:A:H2'	34:BA:150:C:C6	2.39	0.58
42:BI:43:ALA:C	42:BI:45:ALA:H	2.12	0.58
59:BZ:-36:LEU:HD21	59:BZ:-29:LEU:HD22	1.84	0.58
59:DZ:357:ARG:HD2	59:DZ:366:VAL:HG11	1.85	0.58
59:DZ:404:VAL:H	59:DZ:405:PRO:HD3	1.69	0.58
1:AA:551:A:H5"	1:AA:552:C:OP1	2.03	0.58
34:BA:142:G:H2'	34:BA:143:A:H8	1.68	0.58
38:BE:71:LEU:HD21	38:BE:115:VAL:HG22	1.85	0.58
59:BZ:-58:LEU:HD21	59:BZ:-32:LEU:HD22	1.85	0.58
1:CA:1430:C:H2'	1:CA:1431:U:H6	1.69	0.58
4:CD:26:LYS:NZ	4:CD:30:GLU:HG2	2.19	0.58
24:C0:2:ALA:N	65:C0:201:HOH:O	2.37	0.58
34:DA:64:G:H4'	34:DA:65:U:H3'	1.86	0.58
34:DA:834:C:H2'	34:DA:835:U:C6	2.39	0.58
34:DA:978:A:O2'	34:DA:1322:C:N3	2.33	0.58
34:DA:1001:A:H2'	34:DA:1001(A):G:H8	1.68	0.58
47:DN:27:CYS:SG	47:DN:29:ARG:HB2	2.44	0.58
1:AA:173:C:H2'	1:AA:174:U:C6	2.39	0.58
30:A6:14:THR:HB	30:A6:48:VAL:O	2.04	0.58
34:BA:232:G:H1'	34:BA:262:A:N1	2.19	0.58
1:CA:2349:G:OP1	65:CA:3723:HOH:O	2.17	0.58
1:CA:2815:C:H5'	29:C5:29:THR:HG21	1.85	0.58
34:DA:673:G:H2'	34:DA:674:G:C8	2.38	0.58
1:AA:181:C:OP1	65:AA:3924:HOH:O	2.17	0.58
1:AA:1101:G:O2'	1:AA:1131:A:N1	2.30	0.58
1:AA:1123:A:O2'	10:AL:132:ARG:O	2.21	0.58
21:AX:11:PRO:HB3	21:AX:92:LEU:HD11	1.86	0.58
50:BQ:97:SER:O	50:BQ:97:SER:OG	2.21	0.58
1:CA:2788:C:OP1	5:CE:61:ARG:NH2	2.37	0.58
17:CT:23:ARG:HG3	17:CT:120:ARG:NH1	2.19	0.58
25:C1:18:ILE:HG12	25:C1:37:ILE:HG23	1.86	0.58
1:AA:1891:G:H4'	3:AC:206:LYS:HD2	1.25	0.57
1:AA:2227:G:O2'	1:AA:2228:G:OP1	2.22	0.57
1:AA:2787:C:H2'	1:AA:2788:A:O4'	2.03	0.57
11:AN:42:TRP:CE3	18:AU:63:VAL:HG11	2.39	0.57
59:BZ:13:ARG:NH1	59:BZ:280:LEU:O	2.37	0.57
59:BZ:246:ILE:HG23	59:BZ:255:ILE:HD11	1.85	0.57
1:CA:796:C:H2'	1:CA:797:C:C6	2.39	0.57
34:DA:344:A:H5"	34:DA:345:C:C5	2.35	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:DA:1321:C:H4'	46:DM:87:TYR:CE2	2.39	0.57
40:DG:72:ARG:N	40:DG:142:GLU:OE2	2.36	0.57
59:DZ:-62:LEU:HD11	59:DZ:-48:VAL:HG22	1.86	0.57
1:AA:1296:G:N7	13:AP:18:ARG:NH2	2.52	0.57
1:AA:2141:A:O2'	1:AA:2142:G:H5'	2.04	0.57
1:AA:2585:C:OP1	65:AA:3923:HOH:O	2.17	0.57
28:A4:26:SER:OG	28:A4:27:THR:N	2.35	0.57
34:BA:1323:G:H2'	34:BA:1324:A:C8	2.39	0.57
49:BP:56:ALA:O	49:BP:60:LEU:HB2	2.04	0.57
51:BR:32:ARG:HA	51:BR:69:THR:HG21	1.86	0.57
1:CA:1364:G:OP2	25:C1:3:LYS:HG3	2.04	0.57
16:CS:41:ASP:OD2	16:CS:44:LYS:HE2	2.04	0.57
34:DA:1126:U:H4'	34:DA:1281:U:H1'	1.85	0.57
35:DB:77:ALA:HA	35:DB:80:ILE:HG22	1.84	0.57
1:AA:610:C:OP2	13:AP:21:ARG:NH2	2.36	0.57
1:AA:1077:G:H21	33:A9:36:GLN:HE22	1.52	0.57
1:AA:2417:G:P	13:AP:77:ARG:HH22	2.26	0.57
28:A4:61:ARG:HH21	52:BS:42:PRO:HD2	1.69	0.57
42:BI:99:LEU:HB3	42:BI:101:PHE:CE1	2.38	0.57
59:BZ:225:GLU:HA	59:BZ:228:MET:HB3	1.86	0.57
1:CA:2179:C:O4'	3:CC:169:THR:HG22	2.03	0.57
1:CA:2749:A:H1'	8:CH:63:SER:HB3	1.86	0.57
4:CD:130:ALA:C	4:CD:131:LEU:HD12	2.29	0.57
8:CH:143:GLN:O	8:CH:146:ALA:N	2.38	0.57
35:DB:80:ILE:HD11	35:DB:212:GLN:HA	1.87	0.57
37:DD:61:LYS:HB2	37:DD:203:VAL:HG22	1.85	0.57
46:DM:16:ASP:OD1	46:DM:16:ASP:N	2.38	0.57
47:DN:48:ALA:HB2	47:DN:53:LEU:HD12	1.86	0.57
59:DZ:114:VAL:HG21	59:DZ:156:ARG:HB2	1.86	0.57
1:AA:1201:A:OP1	18:AU:55:ARG:HD3	2.04	0.57
7:AG:43:LEU:HD11	7:AG:153:ARG:HG2	1.87	0.57
34:BA:131:C:O2'	34:BA:262:A:N3	2.34	0.57
35:BB:185:ILE:HG23	35:BB:199:TYR:HB2	1.85	0.57
42:BI:70:LYS:O	42:BI:74:ILE:HG13	2.04	0.57
1:CA:1021:A:H3'	1:CA:1021:A:H8	1.70	0.57
1:CA:1062:G:O2'	10:CL:133:SER:O	2.17	0.57
1:CA:1648:C:OP1	65:CA:3724:HOH:O	2.17	0.57
9:CK:69:PRO:O	9:CK:71:LEU:N	2.35	0.57
28:C4:62:ARG:O	28:C4:64:GLY:N	2.37	0.57
34:DA:736:C:H2'	34:DA:737:A:C8	2.39	0.57
35:DB:74:LYS:O	35:DB:78:GLN:HB2	2.04	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1112:U:N3	1:AA:1114:G:OP2	2.37	0.57
1:AA:2735:G:H2'	1:AA:2736:C:C6	2.39	0.57
25:A1:77:ALA:HB2	25:A1:94:LEU:HD21	1.85	0.57
49:BP:17:TYR:CE2	49:BP:41:PRO:HG3	2.40	0.57
59:BZ:-53:ASP:H	59:BZ:-50:GLN:NE2	2.02	0.57
59:BZ:162:VAL:HG21	59:BZ:255:ILE:HD12	1.85	0.57
1:CA:1568:G:N7	65:CA:3771:HOH:O	2.32	0.57
34:DA:1171:G:H2'	34:DA:1172:C:C6	2.40	0.57
35:DB:16:HIS:HB2	35:DB:204:ASN:HB3	1.86	0.57
56:DW:51:U:H2'	56:DW:52:G:C8	2.40	0.57
59:DZ:294:PRO:HG3	59:DZ:396:ARG:HB2	1.85	0.57
1:AA:561:A:H2'	1:AA:562:C:C6	2.40	0.57
1:AA:2158:C:H42	1:AA:2177:G:H1	1.53	0.57
37:BD:162:LEU:HD13	37:BD:181:MET:HG2	1.87	0.57
59:BZ:-53:ASP:H	59:BZ:-50:GLN:HE21	1.53	0.57
1:CA:955:C:OP1	14:CQ:87:LYS:NZ	2.34	0.57
1:CA:2744:G:N2	8:CH:143:GLN:OE1	2.37	0.57
12:CO:24:VAL:HB	12:CO:33:ALA:HB2	1.87	0.57
34:DA:834:C:H2'	34:DA:835:U:H6	1.69	0.57
59:DZ:619:ASP:HB3	59:DZ:662:LYS:HD2	1.86	0.57
1:AA:1067:A:H8	1:AA:1068:G:H5"	1.70	0.57
5:AE:111:ARG:HG3	5:AE:160:TYR:CD2	2.40	0.57
34:BA:167:G:H2'	34:BA:168:G:C8	2.37	0.57
34:BA:395:C:O3'	59:BZ:349:LYS:NZ	2.37	0.57
35:BB:77:ALA:HB2	35:BB:211:ILE:HD13	1.87	0.57
35:BB:111:ARG:HG2	35:BB:111:ARG:NH1	2.17	0.57
37:BD:154:ASN:HA	37:BD:159:ARG:HH21	1.69	0.57
40:BG:18:TYR:CE2	40:BG:59:LEU:HB2	2.40	0.57
43:BJ:8:LEU:HD12	43:BJ:20:ALA:HB2	1.87	0.57
46:BM:3:ARG:HD2	46:BM:9:ILE:HG12	1.86	0.57
6:CF:195:ASP:HB3	6:CF:198:ALA:H	1.70	0.57
26:C2:35:LEU:HD22	26:C2:44:LEU:HD11	1.84	0.57
34:DA:646:U:H2'	34:DA:647:C:C6	2.40	0.57
34:DA:1256:A:H61	34:DA:1278:U:H1'	1.70	0.57
59:DZ:16:GLY:HA3	59:DZ:101:LEU:HD22	1.85	0.57
1:AA:2209:G:O2'	1:AA:2210:C:OP1	2.18	0.57
34:BA:1239:A:H4'	34:BA:1240:U:H5"	1.85	0.57
36:BC:40:ARG:O	36:BC:44:GLU:HB2	2.05	0.57
38:BE:152:ARG:HA	41:BH:64:LYS:NZ	2.19	0.57
59:BZ:74:TRP:CD1	59:BZ:273:LEU:HB3	2.39	0.57
1:CA:1108:U:C6	1:CA:1109:C:C5	2.92	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:1693:U:O2'	4:CD:14:ARG:NH2	2.37	0.57
15:CR:104:ARG:HD2	15:CR:109:ALA:HB3	1.85	0.57
34:DA:188:C:H2'	34:DA:189:G:H8	1.69	0.57
34:DA:316:G:OP2	34:DA:351:G:O2'	2.22	0.57
34:DA:503:C:OP2	45:DL:116:SER:HB3	2.04	0.57
34:DA:1001:A:H2'	34:DA:1001(A):G:C8	2.40	0.57
35:DB:7:VAL:HG12	35:DB:8:LYS:HG2	1.86	0.57
48:DO:56:LEU:O	48:DO:60:VAL:HG23	2.05	0.57
1:AA:469:A:H1'	1:AA:1246:C:O4'	2.04	0.57
5:AE:101:ARG:NH1	5:AE:169:ASN:O	2.34	0.57
33:A9:2:LYS:HE2	33:A9:31:LYS:O	2.04	0.57
35:BB:37:ASN:N	35:BB:37:ASN:OD1	2.38	0.57
1:CA:1899:G:H2'	1:CA:1899:G:N3	2.20	0.57
8:CH:3:ARG:CZ	8:CH:4:ILE:H	2.17	0.57
19:CV:3:ALA:HB3	19:CV:14:VAL:HG23	1.86	0.57
21:CX:41:ASN:O	21:CX:45:THR:HG23	2.05	0.57
30:C6:10:LEU:HD23	30:C6:22:ALA:HB2	1.86	0.57
34:DA:1135:U:H2'	34:DA:1137:C:C2	2.40	0.57
1:AA:185:A:H62	13:AP:38:GLN:HE22	1.51	0.57
3:AC:29:LEU:O	3:AC:30:VAL:C	2.48	0.57
6:AF:184:TYR:O	6:AF:188:ARG:HG3	2.05	0.57
7:AG:38:VAL:HG22	7:AG:93:THR:HG23	1.87	0.57
34:BA:673:G:H2'	34:BA:674:G:C8	2.40	0.57
34:BA:731:G:H5'	34:BA:766:A:H4'	1.87	0.57
6:CF:184:TYR:CE1	13:CP:3:LEU:HD21	2.39	0.57
34:DA:881:G:OP2	45:DL:12:ARG:NH2	2.38	0.57
34:DA:1353:G:OP1	54:DU:10:ARG:NH1	2.38	0.57
35:DB:184:VAL:HG12	35:DB:197:VAL:HG13	1.87	0.57
46:DM:78:ILE:HD12	46:DM:92:HIS:CE1	2.40	0.57
1:AA:990:A:H2	65:AA:4161:HOH:O	1.87	0.56
1:AA:1827:U:H2'	1:AA:1828:C:C6	2.40	0.56
14:AQ:110:THR:HG23	14:AQ:113:GLN:OE1	2.05	0.56
35:BB:97:TRP:CH2	35:BB:101:MET:HB2	2.40	0.56
59:BZ:247:ARG:HE	59:BZ:251:ILE:HD11	1.70	0.56
8:CH:7:LEU:HD23	8:CH:69:ARG:HH12	1.70	0.56
9:CK:26:LEU:HA	9:CK:84:GLU:HA	1.86	0.56
23:CZ:145:GLU:H	23:CZ:148:ASP:HB2	1.70	0.56
34:DA:1106:G:H5"	36:DC:172:ARG:HG2	1.87	0.56
59:DZ:138:LYS:HG2	64:DZ:702:GDP:C5	2.40	0.56
59:DZ:224:ASP:HB3	59:DZ:227:ILE:HG12	1.87	0.56
1:AA:843:C:H2'	1:AA:844:C:C6	2.40	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1067:A:C8	1:AA:1067:A:H3'	2.40	0.56
4:AD:2:ALA:O	4:AD:3:VAL:HB	2.05	0.56
7:AG:61:ALA:O	28:A4:7:PRO:HG2	2.05	0.56
35:BB:55:PHE:HA	35:BB:58:ILE:HG13	1.87	0.56
1:CA:1688:U:O2	1:CA:1700:A:H5'	2.06	0.56
1:CA:1721:G:N1	1:CA:1739:U:OP2	2.38	0.56
13:CP:64:LYS:HA	32:C8:13:ARG:HB3	1.87	0.56
34:DA:527:G:O2'	34:DA:535:A:N1	2.37	0.56
35:DB:16:HIS:CD2	35:DB:204:ASN:HB3	2.40	0.56
46:DM:22:ILE:HG23	46:DM:67:GLU:HG2	1.86	0.56
1:AA:1785:C:OP1	17:AT:96:ARG:NH1	2.35	0.56
3:AC:6:LYS:HG3	3:AC:7:ARG:H	1.69	0.56
37:BD:168:ARG:HB2	37:BD:168:ARG:HH11	1.69	0.56
46:BM:11:ARG:HA	46:BM:45:VAL:HB	1.86	0.56
49:BP:39:TYR:CD2	49:BP:73:LEU:HD11	2.40	0.56
59:BZ:20:HIS:CE1	59:BZ:117:GLN:HG2	2.40	0.56
59:BZ:129:LYS:HA	59:BZ:253:LEU:HD21	1.88	0.56
59:BZ:403:GLU:HG2	59:BZ:404:VAL:HG22	1.86	0.56
1:CA:535:C:O3'	18:CU:53:ARG:NH1	2.38	0.56
1:CA:566:U:H5"	13:CP:29:LYS:HE3	1.86	0.56
1:CA:957:A:H5'	14:CQ:76:LYS:HD2	1.87	0.56
1:CA:1149:G:H2'	1:CA:1150:C:C6	2.41	0.56
1:CA:1794:U:H2'	1:CA:1795:C:H6	1.71	0.56
1:CA:2132:U:C2	3:CC:6:LYS:CD	2.88	0.56
5:CE:111:ARG:HG3	5:CE:160:TYR:CD2	2.40	0.56
6:CF:34:TRP:CE2	13:CP:8:PRO:HG3	2.40	0.56
29:C5:16:ARG:HG2	29:C5:16:ARG:HH11	1.70	0.56
38:DE:9:LYS:HB2	38:DE:112:LEU:HD11	1.87	0.56
59:DZ:150:ILE:O	59:DZ:154:GLN:HG2	2.05	0.56
1:AA:2121:U:H3	1:AA:2212:G:H1	1.54	0.56
34:BA:179:A:H2'	34:BA:180:U:C6	2.41	0.56
39:DF:7:ASN:HD22	39:DF:7:ASN:N	2.04	0.56
55:DV:20:U:H2'	55:DV:21:C:C6	2.40	0.56
59:DZ:138:LYS:HG2	64:DZ:702:GDP:C6	2.41	0.56
1:AA:1068:G:N2	1:AA:1188:A:C2	2.74	0.56
10:AL:115:LEU:HD22	10:AL:126:MET:HE1	1.88	0.56
14:AQ:104:PHE:HE2	14:AQ:125:LEU:HD11	1.70	0.56
22:AY:55:TYR:N	22:AY:55:TYR:CD1	2.74	0.56
34:BA:179:A:H2'	34:BA:180:U:H6	1.70	0.56
37:BD:25:ARG:HA	37:BD:28:SER:HB3	1.88	0.56
43:BJ:37:PRO:HA	43:BJ:72:VAL:HG12	1.86	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:BZ:125:ALA:HB1	59:BZ:132:ARG:NH1	2.20	0.56
59:BZ:555:LEU:HD11	59:BZ:599:PRO:HG2	1.87	0.56
7:CG:145:THR:HG23	7:CG:147:ASP:H	1.71	0.56
21:CX:26:TYR:O	21:CX:81:VAL:HG22	2.06	0.56
22:CY:90:LEU:HB3	22:CY:92:ASN:HB3	1.87	0.56
34:DA:1348:U:H4'	42:DI:120:ARG:HD3	1.85	0.56
34:DA:1441:G:H5"	34:DA:1442:G:H5'	1.88	0.56
59:DZ:369:LEU:HD21	59:DZ:375:GLY:HA3	1.88	0.56
17:AT:56:GLY:O	17:AT:59:THR:HG23	2.05	0.56
34:BA:1103:C:OP1	35:BB:96:ARG:NH2	2.38	0.56
1:CA:1359:A:N6	1:CA:1372:U:H3	2.04	0.56
1:CA:1518:U:H2'	1:CA:1519:G:O4'	2.06	0.56
25:C1:3:LYS:HB2	25:C1:61:ARG:NH1	2.21	0.56
34:DA:748:C:H4'	34:DA:749:C:O5'	2.05	0.56
1:AA:1218:G:O2'	1:AA:1219:A:O5'	2.24	0.56
32:A8:61:LEU:C	32:A8:63:PRO:HD3	2.30	0.56
59:BZ:495:GLY:N	59:BZ:510:VAL:O	2.38	0.56
1:CA:1338:G:N7	21:CX:62:LYS:NZ	2.49	0.56
3:CC:49:GLY:N	3:CC:209:PHE:O	2.39	0.56
16:CS:84:GLN:H	16:CS:111:GLU:HB2	1.71	0.56
19:CV:72:VAL:HG13	19:CV:85:LYS:HB3	1.86	0.56
23:CZ:5:LEU:HD22	23:CZ:6:LYS:H	1.71	0.56
34:DA:1016:A:O2'	34:DA:1217:C:O2'	2.21	0.56
36:DC:57:ILE:HG13	36:DC:66:VAL:HG22	1.88	0.56
1:AA:552:C:C5	1:AA:2792:U:H2'	2.41	0.56
1:AA:1123:A:H4'	10:AL:91:PRO:HB2	1.87	0.56
1:AA:1154:U:O2'	1:AA:1155:C:H5"	2.06	0.56
29:A5:35:GLU:HG3	29:A5:51:TYR:CD2	2.41	0.56
34:BA:159:G:N2	34:BA:161:A:O5'	2.39	0.56
1:CA:1412:A:H2'	1:CA:1413:G:C8	2.40	0.56
1:CA:1782:C:H1'	1:CA:2609:U:H5"	1.86	0.56
1:CA:1803:A:O2'	4:CD:259:THR:HG21	2.06	0.56
3:CC:42:VAL:O	3:CC:216:THR:O	2.24	0.56
4:CD:121:PRO:HB3	4:CD:135:PHE:CE2	2.41	0.56
45:DL:71:PRO:O	45:DL:102:ARG:HD3	2.05	0.56
46:DM:40:ASN:HD22	46:DM:41:PRO:HD2	1.71	0.56
59:DZ:630:GLN:HG2	59:DZ:646:PHE:HB2	1.86	0.56
1:AA:482:C:H4'	65:AA:4069:HOH:O	2.04	0.56
1:AA:1825:U:H2'	1:AA:1826:C:C6	2.41	0.56
18:AU:81:HIS:CE1	18:AU:85:LYS:HD2	2.41	0.56
51:BR:56:THR:HB	51:BR:58:LEU:CD2	2.36	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:1668:A:OP1	12:CO:5:GLN:HG2	2.04	0.56
1:CA:2074:U:H2'	1:CA:2075:U:C6	2.41	0.56
10:CL:89:HIS:O	10:CL:91:PRO:HD3	2.06	0.56
10:CL:134:MET:HG3	10:CL:136:VAL:HG12	1.87	0.56
13:CP:63:PRO:HG2	32:C8:25:MET:HB2	1.86	0.56
18:CU:28:ARG:NH1	18:CU:38:THR:OG1	2.38	0.56
36:DC:12:LEU:HD23	36:DC:16:ARG:HB3	1.86	0.56
44:DK:79:SER:HB2	44:DK:106:LYS:HE3	1.87	0.56
59:DZ:614:GLU:HA	59:DZ:617:MET:HG3	1.86	0.56
1:AA:670:C:H5"	1:AA:671:A:OP2	2.06	0.56
3:AC:49:GLY:N	3:AC:209:PHE:O	2.39	0.56
7:AG:77:ILE:HG22	7:AG:80:PHE:H	1.71	0.56
15:AR:57:ARG:HB3	15:AR:59:ASP:OD1	2.06	0.56
35:BB:21:ARG:HB3	35:BB:39:ILE:HG12	1.88	0.56
35:BB:201:ILE:O	35:BB:203:GLY:N	2.39	0.56
48:BO:16:ALA:HB1	48:BO:21:ASP:HB3	1.87	0.56
59:BZ:-38:TYR:HD2	59:BZ:-37:LEU:HD23	1.71	0.56
1:CA:897:C:H1'	56:DW:56:C:H41	1.71	0.56
30:C6:6:ARG:NH2	65:C6:4001:HOH:O	2.30	0.56
34:DA:1118:C:H2'	34:DA:1119:C:C6	2.41	0.56
34:DA:1326:C:H2'	34:DA:1327:C:C6	2.41	0.56
1:AA:555:G:N3	1:AA:555:G:O4'	2.34	0.55
1:AA:1116:A:H5'	1:AA:1118:C:OP2	2.06	0.55
4:AD:102:LYS:C	4:AD:103:ARG:HG2	2.30	0.55
25:A1:51:VAL:HG11	25:A1:74:VAL:HG21	1.87	0.55
34:BA:1356:G:H2'	34:BA:1357:A:C8	2.40	0.55
44:BK:99:GLN:HG2	44:BK:105:VAL:HG21	1.88	0.55
1:CA:922:U:H2'	1:CA:923:C:C6	2.40	0.55
1:CA:1794:U:H2'	1:CA:1795:C:C6	2.41	0.55
3:CC:6:LYS:HG3	3:CC:7:ARG:H	1.69	0.55
16:CS:39:ILE:HB	16:CS:49:VAL:HG12	1.88	0.55
34:DA:1095:U:OP1	34:DA:1108:G:N2	2.29	0.55
48:DO:54:ARG:O	48:DO:58:MET:HG3	2.06	0.55
1:AA:1423:G:H2'	65:AA:4347:HOH:O	2.06	0.55
6:AF:120:GLU:HB2	6:AF:122:LYS:HG3	1.88	0.55
6:AF:132:VAL:HG22	6:AF:163:VAL:HG22	1.88	0.55
10:AL:105:LEU:HD23	10:AL:120:LEU:HD22	1.87	0.55
34:BA:262:A:H2'	34:BA:263:A:C8	2.41	0.55
34:BA:662:G:H2'	34:BA:663:A:C8	2.41	0.55
41:BH:116:LYS:HD3	41:BH:127:LEU:HD23	1.88	0.55
6:CF:197:ASP:OD1	6:CF:198:ALA:N	2.39	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:CU:91:ASP:O	18:CU:95:LEU:HD13	2.05	0.55
24:C0:53:MET:HG3	24:C0:59:LEU:HD23	1.87	0.55
36:DC:136:GLN:C	36:DC:138:VAL:H	2.13	0.55
1:AA:1539:C:H5"	1:AA:1539:C:O2	2.06	0.55
7:AG:98:ARG:CZ	28:A4:1:MET:HE3	2.36	0.55
17:AT:16:ARG:NH1	17:AT:18:ASP:OD1	2.39	0.55
17:AT:39:ARG:NH2	34:BA:345:C:OP1	2.39	0.55
34:BA:537:G:H5"	45:BL:113:ARG:NH1	2.21	0.55
36:BC:113:ALA:HB2	36:BC:202:ILE:HG13	1.89	0.55
59:BZ:126:GLU:OE2	59:BZ:132:ARG:NH2	2.40	0.55
1:CA:492:A:H2'	1:CA:493:G:O4'	2.06	0.55
1:CA:639:U:H2'	1:CA:640:C:C6	2.40	0.55
1:CA:1689:A:N6	1:CA:1698:A:H2	1.88	0.55
8:CH:46:GLU:HB2	8:CH:49:VAL:HG12	1.88	0.55
10:CL:75:SER:OG	10:CL:134:MET:SD	2.65	0.55
34:DA:742:G:OP2	48:DO:35:ARG:NH2	2.39	0.55
35:DB:16:HIS:CD2	35:DB:17:PHE:H	2.24	0.55
35:DB:91:PRO:HD3	35:DB:154:LEU:HD12	1.88	0.55
44:DK:15:ALA:HB1	44:DK:78:GLN:HG3	1.87	0.55
1:AA:2874:G:OP1	17:AT:119:LYS:HE3	2.06	0.55
35:BB:69:LEU:HD13	35:BB:91:PRO:HB2	1.88	0.55
44:BK:84:VAL:HG21	44:BK:95:ILE:HD11	1.87	0.55
46:BM:3:ARG:HG2	46:BM:8:GLU:HA	1.87	0.55
50:BQ:6:LEU:HG	50:BQ:23:VAL:HG11	1.87	0.55
1:CA:1709:U:H2'	1:CA:1710:C:C6	2.41	0.55
1:CA:2653:U:O2'	8:CH:110:SER:HB3	2.07	0.55
17:CT:2:ASN:O	17:CT:6:LEU:HD22	2.06	0.55
22:CY:23:ARG:HG2	22:CY:42:VAL:HG22	1.88	0.55
28:C4:16:CYS:HA	28:C4:33:VAL:HB	1.88	0.55
45:DL:24:VAL:CG1	45:DL:27:LEU:HD22	2.33	0.55
50:DQ:66:SER:OG	50:DQ:67:LYS:N	2.38	0.55
54:DU:9:ARG:O	54:DU:13:ILE:HG13	2.07	0.55
1:AA:2504:U:H2'	1:AA:2505:U:H6	1.71	0.55
23:AZ:111:VAL:HG23	23:AZ:117:LEU:HD13	1.88	0.55
24:A0:43:THR:O	24:A0:43:THR:HG23	2.07	0.55
36:BC:153:VAL:HG22	36:BC:198:VAL:HG22	1.88	0.55
41:BH:73:ASP:OD1	41:BH:75:ARG:HD3	2.06	0.55
59:BZ:336:THR:O	59:BZ:339:SER:OG	2.24	0.55
1:CA:954:G:H5"	14:CQ:13:GLN:HB3	1.88	0.55
34:DA:957:U:H2'	34:DA:959:A:OP2	2.07	0.55
34:DA:1273:G:H3'	34:DA:1274:G:H8	1.71	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:DB:55:PHE:CD1	35:DB:58:ILE:HD12	2.42	0.55
1:AA:934:A:O2'	1:AA:935:C:OP2	2.23	0.55
1:AA:943:C:O4'	56:BW:56:C:H5	1.89	0.55
1:AA:2146:G:C5'	3:AC:175:PRO:HG3	2.35	0.55
3:AC:42:VAL:O	3:AC:216:THR:O	2.24	0.55
3:AC:52:PRO:HB2	3:AC:168:LYS:O	2.07	0.55
5:AE:7:VAL:HG12	5:AE:51:PHE:HE2	1.72	0.55
11:AN:58:ASP:OD1	11:AN:58:ASP:N	2.33	0.55
35:BB:82:ARG:HG3	35:BB:92:TYR:CZ	2.41	0.55
37:BD:43:HIS:O	37:BD:46:LYS:HB2	2.07	0.55
38:BE:75:THR:OG1	38:BE:76:ILE:N	2.40	0.55
59:BZ:114:VAL:HB	59:BZ:156:ARG:HH12	1.71	0.55
1:CA:1412:A:H2'	1:CA:1413:G:H8	1.72	0.55
1:CA:2572:A:C8	5:CE:144:ARG:HD2	2.42	0.55
3:CC:52:PRO:HB2	3:CC:168:LYS:O	2.07	0.55
6:CF:53:THR:HG23	6:CF:55:GLY:H	1.70	0.55
34:DA:1003:G:H2'	34:DA:1004:A:O4'	2.06	0.55
59:DZ:22:ASP:HA	64:DZ:702:GDP:H5'	1.89	0.55
1:AA:1825:U:H2'	1:AA:1826:C:H6	1.71	0.55
12:AO:35:VAL:HG11	12:AO:103:ALA:HB3	1.89	0.55
38:BE:40:ARG:NH2	38:BE:68:GLU:HA	2.22	0.55
46:BM:122:LYS:HD3	46:BM:123:ALA:H	1.72	0.55
49:BP:43:LYS:HA	49:BP:48:TRP:HB3	1.89	0.55
1:CA:584:C:OP2	18:CU:6:THR:OG1	2.23	0.55
1:CA:1155:A:OP1	18:CU:55:ARG:HD2	2.05	0.55
1:CA:1359:A:H61	1:CA:1372:U:H3	1.54	0.55
3:CC:29:LEU:O	3:CC:30:VAL:C	2.48	0.55
16:CS:48:LEU:HD23	16:CS:82:ILE:HD11	1.89	0.55
34:DA:255:G:H2'	34:DA:256:U:C6	2.41	0.55
34:DA:1218:C:H2'	34:DA:1219:U:C6	2.41	0.55
36:DC:129:ALA:HB3	36:DC:132:ARG:HB3	1.89	0.55
40:DG:115:ARG:HG2	40:DG:118:VAL:HG23	1.87	0.55
1:AA:2346:G:H4'	1:AA:2347:A:OP2	2.06	0.55
1:AA:2699:U:H2'	1:AA:2700:U:O4'	2.07	0.55
36:BC:82:GLU:HA	36:BC:85:ARG:HH21	1.71	0.55
37:BD:8:VAL:HG23	37:BD:11:LEU:HD22	1.88	0.55
58:BY:6:G:O6	58:BY:7:A:N6	2.40	0.55
59:BZ:623:ASP:CG	59:BZ:662:LYS:HE3	2.31	0.55
1:CA:2136:C:HO2'	1:CA:2137:C:C5'	2.19	0.55
1:CA:2345:G:N3	1:CA:2381:C:H2'	2.21	0.55
5:CE:120:TRP:CE3	5:CE:155:LYS:HD3	2.41	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:C4:24:THR:OG1	28:C4:25:TYR:N	2.27	0.55
35:DB:189:ASP:O	35:DB:192:SER:OG	2.24	0.55
42:DI:28:VAL:HA	42:DI:63:ILE:O	2.07	0.55
53:DT:54:LYS:HA	53:DT:57:ARG:NH2	2.22	0.55
59:DZ:303:PRO:O	59:DZ:305:PRO:HD3	2.07	0.55
59:DZ:346:LYS:NZ	59:DZ:384:ILE:HG23	2.22	0.55
1:AA:2221:A:H5"	1:AA:2222:C:OP2	2.07	0.55
36:BC:148:GLY:HA3	36:BC:172:ARG:O	2.07	0.55
38:BE:12:LEU:HD11	38:BE:14:ARG:HD3	1.89	0.55
59:BZ:99:ARG:HG3	59:BZ:128:TYR:HE1	1.71	0.55
59:BZ:608:VAL:HG22	59:BZ:671:MET:HG3	1.89	0.55
1:CA:1336:A:OP2	21:CX:64:LYS:HE3	2.07	0.55
1:CA:2292:C:OP1	16:CS:17:ARG:NH2	2.29	0.55
7:CG:15:VAL:HG21	7:CG:176:LEU:HD23	1.88	0.55
15:CR:38:VAL:HB	15:CR:39:PRO:HD3	1.89	0.55
34:DA:1000:U:H2'	34:DA:1001:A:C8	2.42	0.55
1:AA:354:A:H2	1:AA:1255:A:H2'	1.72	0.55
1:AA:1473:A:H4'	1:AA:1474:C:O5'	2.07	0.55
1:AA:2442:A:H2'	1:AA:2442:A:N3	2.22	0.55
18:AU:76:TYR:CZ	18:AU:80:ILE:HG13	2.41	0.55
34:BA:942:G:H21	42:BI:124:GLN:NE2	2.04	0.55
35:BB:134:GLU:O	35:BB:138:LEU:HG	2.07	0.55
39:BF:19:LEU:HD11	39:BF:59:TYR:CE2	2.42	0.55
40:BG:16:LEU:HD22	40:BG:16:LEU:H	1.71	0.55
46:BM:11:ARG:HG3	46:BM:12:ASN:ND2	2.22	0.55
48:BO:24:SER:OG	48:BO:25:THR:N	2.40	0.55
59:BZ:-38:TYR:O	59:BZ:-35:PRO:HD2	2.07	0.55
59:BZ:363:ARG:HH11	59:BZ:363:ARG:CG	2.17	0.55
34:DA:235:C:H2'	34:DA:236:G:H8	1.72	0.55
34:DA:707:C:H4'	44:DK:20:TYR:CD2	2.42	0.55
34:DA:1239:A:H62	34:DA:1299:A:N6	2.05	0.55
57:DX:75:C:H5"	57:DX:76:31H:OP1	2.07	0.55
1:AA:543:G:H2'	1:AA:544:U:C6	2.42	0.54
1:AA:1109:G:H1	1:AA:1121:C:H42	1.55	0.54
3:AC:54:ARG:CZ	3:AC:56:ASP:HB3	2.38	0.54
3:AC:183:PRO:C	3:AC:185:LYS:H	2.16	0.54
5:AE:116:VAL:HG13	5:AE:122:PHE:HB2	1.89	0.54
18:AU:83:LEU:HD13	18:AU:113:ALA:HB2	1.89	0.54
28:A4:61:ARG:HG3	28:A4:62:ARG:N	2.21	0.54
32:A8:42:ARG:HD2	65:A8:5104:HOH:O	2.06	0.54
34:BA:406:G:H5'	37:BD:5:ILE:HD11	1.87	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:BZ:639:ASN:HA	59:BZ:640:ALA:O	2.07	0.54
1:CA:271(H):G:HO2'	1:CA:271(I):G:H8	1.53	0.54
1:CA:800:A:H8	1:CA:800:A:OP1	1.90	0.54
3:CC:194:ILE:HD11	3:CC:227:PRO:HB3	1.89	0.54
8:CH:3:ARG:NH2	8:CH:4:ILE:H	2.05	0.54
34:DA:174:C:H2'	34:DA:175:C:H6	1.72	0.54
34:DA:1240:U:OP2	40:DG:116:ALA:N	2.39	0.54
42:DI:128:ARG:NH1	57:DX:35:A:OP2	2.40	0.54
50:DQ:4:LYS:HE2	50:DQ:6:LEU:HD11	1.88	0.54
1:AA:1261:G:P	18:AU:12:ARG:HH21	2.29	0.54
7:AG:77:ILE:HD12	7:AG:82:LEU:HD12	1.88	0.54
9:AK:118:THR:N	9:AK:121:ASP:O	2.38	0.54
13:AP:95:VAL:HG22	13:AP:125:VAL:HG12	1.88	0.54
34:BA:189(K):U:H2'	34:BA:189(L):G:C8	2.42	0.54
34:BA:1123:A:O2'	43:BJ:37:PRO:O	2.22	0.54
51:BR:40:LEU:O	51:BR:42:ARG:N	2.40	0.54
1:CA:1106:G:C6	1:CA:1107:G:C5	2.95	0.54
22:CY:30:VAL:HG22	22:CY:37:VAL:HG12	1.89	0.54
34:DA:1316:G:H22	34:DA:1319:A:H5"	1.72	0.54
35:DB:210:SER:OG	35:DB:211:ILE:HG13	2.07	0.54
38:DE:84:PHE:HB3	38:DE:134:ALA:HB2	1.89	0.54
1:AA:469:A:C5	6:AF:45:ARG:HD2	2.43	0.54
1:AA:776:G:C6	4:AD:208:LYS:HB2	2.43	0.54
1:AA:2764:G:H4'	8:AH:4:ILE:HD11	1.88	0.54
34:BA:1435:G:H2'	34:BA:1436:U:C6	2.42	0.54
39:BF:10:LEU:HB2	39:BF:59:TYR:HB3	1.90	0.54
49:BP:3:LYS:N	49:BP:22:THR:O	2.41	0.54
59:BZ:348:ARG:HG2	59:BZ:348:ARG:HH11	1.72	0.54
23:CZ:92:SER:O	23:CZ:130:PRO:HG2	2.07	0.54
34:DA:985:C:H2'	34:DA:986:A:C8	2.43	0.54
34:DA:1053:G:O5'	34:DA:1054:C:H5'	2.07	0.54
34:DA:1104:G:H4'	35:DB:111:ARG:NH1	2.22	0.54
59:DZ:496:LYS:HE2	59:DZ:509:HIS:CE1	2.42	0.54
1:AA:2653:G:H5"	1:AA:2653:G:H8	1.71	0.54
3:AC:52:PRO:HG2	3:AC:53:ARG:H	1.73	0.54
11:AN:121:LYS:HB3	11:AN:123:TYR:HE2	1.72	0.54
28:A4:33:VAL:HG12	28:A4:35:VAL:H	1.71	0.54
34:BA:555:C:H2'	34:BA:556:C:H6	1.73	0.54
37:BD:41:GLY:O	37:BD:43:HIS:N	2.41	0.54
44:BK:48:ILE:O	44:BK:48:ILE:HG12	2.05	0.54
50:BQ:41:LYS:NZ	50:BQ:92:ARG:HH21	2.05	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:1149:G:H2'	1:CA:1150:C:H6	1.71	0.54
16:CS:15:ARG:HB3	16:CS:19:LYS:NZ	2.22	0.54
32:C8:9:GLY:O	32:C8:13:ARG:HG2	2.08	0.54
34:DA:1316:G:H4'	47:DN:18:VAL:HG13	1.90	0.54
59:DZ:116:PRO:HA	59:DZ:119:GLU:HG3	1.89	0.54
1:AA:559:U:H2'	1:AA:560:C:C6	2.43	0.54
3:AC:194:ILE:HD11	3:AC:227:PRO:HB3	1.89	0.54
16:AS:10:ARG:O	16:AS:14:VAL:HG13	2.07	0.54
34:BA:1505:G:O2'	55:BV:13:A:O2'	2.26	0.54
43:BJ:11:PHE:HE1	43:BJ:67:THR:HG22	1.73	0.54
1:CA:2882:A:OP1	15:CR:96:ARG:NE	2.30	0.54
3:CC:183:PRO:C	3:CC:185:LYS:H	2.16	0.54
4:CD:121:PRO:HB3	4:CD:135:PHE:CD2	2.42	0.54
7:CG:145:THR:HG22	7:CG:148:MET:HG2	1.89	0.54
12:CO:64:ARG:HB2	12:CO:83:ALA:HB3	1.90	0.54
27:C3:46:ASN:O	27:C3:50:VAL:HG22	2.08	0.54
34:DA:1133:G:H2'	34:DA:1134:G:C8	2.42	0.54
34:DA:1387:G:H2'	34:DA:1388:C:C6	2.42	0.54
45:DL:83:VAL:HG21	45:DL:100:ILE:HD13	1.90	0.54
59:DZ:603:GLU:OE2	59:DZ:628:ARG:NH2	2.28	0.54
1:AA:2576:A:C2	1:AA:2659:U:H4'	2.43	0.54
34:BA:1191:A:H5"	36:BC:4:LYS:NZ	2.22	0.54
35:BB:16:HIS:CG	35:BB:17:PHE:N	2.76	0.54
46:BM:9:ILE:HB	46:BM:18:ALA:HB1	1.88	0.54
3:CC:44:VAL:HG23	3:CC:176:VAL:HG21	1.89	0.54
14:CQ:21:THR:HG21	14:CQ:101:ARG:HD3	1.90	0.54
34:DA:858:G:O6	34:DA:869:G:H3'	2.07	0.54
38:DE:12:LEU:HD12	38:DE:128:PRO:HB2	1.90	0.54
49:DP:28:ARG:HG3	49:DP:29:ASP:OD1	2.07	0.54
52:DS:12:ASP:OD1	52:DS:37:ARG:NH1	2.40	0.54
1:AA:714:U:O2	32:A8:2:PRO:HD2	2.07	0.54
11:AN:96:GLU:H	11:AN:96:GLU:CD	2.16	0.54
34:BA:1239:A:H62	34:BA:1299:A:N6	2.06	0.54
59:BZ:227:ILE:HD13	59:BZ:242:LEU:HD23	1.89	0.54
4:CD:206:LEU:HD22	4:CD:211:ARG:HG2	1.88	0.54
34:DA:353:A:H5'	34:DA:353:A:C8	2.42	0.54
59:DZ:404:VAL:H	59:DZ:405:PRO:CD	2.21	0.54
1:AA:486:A:H2'	1:AA:487:C:O4'	2.08	0.54
22:AY:92:ASN:N	22:AY:93:GLY:HA2	2.23	0.54
34:BA:134:A:H61	49:BP:25:ARG:NH1	2.06	0.54
41:BH:120:THR:H	41:BH:123:GLU:HB3	1.72	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:BQ:77:VAL:HG12	50:BQ:78:GLU:HB2	1.89	0.54
59:BZ:-25:SER:O	59:BZ:-22:LYS:HB2	2.07	0.54
59:BZ:239:GLU:O	59:BZ:243:VAL:HG23	2.07	0.54
1:CA:774:A:H2'	1:CA:774:A:N3	2.22	0.54
3:CC:6:LYS:HA	3:CC:9:ARG:HH11	1.72	0.54
17:CT:108:ARG:NH2	34:DA:1465:C:OP2	2.41	0.54
34:DA:255:G:H2'	34:DA:256:U:H6	1.73	0.54
34:DA:1321:C:H4'	46:DM:87:TYR:HE2	1.72	0.54
46:DM:25:ILE:HG13	46:DM:29:ARG:HG2	1.90	0.54
59:DZ:264:LEU:HB2	64:DZ:702:GDP:C5	2.42	0.54
1:AA:715:G:H5'	1:AA:716:G:OP2	2.07	0.54
1:AA:2023:A:H2'	1:AA:2024:G:C8	2.43	0.54
34:BA:49:U:O4	34:BA:365:U:H5	1.90	0.54
39:BF:86:ARG:O	39:BF:87:ARG:HG2	2.07	0.54
1:CA:323:G:O2'	1:CA:1205:U:N3	2.29	0.54
1:CA:1063:G:H2'	1:CA:1064:C:H6	1.72	0.54
1:CA:2132:U:C2	3:CC:6:LYS:HD2	2.42	0.54
10:CL:112:MET:H	10:CL:113:PRO:HD2	1.73	0.54
14:CQ:76:LYS:HB3	14:CQ:91:GLU:HG3	1.89	0.54
23:CZ:132:ASN:HD21	23:CZ:160:GLY:H	1.54	0.54
47:DN:23:ARG:NH1	47:DN:30:ALA:HB2	2.22	0.54
59:DZ:38:ARG:HH12	59:DZ:270:GLN:NE2	2.05	0.54
59:DZ:276:VAL:HG13	59:DZ:280:LEU:HD12	1.90	0.54
1:AA:664:U:H2'	1:AA:665:C:C6	2.43	0.54
1:AA:1065:U:O2'	1:AA:1067:A:H2	1.90	0.54
1:AA:1452:U:H2'	1:AA:1453:C:C6	2.42	0.54
1:AA:1846:A:H8	1:AA:1846:A:OP1	1.91	0.54
1:AA:2349:G:OP1	65:AA:3926:HOH:O	2.18	0.54
34:BA:1238:A:OP2	65:BA:1909:HOH:O	2.19	0.54
59:BZ:85:PRO:HD2	59:BZ:94:VAL:HG13	1.89	0.54
59:BZ:114:VAL:CB	59:BZ:156:ARG:HH12	2.21	0.54
1:CA:956:G:OP2	14:CQ:14:ARG:NH2	2.35	0.54
1:CA:1165:U:H2'	1:CA:1166:C:C6	2.43	0.54
41:DH:39:LEU:HD12	41:DH:44:PHE:HB2	1.90	0.54
51:DR:53:ARG:HD2	51:DR:59:SER:O	2.07	0.54
59:DZ:5:LEU:HD13	59:DZ:305:PRO:HG2	1.90	0.54
1:AA:553:A:H2'	1:AA:554:A:H5'	1.90	0.53
1:AA:1102:G:H5"	1:AA:1103:A:O4'	2.08	0.53
1:AA:2658:C:H2'	1:AA:2659:U:O4'	2.08	0.53
3:AC:30:VAL:HG23	3:AC:31:LYS:HG2	1.89	0.53
34:BA:159:G:H2'	34:BA:161:A:OP2	2.07	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:BH:121:ASP:OD2	41:BH:121:ASP:N	2.37	0.53
1:CA:1495:A:OP2	65:CA:3725:HOH:O	2.19	0.53
3:CC:48:LEU:CB	3:CC:50:ILE:HD12	2.38	0.53
7:CG:13:GLU:O	7:CG:15:VAL:N	2.40	0.53
30:C6:9:LEU:HA	30:C6:54:ILE:HB	1.89	0.53
34:DA:1218:C:OP2	47:DN:9:LYS:NZ	2.39	0.53
59:DZ:96:ARG:NH1	59:DZ:96:ARG:HB2	2.23	0.53
8:AH:3:ARG:HG2	8:AH:6:ARG:HD2	1.90	0.53
34:BA:1014:A:H4'	52:BS:14:HIS:NE2	2.24	0.53
34:BA:1349:A:OP2	42:BI:118:LYS:HE3	2.08	0.53
34:BA:1355:G:H2'	34:BA:1356:G:C8	2.43	0.53
43:BJ:49:VAL:CG2	47:BN:41:ARG:HB2	2.38	0.53
52:BS:11:VAL:HG11	52:BS:16:LEU:HB2	1.90	0.53
59:BZ:165:GLN:NE2	59:BZ:259:PHE:HB3	2.22	0.53
1:CA:127:A:H5"	1:CA:128:C:C6	2.44	0.53
1:CA:856:C:H2'	1:CA:857:C:C6	2.43	0.53
1:CA:880:G:N2	1:CA:898:C:H1'	2.20	0.53
1:CA:910:A:H62	14:CQ:12:GLN:HA	1.72	0.53
12:CO:7:TYR:HE1	12:CO:20:MET:HE3	1.74	0.53
22:CY:49:VAL:HG11	22:CY:55:TYR:CD2	2.44	0.53
34:DA:688:G:H2'	34:DA:689:C:H6	1.73	0.53
34:DA:1402:C:H2'	34:DA:1403:C:O4'	2.08	0.53
46:DM:5:ALA:HB3	46:DM:22:ILE:HD12	1.90	0.53
59:DZ:639:ASN:N	59:DZ:640:ALA:HB3	2.23	0.53
1:AA:139:A:H8	1:AA:1454:C:O2'	1.91	0.53
1:AA:2289:G:P	24:A0:10:THR:HG21	2.49	0.53
5:AE:143:ASN:HD22	5:AE:147:PRO:HD3	1.73	0.53
6:AF:24:LEU:HB3	6:AF:115:ALA:HB2	1.90	0.53
52:BS:3:ARG:NH1	52:BS:8:GLY:O	2.42	0.53
59:BZ:181:LEU:HD12	59:BZ:216:LEU:HD21	1.90	0.53
1:CA:184:C:H2'	1:CA:185:U:C6	2.43	0.53
1:CA:247:G:H4'	1:CA:386:G:C5	2.43	0.53
1:CA:997:G:OP1	18:CU:92:ARG:HG2	2.09	0.53
1:CA:2207:G:H3'	1:CA:2208:A:H5"	1.90	0.53
1:CA:2305:A:H5"	7:CG:134:GLY:HA3	1.90	0.53
3:CC:30:VAL:HG23	3:CC:31:LYS:HG2	1.89	0.53
40:DG:111:ARG:NH2	40:DG:126:ASP:OD2	2.41	0.53
42:DI:8:GLY:O	42:DI:15:ALA:N	2.27	0.53
46:DM:20:THR:HA	46:DM:25:ILE:HG22	1.89	0.53
59:DZ:165:GLN:HE21	59:DZ:260:LEU:N	2.04	0.53
3:AC:6:LYS:HA	3:AC:9:ARG:HH11	1.72	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:171:ALA:HB1	3:AC:173:HIS:CE1	2.44	0.53
12:AO:104:ARG:HH12	17:AT:43:GLN:HE22	1.57	0.53
24:A0:27:GLU:HG3	24:A0:68:GLU:HA	1.89	0.53
34:BA:354:G:H2'	34:BA:355:C:H5'	1.90	0.53
34:BA:1030(D):A:N6	34:BA:1031:G:H21	2.07	0.53
34:BA:1367:C:H4'	43:BJ:48:THR:HG21	1.89	0.53
59:BZ:138:LYS:HE2	64:BZ:702:GDP:C4	2.44	0.53
1:CA:2277:G:H5"	14:CQ:87:LYS:HB3	1.90	0.53
4:CD:129:ASN:O	4:CD:193:VAL:HG13	2.08	0.53
14:CQ:26:TYR:CD1	14:CQ:28:ALA:HB2	2.44	0.53
21:CX:29:TRP:CZ3	21:CX:78:LYS:HB3	2.44	0.53
36:DC:63:ASN:HB2	36:DC:98:ASN:HB2	1.91	0.53
57:DX:50:U:H3	57:DX:64:G:H1	1.56	0.53
1:AA:704:U:H2'	1:AA:705:C:C6	2.44	0.53
1:AA:2053:A:C6	1:AA:2510:C:H1'	2.43	0.53
1:AA:2296:C:OP1	30:A6:3:SER:OG	2.15	0.53
34:BA:381:C:H2'	34:BA:382:A:O4'	2.09	0.53
34:BA:404:U:H5'	37:BD:122:ARG:HD3	1.89	0.53
34:BA:507:C:OP2	34:BA:508:C:O2'	2.20	0.53
41:BH:87:SER:HA	41:BH:93:VAL:HG23	1.90	0.53
49:BP:58:TYR:O	49:BP:61:SER:OG	2.22	0.53
53:BT:26:ASN:ND2	53:BT:71:THR:OG1	2.41	0.53
59:BZ:213:HIS:O	59:BZ:217:VAL:HG23	2.09	0.53
1:CA:2166:G:H3'	1:CA:2167:U:C5'	2.38	0.53
35:DB:119:GLU:OE2	35:DB:153:ARG:NH1	2.32	0.53
36:DC:137:ALA:HA	36:DC:140:ARG:HH11	1.72	0.53
42:DI:26:VAL:HG13	42:DI:61:ALA:HB3	1.88	0.53
1:AA:2389:A:H2'	1:AA:2390:A:C8	2.43	0.53
1:AA:2798:C:OP1	5:AE:41:LYS:NZ	2.35	0.53
65:AA:4571:HOH:O	25:A1:20:ARG:HD3	2.07	0.53
3:AC:64:SER:HA	3:AC:161:ARG:H	1.74	0.53
4:AD:68:LYS:HD2	4:AD:70:TRP:CZ2	2.44	0.53
34:BA:1024:G:H2'	34:BA:1025:U:H5"	1.90	0.53
51:BR:37:VAL:O	51:BR:41:LYS:HG2	2.09	0.53
52:BS:22:LEU:HB3	52:BS:27:GLU:HG3	1.91	0.53
52:BS:27:GLU:HB3	52:BS:28:LYS:HB3	1.91	0.53
3:CC:42:VAL:HG13	3:CC:43:GLU:H	1.73	0.53
5:CE:47:VAL:HG11	5:CE:86:PRO:HD2	1.89	0.53
7:CG:49:ASP:OD1	7:CG:49:ASP:N	2.41	0.53
8:CH:154:PRO:HB3	8:CH:163:TYR:CE2	2.44	0.53
34:DA:977:A:O2'	34:DA:979:C:OP2	2.22	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:DA:1286:A:C8	34:DA:1287:A:H4'	2.44	0.53
35:DB:28:PHE:CD1	35:DB:190:THR:HG22	2.44	0.53
59:DZ:284:LEU:HD22	59:DZ:284:LEU:H	1.74	0.53
1:AA:1381:U:H2'	1:AA:1382:A:O4'	2.09	0.53
1:AA:2287:C:C2	14:AQ:85:LYS:HE2	2.44	0.53
22:AY:92:ASN:H	22:AY:92:ASN:ND2	2.02	0.53
34:BA:1456:G:O3'	53:BT:39:LYS:NZ	2.41	0.53
35:BB:97:TRP:CZ2	35:BB:102:LEU:HD13	2.43	0.53
42:BI:9:ARG:HD3	42:BI:14:VAL:HG22	1.91	0.53
1:CA:668:G:H5'	1:CA:669:G:OP2	2.09	0.53
1:CA:1359:A:C2	1:CA:1372:U:O4	2.61	0.53
3:CC:54:ARG:CZ	3:CC:56:ASP:HB3	2.37	0.53
16:CS:14:VAL:O	16:CS:18:ILE:HG12	2.08	0.53
16:CS:67:ARG:HH11	16:CS:67:ARG:HB2	1.73	0.53
34:DA:45:U:H2'	34:DA:46:G:C8	2.44	0.53
34:DA:857:C:H2'	34:DA:858:G:O4'	2.09	0.53
35:DB:164:VAL:HB	35:DB:186:ALA:HB2	1.90	0.53
1:AA:1157:A:H8	1:AA:1158:G:H1'	1.73	0.53
1:AA:2146:G:H5'	3:AC:175:PRO:HG3	1.90	0.53
3:AC:44:VAL:HG23	3:AC:176:VAL:HG21	1.89	0.53
6:AF:162:LEU:HA	6:AF:165:ARG:HD3	1.91	0.53
10:AL:88:ALA:HB3	10:AL:135:GLY:HA3	1.90	0.53
32:A8:61:LEU:O	32:A8:63:PRO:HD3	2.09	0.53
34:BA:250:A:H4'	34:BA:251:G:O5'	2.08	0.53
34:BA:677:U:H3	34:BA:713:G:H22	1.55	0.53
34:BA:790:A:OP1	57:BX:38:A:O2'	2.25	0.53
49:BP:17:TYR:HE2	49:BP:41:PRO:HG3	1.72	0.53
59:BZ:138:LYS:HG2	64:BZ:702:GDP:C5	2.43	0.53
1:CA:489:G:N7	20:CW:49:LYS:NZ	2.57	0.53
1:CA:636:G:O2'	1:CA:638:G:O2'	2.19	0.53
1:CA:637:A:H8	13:CP:117:GLU:HG3	1.73	0.53
34:DA:1388:C:H2'	34:DA:1389:C:C6	2.44	0.53
35:DB:72:GLY:O	35:DB:94:ASN:HA	2.09	0.53
59:DZ:435:ASP:OD2	59:DZ:437:THR:OG1	2.26	0.53
1:AA:602:G:H2'	1:AA:603:C:C6	2.44	0.53
3:AC:42:VAL:HG13	3:AC:43:GLU:H	1.73	0.53
44:BK:44:SER:OG	44:BK:47:VAL:HG23	2.09	0.53
56:BW:43:C:H2'	56:BW:44:G:C8	2.44	0.53
1:CA:958:U:OP2	14:CQ:14:ARG:NH1	2.42	0.53
3:CC:65:LEU:HD22	3:CC:189:ASN:HB3	1.91	0.53
7:CG:79:ASN:OD1	7:CG:79:ASN:N	2.40	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:CV:1:MET:HE3	19:CV:44:LYS:H	1.74	0.53
34:DA:972:C:O2'	43:DJ:55:LYS:O	2.27	0.53
36:DC:152:ILE:HB	36:DC:167:TRP:HB3	1.90	0.53
43:DJ:78:ASN:O	43:DJ:80:LYS:N	2.41	0.53
59:DZ:168:ILE:HG12	59:DZ:205:TYR:CE2	2.44	0.53
1:AA:1495:G:O2'	1:AA:1575:A:N1	2.41	0.53
1:AA:2204:G:H2'	1:AA:2205:C:C6	2.44	0.53
3:AC:65:LEU:HD22	3:AC:189:ASN:HB3	1.91	0.53
6:AF:123:LEU:HD13	6:AF:192:LEU:HD13	1.90	0.53
34:BA:67:C:H2'	34:BA:68:G:C8	2.44	0.53
34:BA:452:A:H62	34:BA:480:U:H3	1.56	0.53
35:BB:175:ARG:O	35:BB:179:LYS:N	2.36	0.53
37:BD:57:ARG:HE	37:BD:202:LEU:HD22	1.74	0.53
59:BZ:264:LEU:HB2	64:BZ:702:GDP:C5	2.43	0.53
1:CA:673:C:H5"	6:CF:81:PRO:HD2	1.91	0.53
6:CF:165:ARG:HG2	6:CF:168:ARG:HH21	1.74	0.53
22:CY:77:PRO:HD3	22:CY:106:LEU:HD23	1.90	0.53
28:A4:63:TYR:CD1	28:A4:63:TYR:N	2.77	0.52
34:BA:1458:G:H5"	53:BT:31:SER:HB2	1.91	0.52
35:BB:231:GLU:HB3	35:BB:232:PRO:HD3	1.90	0.52
42:BI:50:LEU:HB2	42:BI:81:ILE:HD11	1.89	0.52
53:BT:9:ASN:O	53:BT:10:LEU:HB2	2.08	0.52
59:BZ:682:GLN:O	59:BZ:686:LYS:HB3	2.09	0.52
1:CA:1144:G:H2'	1:CA:1145:C:C6	2.44	0.52
1:CA:2287:A:N6	1:CA:2344:U:H3	2.02	0.52
1:CA:2291:U:H2'	1:CA:2292:C:C6	2.44	0.52
3:CC:52:PRO:HG2	3:CC:53:ARG:H	1.73	0.52
5:CE:116:VAL:HG13	5:CE:122:PHE:HB2	1.90	0.52
6:CF:24:LEU:HD21	6:CF:114:VAL:HG12	1.90	0.52
34:DA:201:C:H42	34:DA:216:G:H1	1.57	0.52
40:DG:54:THR:O	40:DG:56:GLN:N	2.41	0.52
53:DT:57:ARG:HH12	53:DT:100:ILE:HD12	1.74	0.52
34:BA:976:G:N2	34:BA:1363:C:OP2	2.36	0.52
3:CC:51:ASP:OD2	3:CC:54:ARG:HB2	2.09	0.52
3:CC:171:ALA:HB1	3:CC:173:HIS:CE1	2.43	0.52
30:C6:23:THR:OG1	30:C6:24:GLU:N	2.34	0.52
34:DA:1062:U:H2'	34:DA:1063:C:C5	2.45	0.52
34:DA:1435:G:H2'	34:DA:1436:U:C6	2.44	0.52
45:DL:28:LYS:N	45:DL:29:GLY:HA2	2.24	0.52
58:DY:55:PSU:HN1	58:DY:57:G:H5'	1.75	0.52
1:AA:1157:A:O2'	1:AA:1158:G:H4'	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:2638:C:H2'	1:AA:2639:G:O4'	2.08	0.52
23:AZ:151:HIS:O	23:AZ:153:SER:N	2.35	0.52
34:BA:8:A:N6	37:BD:205:GLU:O	2.43	0.52
34:BA:1125:U:H4'	43:BJ:5:ARG:HH22	1.74	0.52
1:CA:1057:A:HO2'	1:CA:1058:G:P	2.32	0.52
1:CA:1068:G:H21	1:CA:1096:A:H5'	1.74	0.52
1:CA:1721:G:H8	1:CA:1741:A:H62	1.55	0.52
2:CB:46:A:H2'	2:CB:47:C:C6	2.44	0.52
24:C0:70:GLN:NE2	24:C0:72:ARG:HD2	2.24	0.52
33:C9:17:ILE:HG22	33:C9:24:TYR:HB2	1.92	0.52
34:DA:620:C:H2'	34:DA:621:A:O4'	2.10	0.52
46:DM:3:ARG:NH1	46:DM:3:ARG:O	2.42	0.52
1:AA:470:C:H4'	6:AF:49:ALA:HB2	1.91	0.52
1:AA:1525:G:O2'	1:AA:1605:A:C2	2.62	0.52
1:AA:1921:G:H2'	1:AA:1921:G:N3	2.25	0.52
3:AC:48:LEU:CB	3:AC:50:ILE:HD12	2.38	0.52
25:A1:15:ALA:HB3	25:A1:40:ARG:HD3	1.91	0.52
36:BC:11:ARG:NH2	36:BC:177:THR:O	2.41	0.52
43:BJ:17:ASP:OD1	43:BJ:70:ARG:NH1	2.43	0.52
59:BZ:428:LEU:O	59:BZ:432:ALA:N	2.42	0.52
1:CA:335:C:H4'	22:CY:73:ARG:CZ	2.40	0.52
1:CA:1237:A:OP1	65:CA:3726:HOH:O	2.19	0.52
1:CA:1453:U:O2'	1:CA:1455:G:N7	2.40	0.52
1:CA:1815:A:OP2	4:CD:54:ARG:NH2	2.40	0.52
14:CQ:32:TYR:CE1	14:CQ:133:ARG:HD3	2.45	0.52
1:AA:939:C:H2'	1:AA:940:C:C6	2.44	0.52
1:AA:1648:U:O4	65:AA:3914:HOH:O	2.10	0.52
3:AC:51:ASP:OD2	3:AC:54:ARG:HB2	2.09	0.52
4:AD:101:GLU:OE1	4:AD:103:ARG:HD3	2.10	0.52
34:BA:1165:C:H2'	34:BA:1166:G:O4'	2.08	0.52
36:BC:77:ILE:O	36:BC:84:ILE:N	2.34	0.52
40:BG:113:GLU:HG2	40:BG:119:ARG:HG2	1.92	0.52
59:BZ:405:PRO:HB2	59:BZ:406:GLU:HA	1.92	0.52
1:CA:607:U:OP1	6:CF:102:PRO:HA	2.10	0.52
1:CA:811:U:H2'	13:CP:21:ARG:HA	1.91	0.52
1:CA:2695:C:H2'	1:CA:2696:U:H6	1.75	0.52
3:CC:67:HIS:CG	3:CC:185:LYS:HD2	2.45	0.52
9:CK:74:LEU:O	9:CK:76:GLY:N	2.40	0.52
19:CV:40:LEU:HB2	19:CV:46:VAL:HG13	1.91	0.52
21:CX:11:PRO:HB3	21:CX:92:LEU:HD11	1.91	0.52
34:DA:921:U:O2	38:DE:19:MET:HB2	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:DB:97:TRP:CZ3	35:DB:101:MET:HB2	2.45	0.52
52:DS:27:GLU:HB2	52:DS:28:LYS:HZ2	1.75	0.52
1:AA:11:G:H2'	1:AA:12:U:H5"	1.91	0.52
1:AA:2343:G:H4'	24:A0:43:THR:H	1.74	0.52
4:AD:17:THR:O	4:AD:211:ARG:NH2	2.40	0.52
34:BA:186:C:H2'	34:BA:187:C:C6	2.45	0.52
35:BB:197:VAL:HG12	35:BB:200:ILE:HD13	1.90	0.52
36:BC:58:GLU:H	36:BC:65:ALA:HB3	1.75	0.52
49:BP:18:ARG:O	49:BP:20:VAL:HB	2.09	0.52
59:BZ:156:ARG:NH1	59:BZ:156:ARG:HB3	2.25	0.52
1:CA:491:G:H2'	1:CA:492:A:C8	2.44	0.52
2:CB:105:A:H2'	2:CB:106:G:O4'	2.08	0.52
6:CF:21:ALA:HB3	6:CF:22:ALA:HA	1.92	0.52
9:CK:40:LEU:HA	9:CK:43:ALA:HB3	1.91	0.52
16:CS:27:SER:HA	16:CS:88:ASP:HB3	1.92	0.52
34:DA:1012:U:H2'	34:DA:1013:G:C8	2.44	0.52
34:DA:1317:C:OP1	47:DN:17:LYS:HG2	2.09	0.52
37:DD:189:PRO:HB2	37:DD:194:LEU:HD11	1.92	0.52
38:DE:139:LEU:O	38:DE:141:GLN:N	2.42	0.52
38:DE:152:ARG:HG3	41:DH:43:GLY:O	2.09	0.52
59:DZ:165:GLN:NE2	59:DZ:260:LEU:H	2.04	0.52
59:DZ:592:GLU:HA	59:DZ:595:GLN:HB3	1.92	0.52
34:BA:527:G:O2'	34:BA:535:A:N1	2.39	0.52
34:BA:1399:C:C2	34:BA:1502:A:N6	2.77	0.52
36:BC:22:TRP:CE2	47:BN:54:PRO:HG3	2.45	0.52
49:BP:3:LYS:O	49:BP:21:VAL:HA	2.09	0.52
1:CA:1059:G:H3'	1:CA:1060:U:C6	2.45	0.52
34:DA:859:A:H2'	34:DA:860:A:O4'	2.09	0.52
35:DB:178:ARG:NH1	35:DB:196:LEU:O	2.42	0.52
36:DC:7:PRO:HG3	36:DC:201:TYR:HE2	1.75	0.52
45:DL:69:TYR:HB2	45:DL:96:VAL:HG11	1.91	0.52
46:DM:84:ILE:O	46:DM:86:CYS:N	2.40	0.52
49:DP:23:ASP:OD1	49:DP:25:ARG:HD3	2.10	0.52
1:AA:1221:G:H1'	1:AA:1222:A:C5'	2.39	0.52
1:AA:1834:A:O2'	4:AD:259:THR:HG21	2.09	0.52
1:AA:2734:A:H5"	65:AA:4178:HOH:O	2.10	0.52
34:BA:418:C:H1'	34:BA:540:G:O2'	2.09	0.52
34:BA:600:C:H2'	34:BA:601:C:H6	1.73	0.52
40:BG:46:ALA:O	40:BG:50:ILE:HG23	2.10	0.52
1:CA:1028:A:N6	1:CA:1125:G:H2'	2.25	0.52
2:CB:20:C:H42	2:CB:63:G:H1	1.57	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:CC:64:SER:HA	3:CC:161:ARG:H	1.74	0.52
7:CG:43:LEU:HD12	7:CG:45:GLU:HG3	1.92	0.52
8:CH:12:PRO:O	8:CH:15:VAL:HG12	2.09	0.52
14:CQ:16:ARG:HG2	14:CQ:16:ARG:NH1	2.24	0.52
17:CT:19:LEU:HD13	17:CT:86:ILE:HD12	1.90	0.52
20:CW:59:VAL:HG12	20:CW:60:ASN:HD22	1.75	0.52
31:C7:30:VAL:O	31:C7:34:ARG:HG3	2.10	0.52
34:DA:539:A:H2'	34:DA:540:G:H8	1.75	0.52
34:DA:1008:C:H2'	34:DA:1009:G:O4'	2.10	0.52
44:DK:48:ILE:O	44:DK:50:TYR:N	2.43	0.52
1:AA:2331:G:N2	16:AS:3:ARG:HA	2.25	0.52
1:AA:2643:G:O2'	1:AA:2820:A:N1	2.32	0.52
34:BA:1068:G:H8	34:BA:1068:G:OP2	1.92	0.52
34:BA:1106:G:C6	34:BA:1107:C:C4	2.98	0.52
35:BB:77:ALA:O	35:BB:81:VAL:HG22	2.10	0.52
37:BD:190:ASP:OD1	37:BD:190:ASP:N	2.42	0.52
59:BZ:399:LEU:C	59:BZ:401:SER:H	2.17	0.52
1:CA:1815:A:H8	1:CA:1815:A:OP1	1.92	0.52
1:CA:1932:A:H2'	1:CA:1933:G:O4'	2.10	0.52
1:CA:2871:C:N4	65:CA:3811:HOH:O	2.42	0.52
6:CF:184:TYR:CE2	6:CF:188:ARG:HD2	2.45	0.52
18:CU:81:HIS:HB3	18:CU:117:GLN:HE22	1.73	0.52
25:C1:8:SER:HB3	25:C1:66:HIS:CD2	2.45	0.52
34:DA:278:G:OP2	50:DQ:41:LYS:NZ	2.43	0.52
36:DC:18:TRP:CD1	47:DN:54:PRO:HA	2.45	0.52
38:DE:11:ILE:HG21	38:DE:105:VAL:HG22	1.92	0.52
6:AF:129:PHE:HB3	6:AF:132:VAL:HG13	1.92	0.52
30:A6:40:CYS:SG	30:A6:42:TRP:HB2	2.50	0.52
34:BA:368:U:N3	59:BZ:354:ARG:NH1	2.58	0.52
39:BF:60:PHE:CE2	51:BR:78:LEU:HD21	2.45	0.52
1:CA:1110:G:H2'	1:CA:1110:G:N3	2.25	0.52
1:CA:2275:C:H5'	1:CA:2275:C:H6	1.74	0.52
7:CG:23:PHE:HB2	7:CG:25:TYR:CZ	2.44	0.52
8:CH:96:ALA:HB2	8:CH:105:LEU:HD23	1.92	0.52
14:CQ:85:LYS:HB2	24:C0:7:LEU:HD12	1.91	0.52
34:DA:539:A:H2'	34:DA:540:G:C8	2.45	0.52
34:DA:1352:C:H2'	34:DA:1353:G:C8	2.45	0.52
38:DE:110:LEU:HD13	38:DE:118:ILE:HG21	1.92	0.52
1:AA:1882:U:H2'	1:AA:1883:C:O4'	2.10	0.51
3:AC:67:HIS:CG	3:AC:185:LYS:HD2	2.45	0.51
41:BH:87:SER:HB2	41:BH:93:VAL:H	1.75	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:BZ:2:LYS:O	59:BZ:6:GLU:N	2.42	0.51
59:BZ:78:ARG:HH21	59:BZ:357:ARG:CZ	2.23	0.51
59:BZ:494:GLU:HG2	59:BZ:511:LYS:HG2	1.91	0.51
1:CA:65:C:H2'	1:CA:66:C:C6	2.45	0.51
1:CA:1101:U:H2'	1:CA:1102:C:C6	2.45	0.51
1:CA:1340:U:OP1	21:CX:16:LYS:NZ	2.43	0.51
1:CA:2173:A:C2	3:CC:219:MET:HE1	2.45	0.51
7:CG:44:GLY:O	7:CG:47:LYS:HB2	2.10	0.51
34:DA:130:A:O2'	34:DA:131:C:O5'	2.23	0.51
34:DA:1316:G:N2	34:DA:1319:A:H5"	2.25	0.51
35:DB:122:PHE:HA	35:DB:127:ILE:HD12	1.92	0.51
57:DX:75:C:H5"	57:DX:76:31H:P	2.49	0.51
59:DZ:238:THR:O	59:DZ:241:GLU:HG2	2.10	0.51
1:AA:1091:A:H4'	1:AA:1092:A:H5'	1.93	0.51
1:AA:2304:C:P	16:AS:17:ARG:HH12	2.33	0.51
4:AD:3:VAL:HG13	4:AD:17:THR:HB	1.92	0.51
18:AU:104:GLN:CD	18:AU:104:GLN:H	2.16	0.51
30:A6:18:ARG:HD2	30:A6:42:TRP:CD1	2.45	0.51
34:BA:10:A:OP2	38:BE:126:ARG:HD2	2.09	0.51
34:BA:767:A:H2'	34:BA:768:A:O4'	2.11	0.51
50:BQ:12:SER:HB3	50:BQ:20:THR:HB	1.91	0.51
50:BQ:67:LYS:O	50:BQ:68:ARG:HG2	2.10	0.51
59:BZ:114:VAL:HG11	59:BZ:156:ARG:HH12	1.75	0.51
59:BZ:247:ARG:HG3	59:BZ:247:ARG:HH11	1.75	0.51
1:CA:1359:A:N1	1:CA:1372:U:C4	2.78	0.51
3:CC:218:THR:HG22	3:CC:219:MET:SD	2.50	0.51
13:CP:37:GLY:C	13:CP:38:GLN:O	2.49	0.51
1:AA:2564:U:C2	1:AA:2566:U:H5'	2.45	0.51
2:AB:77:U:H4'	23:AZ:84:GLU:OE2	2.10	0.51
5:AE:59:VAL:HG12	5:AE:64:LYS:HG3	1.91	0.51
26:A2:32:LEU:HD11	26:A2:54:LYS:HG3	1.93	0.51
34:BA:882:C:O2'	34:BA:883:C:H5'	2.11	0.51
34:BA:1305:G:H5"	54:BU:4:GLY:HA3	1.93	0.51
3:CC:65:LEU:HB3	3:CC:189:ASN:HD22	1.75	0.51
4:CD:71:ASP:HB3	4:CD:103:ARG:HH22	1.75	0.51
20:CW:41:LYS:HE3	29:C5:25:LEU:HD21	1.91	0.51
34:DA:437:U:O2'	37:DD:123:HIS:HD2	1.94	0.51
34:DA:1004:A:H8	34:DA:1005:A:H4'	1.75	0.51
34:DA:1227:A:OP1	52:DS:80:TYR:OH	2.23	0.51
46:DM:84:ILE:HB	52:DS:66:MET:HE2	1.92	0.51
1:AA:1072:U:H4'	1:AA:1073:A:OP1	2.09	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:2123:G:H1	1:AA:2210:C:H42	1.58	0.51
1:AA:2149:G:H21	1:AA:2195:A:H1'	1.76	0.51
34:BA:976:G:OP1	47:BN:32:SER:N	2.44	0.51
34:BA:1353:G:OP1	54:BU:10:ARG:NH1	2.43	0.51
39:BF:1:MET:HA	39:BF:67:MET:O	2.10	0.51
43:BJ:8:LEU:HB2	43:BJ:70:ARG:HB2	1.92	0.51
1:CA:208:C:H2'	1:CA:209:C:H6	1.74	0.51
1:CA:1796:U:H2'	1:CA:1797:C:C6	2.45	0.51
1:CA:2312:U:H5'	7:CG:88:ILE:HD11	1.92	0.51
15:CR:37:THR:OG1	15:CR:40:LYS:HG3	2.09	0.51
21:CX:12:VAL:HG22	21:CX:29:TRP:CE2	2.45	0.51
34:DA:392:G:H2'	34:DA:393:A:H8	1.76	0.51
34:DA:1305:G:H22	34:DA:1331:G:H1'	1.74	0.51
35:DB:9:GLU:O	35:DB:11:LEU:N	2.44	0.51
36:DC:125:GLU:N	36:DC:125:GLU:OE2	2.43	0.51
36:DC:140:ARG:HH12	36:DC:141:VAL:HG23	1.76	0.51
40:DG:151:TYR:OH	44:DK:54:ARG:HD2	2.11	0.51
53:DT:39:LYS:O	53:DT:42:GLN:N	2.42	0.51
1:AA:509:A:O4'	22:AY:48:ALA:HB1	2.10	0.51
2:AB:105:A:OP1	23:AZ:72:ARG:NH1	2.44	0.51
3:AC:65:LEU:HB3	3:AC:189:ASN:HD22	1.74	0.51
3:AC:218:THR:HG22	3:AC:219:MET:SD	2.50	0.51
13:AP:89:ALA:HA	13:AP:121:LYS:HE2	1.92	0.51
17:AT:119:LYS:O	17:AT:123:GLN:HG3	2.10	0.51
34:BA:45:U:H2'	34:BA:46:G:C8	2.46	0.51
34:BA:103:C:OP2	53:BT:17:ARG:NH2	2.43	0.51
34:BA:1379:G:O6	40:BG:2:ALA:HB3	2.10	0.51
1:CA:323:G:C8	6:CF:171:PRO:HG3	2.46	0.51
1:CA:2784:C:H1'	5:CE:37:ARG:HH12	1.75	0.51
4:CD:69:ARG:NH2	4:CD:128:GLY:O	2.43	0.51
4:CD:77:ALA:HB2	4:CD:97:TYR:CD2	2.44	0.51
34:DA:1152:A:H2'	34:DA:1153:C:H6	1.76	0.51
34:DA:1178:G:N2	34:DA:1181:G:OP2	2.42	0.51
38:DE:33:VAL:HG13	38:DE:112:LEU:HD12	1.92	0.51
41:DH:4:ASP:OD2	41:DH:85:ARG:NH1	2.44	0.51
49:DP:28:ARG:NH1	49:DP:29:ASP:OD2	2.43	0.51
52:DS:63:THR:OG1	52:DS:64:GLU:N	2.35	0.51
57:DX:2:G:N3	57:DX:2:G:H2'	2.25	0.51
59:DZ:264:LEU:HD12	64:DZ:702:GDP:N3	2.25	0.51
1:AA:1476:C:H2'	1:AA:1477:U:C6	2.46	0.51
3:AC:6:LYS:N	3:AC:9:ARG:NH1	2.58	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:50:ILE:H	3:AC:50:ILE:HD13	1.76	0.51
9:AK:56:ASN:HA	9:AK:83:TYR:HA	1.93	0.51
10:AL:98:ARG:HA	10:AL:136:VAL:HG23	1.91	0.51
38:BE:135:THR:O	38:BE:139:LEU:HG	2.11	0.51
59:BZ:145:ASP:HB3	59:BZ:148:LEU:HD23	1.92	0.51
1:CA:1102:C:H2'	1:CA:1103:A:C8	2.45	0.51
1:CA:1653:G:H3'	15:CR:2:ARG:HD3	1.93	0.51
8:CH:143:GLN:O	8:CH:145:ALA:N	2.43	0.51
11:CN:94:HIS:O	11:CN:97:ARG:HB2	2.11	0.51
22:CY:99:CYS:SG	22:CY:100:ALA:N	2.84	0.51
34:DA:280:C:OP1	50:DQ:91:ARG:NH1	2.43	0.51
34:DA:828:A:H2'	34:DA:829:G:O4'	2.11	0.51
51:DR:32:ARG:HD2	51:DR:65:ILE:HG21	1.92	0.51
1:AA:95:G:OP1	26:A2:46:GLN:NE2	2.39	0.51
3:AC:68:GLY:H	3:AC:189:ASN:ND2	2.09	0.51
4:AD:2:ALA:N	4:AD:20:ASP:OD2	2.44	0.51
59:BZ:78:ARG:HE	59:BZ:357:ARG:NH1	2.08	0.51
59:BZ:485:GLU:HB3	59:BZ:560:VAL:HG22	1.93	0.51
1:CA:221:A:O2'	1:CA:266:G:N7	2.42	0.51
1:CA:236:C:H2'	1:CA:237:C:C6	2.44	0.51
1:CA:297:C:OP1	22:CY:95:LYS:NZ	2.43	0.51
1:CA:863:A:H2'	1:CA:864:G:C8	2.46	0.51
1:CA:2572:A:N7	5:CE:144:ARG:HD2	2.26	0.51
1:CA:2880:C:O3'	15:CR:90:ARG:NH1	2.43	0.51
2:CB:7:G:H4'	16:CS:29:PHE:CD2	2.46	0.51
3:CC:50:ILE:H	3:CC:50:ILE:HD13	1.76	0.51
8:CH:86:GLU:OE2	8:CH:132:ARG:NH2	2.43	0.51
16:CS:88:ASP:C	16:CS:90:GLY:H	2.19	0.51
34:DA:1401:G:C2	34:DA:1402:C:H1'	2.46	0.51
1:AA:1387:U:O2	21:AX:80:ILE:HD12	2.10	0.51
1:AA:1496:A:H5'	1:AA:1497:G:OP2	2.11	0.51
8:AH:89:ILE:CD1	8:AH:96:ALA:HB2	2.41	0.51
34:BA:17:U:H2'	34:BA:18:C:C6	2.46	0.51
36:BC:52:LEU:HD23	36:BC:53:ALA:N	2.25	0.51
39:BF:8:ILE:HD13	39:BF:26:ILE:HD13	1.93	0.51
59:BZ:417:THR:HA	59:BZ:418:LYS:HG2	1.93	0.51
1:CA:706:A:OP1	4:CD:7:LYS:NZ	2.42	0.51
1:CA:1448:G:H4'	1:CA:1542:A:OP1	2.11	0.51
1:CA:2638:G:P	5:CE:82:ARG:NH2	2.84	0.51
1:CA:2815:C:H2'	1:CA:2816:C:H6	1.75	0.51
3:CC:6:LYS:N	3:CC:9:ARG:NH1	2.59	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:CD:275:LYS:HA	4:CD:276:LYS:C	2.36	0.51
21:CX:36:LYS:HA	21:CX:39:ILE:HD12	1.93	0.51
37:DD:150:GLU:O	37:DD:153:ARG:HG2	2.10	0.51
45:DL:24:VAL:HG13	45:DL:98:TYR:CE1	2.46	0.51
53:DT:63:ILE:HD13	53:DT:80:ARG:HB3	1.93	0.51
59:DZ:373:ASP:OD2	59:DZ:374:LEU:N	2.44	0.51
59:DZ:539:ILE:O	59:DZ:542:VAL:HG12	2.11	0.51
1:AA:212:A:O2'	1:AA:447:C:O2	2.28	0.51
1:AA:1040:C:OP1	18:AU:53:ARG:NH2	2.44	0.51
11:AN:30:ILE:HG22	11:AN:34:LEU:HD22	1.93	0.51
16:AS:58:LEU:HD22	16:AS:59:LYS:HG3	1.92	0.51
34:BA:523:A:H61	45:BL:92:ASP:HB2	1.75	0.51
34:BA:976:G:H5'	34:BA:1358:U:O2'	2.11	0.51
49:BP:20:VAL:HG21	49:BP:32:TYR:CD2	2.46	0.51
1:CA:1247:A:OP1	6:CF:95:ARG:NH2	2.43	0.51
1:CA:1547:C:H2'	1:CA:1548:C:C6	2.43	0.51
1:CA:1786:A:H1'	1:CA:1938:A:N6	2.25	0.51
1:CA:1877:A:H5'	1:CA:1878:G:OP2	2.11	0.51
1:CA:2836:U:H2'	1:CA:2837:G:C8	2.45	0.51
3:CC:54:ARG:HD2	3:CC:55:SER:H	1.76	0.51
4:CD:10:THR:OG1	4:CD:13:ARG:HB2	2.10	0.51
7:CG:18:GLU:HG2	7:CG:175:LEU:HD21	1.93	0.51
13:CP:39:LYS:HD2	13:CP:45:LEU:HD11	1.93	0.51
34:DA:979:C:H42	47:DN:18:VAL:HB	1.76	0.51
34:DA:1166:G:H5'	34:DA:1168:A:OP2	2.11	0.51
39:DF:87:ARG:HH11	39:DF:87:ARG:CG	2.20	0.51
59:DZ:129:LYS:NZ	59:DZ:517:LEU:HG	2.26	0.51
59:DZ:169:GLY:N	59:DZ:170:ARG:HH12	2.09	0.51
1:AA:553:A:C2'	1:AA:554:A:H5'	2.41	0.51
1:AA:1289:G:O2'	13:AP:7:ARG:NH2	2.43	0.51
1:AA:2434:A:O4'	58:BY:76:A:N6	2.44	0.51
6:AF:53:THR:CG2	6:AF:55:GLY:H	2.24	0.51
15:AR:33:ARG:HD2	15:AR:113:LEU:HD13	1.91	0.51
34:BA:8:A:N6	37:BD:209:ARG:HB2	2.26	0.51
34:BA:134:A:H61	49:BP:25:ARG:HH12	1.58	0.51
34:BA:1278:U:H5'	34:BA:1279:A:O4'	2.11	0.51
37:BD:190:ASP:HB2	37:BD:193:ASP:HB2	1.93	0.51
1:CA:1429:G:H2'	1:CA:1430:C:C6	2.46	0.51
1:CA:1939:U:OP1	1:CA:2604:U:O2'	2.26	0.51
2:CB:31:C:C2'	2:CB:32:C:H5'	2.41	0.51
34:DA:427:U:H3'	34:DA:428:G:H2'	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:DA:892:A:O2'	34:DA:1415:G:H4'	2.11	0.51
35:DB:97:TRP:CH2	35:DB:101:MET:HB2	2.45	0.51
41:DH:28:ALA:HB3	41:DH:57:PRO:HB2	1.93	0.51
43:DJ:8:LEU:HD23	43:DJ:96:ILE:HG23	1.93	0.51
59:DZ:18:ALA:HB1	59:DZ:121:VAL:HG21	1.93	0.51
59:DZ:610:VAL:HG22	59:DZ:669:PHE:HB3	1.92	0.51
1:AA:553:A:H2	1:AA:2065:C:H5'	1.75	0.50
1:AA:597:C:N3	5:AE:145:LYS:NZ	2.53	0.50
1:AA:1686:U:O2'	1:AA:1687:C:H5'	2.11	0.50
3:AC:42:VAL:CG1	3:AC:43:GLU:N	2.73	0.50
18:AU:61:TRP:CH2	18:AU:93:LYS:HB2	2.46	0.50
20:AW:1:MET:HA	20:AW:1:MET:HE3	1.94	0.50
34:BA:114:U:O2'	34:BA:115:G:H5'	2.10	0.50
35:BB:160:ASP:N	35:BB:160:ASP:OD1	2.44	0.50
46:BM:60:VAL:HG13	46:BM:64:TRP:HZ3	1.76	0.50
59:BZ:177:ILE:HD12	59:BZ:188:TYR:CE2	2.46	0.50
1:CA:1778:U:H2'	1:CA:1784:A:N6	2.26	0.50
3:CC:42:VAL:CG1	3:CC:43:GLU:N	2.73	0.50
16:CS:31:SER:OG	16:CS:32:LEU:N	2.41	0.50
16:CS:66:ALA:O	16:CS:69:VAL:HG13	2.11	0.50
34:DA:1279:A:H5"	34:DA:1280:A:OP1	2.11	0.50
35:DB:84:GLU:HB3	35:DB:219:VAL:HG21	1.93	0.50
35:DB:96:ARG:O	35:DB:98:LEU:HD22	2.11	0.50
35:DB:229:VAL:HG12	35:DB:230:VAL:H	1.76	0.50
36:DC:28:GLN:O	36:DC:32:LEU:HD23	2.11	0.50
37:DD:117:ALA:O	37:DD:121:VAL:HG23	2.10	0.50
59:DZ:491:VAL:HG12	59:DZ:493:VAL:HG13	1.93	0.50
1:AA:484:G:O2'	1:AA:495:G:O6	2.24	0.50
1:AA:515:G:N7	20:AW:49:LYS:NZ	2.59	0.50
1:AA:1553:A:O2'	1:AA:1554:A:O4'	2.29	0.50
10:AL:108:ALA:O	10:AL:112:MET:HB3	2.11	0.50
11:AN:121:LYS:HB3	11:AN:123:TYR:CE2	2.47	0.50
23:AZ:70:LEU:HG	23:AZ:91:LEU:HD21	1.92	0.50
40:BG:66:VAL:HG12	40:BG:70:LYS:HE3	1.93	0.50
48:BO:35:ARG:CZ	48:BO:59:MET:HE2	2.41	0.50
59:BZ:75:LYS:H	59:BZ:75:LYS:HZ3	1.59	0.50
59:BZ:76:ASP:OD2	59:BZ:76:ASP:N	2.42	0.50
1:CA:176:G:O2'	1:CA:177:G:H5'	2.11	0.50
1:CA:1204:A:H2	1:CA:1241:A:N6	1.97	0.50
1:CA:2061:G:OP2	65:CA:3728:HOH:O	2.19	0.50
7:CG:98:ARG:HA	7:CG:101:ILE:HD12	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:CQ:109:VAL:HG22	14:CQ:113:GLN:OE1	2.11	0.50
34:DA:23:C:OP2	34:DA:561:U:N3	2.34	0.50
34:DA:559:A:OP1	38:DE:126:ARG:NH2	2.44	0.50
34:DA:1118:C:H1'	34:DA:1179:A:C4	2.46	0.50
59:DZ:169:GLY:O	59:DZ:173:THR:OG1	2.28	0.50
59:DZ:302:HIS:CD2	59:DZ:303:PRO:HD2	2.45	0.50
1:AA:943:C:H4'	56:BW:55:PSU:O3'	2.11	0.50
3:AC:54:ARG:HD2	3:AC:55:SER:H	1.76	0.50
3:AC:57:GLN:HB2	3:AC:202:PRO:HG2	1.93	0.50
23:AZ:111:VAL:HG12	23:AZ:112:ARG:H	1.77	0.50
59:BZ:329:ARG:HD2	59:BZ:331:TYR:CE1	2.47	0.50
1:CA:34:C:O2	1:CA:34:C:H2'	2.10	0.50
1:CA:86:C:OP1	22:CY:32:PRO:HG2	2.11	0.50
1:CA:1044:G:H21	1:CA:1111:A:H2	1.59	0.50
1:CA:1052:C:N4	1:CA:1053:C:H41	2.09	0.50
1:CA:1288:U:O4	15:CR:106:GLY:HA3	2.12	0.50
1:CA:2567:G:H2'	1:CA:2568:C:C6	2.47	0.50
1:CA:2805:G:H2'	1:CA:2807:G:H8	1.74	0.50
3:CC:44:VAL:HG21	3:CC:176:VAL:HG21	1.92	0.50
5:CE:9:VAL:HG13	5:CE:25:VAL:O	2.11	0.50
34:DA:665:A:H1'	34:DA:733:A:O4'	2.11	0.50
34:DA:1346:A:H5"	42:DI:120:ARG:HH12	1.76	0.50
35:DB:178:ARG:HH22	41:DH:68:ARG:NH2	2.05	0.50
40:DG:111:ARG:NH1	40:DG:113:GLU:OE1	2.44	0.50
42:DI:88:TYR:CD2	42:DI:89:ASN:HB2	2.46	0.50
50:DQ:65:ILE:HB	50:DQ:69:LYS:HB3	1.93	0.50
59:DZ:629:GLY:HA3	59:DZ:647:VAL:HG12	1.93	0.50
1:AA:1211:U:H2'	1:AA:1212:C:C6	2.46	0.50
1:AA:1410:G:P	25:A1:3:LYS:HG3	2.51	0.50
1:AA:2860:A:OP2	1:AA:2876:U:H5	1.93	0.50
5:AE:5:LEU:HD12	5:AE:51:PHE:HB2	1.92	0.50
28:A4:59:PHE:HB3	52:BS:67:VAL:HG11	1.94	0.50
32:A8:62:LEU:HB3	32:A8:65:GLU:HG2	1.93	0.50
34:BA:200:G:H1	34:BA:217:C:N4	2.10	0.50
34:BA:353:A:H5'	34:BA:353:A:C8	2.42	0.50
34:BA:955:U:O2'	52:BS:83:HIS:HD2	1.94	0.50
34:BA:1179:A:H2'	34:BA:1180:A:O4'	2.12	0.50
1:CA:11:G:H2'	1:CA:12:U:H5"	1.93	0.50
1:CA:1371:G:H2'	1:CA:1372:U:H5	1.77	0.50
1:CA:1482:G:H2'	1:CA:1484:G:H8	1.76	0.50
1:CA:1798:U:H5'	4:CD:259:THR:CG2	2.24	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:2031:A:C6	1:CA:2498:C:H1'	2.47	0.50
3:CC:68:GLY:H	3:CC:189:ASN:ND2	2.08	0.50
15:CR:1:MET:HE3	15:CR:3:HIS:CE1	2.46	0.50
19:CV:24:LYS:HA	19:CV:92:THR:OG1	2.11	0.50
21:CX:25:LYS:HA	21:CX:81:VAL:O	2.12	0.50
25:C1:89:GLU:O	25:C1:93:GLU:HG2	2.11	0.50
34:DA:1070:U:H2'	34:DA:1071:C:H6	1.75	0.50
34:DA:1412:C:H2'	34:DA:1413:A:C8	2.47	0.50
36:DC:113:ALA:O	36:DC:116:VAL:N	2.44	0.50
48:DO:15:PHE:CZ	48:DO:85:LEU:HD21	2.47	0.50
59:DZ:154:GLN:O	59:DZ:158:GLY:HA2	2.12	0.50
1:AA:721:G:H1'	6:AF:74:ARG:HD3	1.92	0.50
1:AA:2843:G:H8	1:AA:2843:G:OP1	1.95	0.50
12:AO:48:PRO:HB3	34:BA:1422:G:H5'	1.94	0.50
34:BA:1511:G:H2'	34:BA:1512:U:O4'	2.10	0.50
35:BB:153:ARG:NH1	35:BB:153:ARG:HB3	2.26	0.50
38:BE:51:VAL:O	38:BE:55:VAL:HG23	2.11	0.50
44:BK:41:THR:OG1	44:BK:42:TRP:N	2.43	0.50
48:BO:81:LEU:O	48:BO:85:LEU:HB2	2.11	0.50
59:BZ:21:ILE:HD13	59:BZ:21:ILE:N	2.25	0.50
59:BZ:554:PRO:HG3	59:BZ:594:VAL:HG12	1.93	0.50
1:CA:81:G:HO2'	1:CA:295:G:HO2'	1.55	0.50
1:CA:298:G:H5"	1:CA:299:A:OP1	2.10	0.50
1:CA:733:G:OP2	65:CA:3729:HOH:O	2.20	0.50
1:CA:987:G:O2'	1:CA:1000:A:N3	2.41	0.50
1:CA:2113:U:H3	1:CA:2170:A:H61	1.59	0.50
1:CA:2126:A:N6	1:CA:2172:U:H5'	2.27	0.50
1:CA:2572:A:N7	5:CE:145:LYS:HB2	2.27	0.50
1:CA:2876:G:H4'	17:CT:2:ASN:ND2	2.26	0.50
3:CC:191:ARG:O	3:CC:195:ARG:HG2	2.11	0.50
13:CP:111:ARG:HD3	13:CP:128:HIS:CD2	2.47	0.50
34:DA:728:A:N7	48:DO:54:ARG:HD2	2.26	0.50
34:DA:1095:U:P	34:DA:1108:G:H1	2.35	0.50
34:DA:1509:C:H2'	34:DA:1510:U:O4'	2.12	0.50
50:DQ:48:GLU:OE2	50:DQ:50:LYS:HE3	2.12	0.50
1:AA:2574:U:O2'	12:AO:23:ARG:HD3	2.11	0.50
4:AD:155:LEU:HD23	4:AD:177:LEU:HD22	1.94	0.50
6:AF:64:ILE:HD12	6:AF:65:TRP:CD2	2.47	0.50
34:BA:52:G:H2'	34:BA:53:A:H8	1.75	0.50
34:BA:765:G:H5"	34:BA:766:A:OP1	2.12	0.50
38:BE:20:GLN:HG2	38:BE:25:ARG:HD2	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:1098:A:H2'	1:CA:1099:G:O4'	2.11	0.50
1:CA:2150:U:H2'	1:CA:2151:G:C8	2.47	0.50
3:CC:54:ARG:HH22	3:CC:56:ASP:HB3	1.75	0.50
3:CC:57:GLN:HB2	3:CC:202:PRO:HG2	1.93	0.50
23:CZ:96:VAL:N	23:CZ:128:VAL:O	2.44	0.50
1:AA:1284:G:OP2	65:AA:3929:HOH:O	2.19	0.50
1:AA:1846:A:O3'	65:AA:3928:HOH:O	2.18	0.50
1:AA:2287:C:O2	14:AQ:85:LYS:HG3	2.12	0.50
3:AC:44:VAL:HG21	3:AC:176:VAL:HG21	1.92	0.50
3:AC:191:ARG:O	3:AC:195:ARG:HG2	2.11	0.50
10:AL:99:ILE:O	10:AL:139:VAL:N	2.39	0.50
11:AN:5:VAL:HG23	11:AN:6:PRO:HD2	1.94	0.50
12:AO:1:MET:HE3	12:AO:32:TYR:CE1	2.46	0.50
34:BA:109:A:H2'	34:BA:326:G:N2	2.27	0.50
34:BA:1312:G:N7	52:BS:2:PRO:HD2	2.27	0.50
37:BD:134:ASP:O	37:BD:136:PRO:HD3	2.11	0.50
54:BU:3:LYS:HB3	54:BU:14:TRP:CG	2.47	0.50
59:BZ:517:LEU:HD13	59:BZ:564:LYS:HB2	1.94	0.50
1:CA:271(E):U:H2'	1:CA:271(F):C:C6	2.46	0.50
1:CA:2365:G:O6	32:C8:39:LYS:NZ	2.45	0.50
16:CS:12:PHE:O	16:CS:16:ASN:ND2	2.44	0.50
18:CU:79:PHE:CZ	18:CU:83:LEU:HD21	2.46	0.50
34:DA:17:U:H2'	34:DA:18:C:C6	2.47	0.50
34:DA:1152:A:H2'	34:DA:1153:C:C6	2.47	0.50
35:DB:102:LEU:HB3	35:DB:180:LEU:HD12	1.93	0.50
35:DB:142:LEU:HA	35:DB:145:LEU:HB2	1.94	0.50
36:DC:97:LYS:O	36:DC:99:VAL:N	2.45	0.50
59:DZ:127:LYS:HG3	59:DZ:520:GLY:HA3	1.93	0.50
1:AA:553:A:C8	1:AA:553:A:C3'	2.94	0.50
1:AA:1553:A:O2'	1:AA:1554:A:O5'	2.29	0.50
1:AA:2152:U:H1'	1:AA:2180:A:N1	2.27	0.50
7:AG:114:ILE:HA	7:AG:140:ILE:HD11	1.93	0.50
25:A1:80:LEU:HB3	25:A1:82:LEU:HG	1.93	0.50
34:BA:1255:G:C2	34:BA:1283:G:C2	3.00	0.50
34:BA:1260:C:OP1	34:BA:1284:C:O2'	2.24	0.50
34:BA:1436:U:OP1	53:BT:23:ARG:NH2	2.44	0.50
34:BA:1509:C:H2'	34:BA:1510:U:O4'	2.12	0.50
35:BB:16:HIS:C	35:BB:18:GLY:H	2.18	0.50
59:BZ:-62:LEU:HD11	59:BZ:-48:VAL:HG22	1.93	0.50
59:BZ:216:LEU:HD11	59:BZ:246:ILE:HD11	1.93	0.50
59:BZ:438:PHE:HB3	59:BZ:458:HIS:HE1	1.77	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:627:A:C6	1:CA:637:A:C8	3.00	0.50
1:CA:1070:A:H2'	1:CA:1097:U:OP1	2.11	0.50
1:CA:2131:G:N7	1:CA:2133:G:N2	2.59	0.50
1:CA:2506:U:O2	56:DW:76:F3N:HD2	2.11	0.50
9:CK:85:ASP:O	9:CK:87:VAL:N	2.45	0.50
23:CZ:69:THR:HG22	23:CZ:90:VAL:HA	1.94	0.50
34:DA:20:U:H2'	34:DA:21:G:O4'	2.12	0.50
34:DA:1203:C:H2'	34:DA:1204:A:C8	2.47	0.50
35:DB:16:HIS:CG	35:DB:17:PHE:N	2.80	0.50
38:DE:69:VAL:HG22	38:DE:71:LEU:HD13	1.94	0.50
48:DO:71:GLN:HB2	48:DO:78:TYR:CD2	2.47	0.50
51:DR:32:ARG:HA	51:DR:69:THR:HG21	1.93	0.50
1:AA:70:A:N7	21:AX:31:HIS:HE1	2.09	0.50
4:AD:79:VAL:HG12	4:AD:113:VAL:HA	1.94	0.50
10:AL:106:GLU:O	10:AL:109:LYS:HB2	2.12	0.50
34:BA:406:G:C2	34:BA:407:G:C8	3.00	0.50
34:BA:714:G:H2'	34:BA:715:A:C8	2.47	0.50
34:BA:1010:G:N2	34:BA:1020:U:H1'	2.26	0.50
55:BV:14:A:C6	58:BY:34:G:C6	3.00	0.50
1:CA:30:G:H2'	1:CA:31:C:C6	2.46	0.50
1:CA:1237:A:OP1	65:CA:3727:HOH:O	2.19	0.50
1:CA:1300:U:H4'	1:CA:1301:A:C5'	2.42	0.50
1:CA:2298:A:H2'	1:CA:2299:G:O4'	2.12	0.50
1:CA:2364:C:OP1	24:C0:55:ARG:HD3	2.11	0.50
3:CC:15:VAL:O	3:CC:21:TYR:OH	2.29	0.50
3:CC:203:GLU:CD	3:CC:203:GLU:N	2.70	0.50
5:CE:77:ILE:HD11	5:CE:79:ARG:NH1	2.27	0.50
29:C5:16:ARG:HD2	29:C5:20:ARG:NH1	2.27	0.50
34:DA:572:A:OP1	65:DA:1805:HOH:O	2.18	0.50
34:DA:1355:G:H2'	34:DA:1356:G:C8	2.46	0.50
35:DB:112:VAL:O	35:DB:116:GLU:HB3	2.12	0.50
53:DT:43:LEU:O	53:DT:47:GLY:N	2.45	0.50
1:AA:1387:U:O4'	21:AX:57:LEU:HD12	2.12	0.49
1:AA:2343:G:O2'	1:AA:2348:A:N1	2.41	0.49
1:AA:2518:U:C2	1:AA:2597:U:O4	2.65	0.49
2:AB:1:U:O2	2:AB:1:U:H2'	2.11	0.49
14:AQ:14:ARG:HG2	14:AQ:41:TRP:CH2	2.41	0.49
19:AV:14:VAL:HB	19:AV:96:ILE:HG13	1.93	0.49
34:BA:560:U:H5'	34:BA:566:G:N2	2.26	0.49
34:BA:645:C:H2'	34:BA:646:U:C6	2.46	0.49
12:CO:23:ARG:HG3	12:CO:24:VAL:N	2.27	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:CU:49:HIS:HA	18:CU:52:ARG:HB3	1.94	0.49
34:DA:583:A:H2'	34:DA:584:G:O4'	2.12	0.49
35:DB:54:THR:O	35:DB:58:ILE:HG13	2.12	0.49
36:DC:15:THR:HG21	36:DC:181:ASN:HA	1.94	0.49
59:DZ:225:GLU:CD	59:DZ:225:GLU:H	2.18	0.49
59:DZ:388:THR:HG21	59:DZ:397:VAL:O	2.12	0.49
59:DZ:526:VAL:HG23	59:DZ:566:THR:HA	1.94	0.49
1:AA:346:A:H5'	1:AA:364:A:H1'	1.93	0.49
1:AA:1249:A:N1	1:AA:1287:A:N7	2.59	0.49
2:AB:29:A:O2'	2:AB:58:A:N1	2.39	0.49
14:AQ:24:GLY:O	14:AQ:102:VAL:HG23	2.12	0.49
22:AY:54:LYS:H	22:AY:56:PRO:HG3	1.77	0.49
34:BA:129:U:H5'	50:BQ:3:LYS:NZ	2.27	0.49
34:BA:1228:C:P	46:BM:108:ARG:HH22	2.35	0.49
59:BZ:396:ARG:HH21	59:BZ:396:ARG:CG	2.23	0.49
1:CA:1026:U:H4'	1:CA:1027:A:OP1	2.11	0.49
1:CA:1637:A:H4'	1:CA:2711:A:O2'	2.11	0.49
1:CA:2600:A:H2'	1:CA:2601:C:C6	2.48	0.49
1:CA:2815:C:H2'	1:CA:2816:C:C6	2.47	0.49
4:CD:148:GLU:CB	4:CD:151:LYS:HD2	2.40	0.49
8:CH:75:ALA:O	8:CH:79:VAL:HG22	2.12	0.49
34:DA:1063:C:OP2	34:DA:1064:G:O2'	2.23	0.49
35:DB:150:SER:O	35:DB:153:ARG:HG2	2.12	0.49
43:DJ:47:PHE:HB2	43:DJ:63:PHE:HB2	1.93	0.49
56:DW:21:A:N6	56:DW:46:7MG:N3	2.60	0.49
59:DZ:36:THR:HB	59:DZ:72:CYS:HB2	1.93	0.49
1:AA:225:C:H2'	1:AA:226:C:C6	2.47	0.49
3:AC:191:ARG:O	3:AC:194:ILE:HG22	2.12	0.49
3:AC:203:GLU:CD	3:AC:203:GLU:N	2.70	0.49
13:AP:62:LEU:O	32:A8:13:ARG:HD3	2.11	0.49
17:AT:65:LYS:HE2	17:AT:67:SER:HB2	1.94	0.49
34:BA:129:U:H5'	50:BQ:3:LYS:HZ3	1.77	0.49
34:BA:539:A:H2'	34:BA:540:G:C8	2.47	0.49
35:BB:218:ALA:O	35:BB:222:ILE:HG13	2.13	0.49
38:BE:7:GLU:N	38:BE:35:GLY:O	2.45	0.49
53:BT:13:LEU:O	53:BT:17:ARG:HG3	2.12	0.49
1:CA:1188:U:H4'	19:CV:79:VAL:HG22	1.94	0.49
1:CA:1418:G:N7	65:CA:3779:HOH:O	2.35	0.49
1:CA:2116:G:H5'	1:CA:2117:A:OP2	2.11	0.49
12:CO:48:PRO:HB3	34:DA:1422:G:H5'	1.95	0.49
17:CT:83:ILE:HD13	17:CT:86:ILE:HD11	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:DA:1084:G:H5'	34:DA:1102:A:OP2	2.12	0.49
36:DC:131:ARG:NH1	38:DE:50:GLU:HG3	2.27	0.49
43:DJ:38:ILE:CG1	43:DJ:71:LEU:HB3	2.42	0.49
53:DT:40:ALA:HB2	53:DT:55:ILE:HG22	1.93	0.49
59:DZ:119:GLU:HB3	59:DZ:123:ARG:HH21	1.77	0.49
59:DZ:523:PHE:HB2	59:DZ:550:MET:HE1	1.94	0.49
1:AA:841:G:H2'	1:AA:842:C:C6	2.47	0.49
1:AA:1074:A:N6	1:AA:1171:G:H2'	2.27	0.49
1:AA:1095:C:H2'	1:AA:1096:A:H5'	1.95	0.49
13:AP:27:HIS:HB2	65:AP:306:HOH:O	2.11	0.49
32:A8:37:SER:OG	32:A8:38:GLY:N	2.45	0.49
34:BA:674:G:H2'	34:BA:675:A:H8	1.76	0.49
34:BA:688:G:H2'	34:BA:689:C:H6	1.77	0.49
34:BA:1171:G:H2'	34:BA:1172:C:C6	2.47	0.49
59:BZ:328:ILE:HD12	59:BZ:377:VAL:HG12	1.93	0.49
1:CA:1480:G:C6	1:CA:1481:U:N3	2.80	0.49
4:CD:96:HIS:NE2	4:CD:102:LYS:HE2	2.27	0.49
23:CZ:110:GLY:HA3	23:CZ:145:GLU:HA	1.93	0.49
34:DA:1299:A:N3	34:DA:1299:A:H2'	2.27	0.49
35:DB:77:ALA:HB2	35:DB:211:ILE:HD13	1.95	0.49
36:DC:47:LEU:HG	36:DC:68:VAL:HG11	1.93	0.49
37:DD:13:ARG:HD3	37:DD:32:ALA:HB1	1.95	0.49
42:DI:46:ALA:HB2	42:DI:74:ILE:HG23	1.94	0.49
43:DJ:30:SER:O	43:DJ:30:SER:OG	2.29	0.49
45:DL:88:GLY:O	45:DL:99:HIS:HD2	1.96	0.49
59:DZ:160:ARG:NH1	59:DZ:256:THR:OG1	2.37	0.49
1:AA:1140:U:O2'	1:AA:1142:A:N7	2.41	0.49
1:AA:1466:U:O2'	1:AA:1467:G:OP1	2.28	0.49
4:AD:12:SER:HB3	4:AD:208:LYS:HB3	1.95	0.49
22:AY:79:CYS:SG	22:AY:81:LYS:HG3	2.52	0.49
35:BB:178:ARG:HH22	41:BH:68:ARG:NH1	2.11	0.49
53:BT:40:ALA:HB2	53:BT:55:ILE:HG22	1.95	0.49
58:BY:34:G:H8	58:BY:34:G:O5'	1.96	0.49
59:BZ:75:LYS:O	59:BZ:77:HIS:HD2	1.95	0.49
59:BZ:358:MET:HE1	59:BZ:363:ARG:NH1	2.27	0.49
1:CA:18:C:H2'	1:CA:19:C:C6	2.48	0.49
1:CA:1782:C:H1'	1:CA:2609:U:C5'	2.43	0.49
1:CA:2758:A:C2	1:CA:2759:G:H1'	2.46	0.49
1:CA:2787:C:HO2'	1:CA:2810:A:HO2'	1.61	0.49
3:CC:191:ARG:O	3:CC:194:ILE:HG22	2.12	0.49
13:CP:38:GLN:O	13:CP:39:LYS:HB3	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:DA:259:G:H2'	34:DA:260:G:O4'	2.13	0.49
34:DA:1107:C:C4	34:DA:1108:G:C8	3.00	0.49
35:DB:46:LYS:O	35:DB:50:GLU:HB2	2.13	0.49
37:DD:59:ARG:O	37:DD:63:LYS:HD3	2.12	0.49
50:DQ:45:HIS:CD2	50:DQ:47:PRO:HD3	2.47	0.49
59:DZ:511:LYS:HB2	59:DZ:569:ASP:HB3	1.94	0.49
1:AA:826:U:OP1	4:AD:49:ILE:HD12	2.13	0.49
1:AA:1834:A:H4'	4:AD:259:THR:CG2	2.41	0.49
1:AA:2200:C:O2'	3:AC:169:THR:CB	2.59	0.49
3:AC:55:SER:C	3:AC:57:GLN:N	2.71	0.49
13:AP:52:GLU:HG2	32:A8:57:ARG:HH22	1.77	0.49
43:BJ:11:PHE:CE1	43:BJ:67:THR:HG22	2.47	0.49
48:BO:33:THR:HG21	48:BO:85:LEU:HD22	1.93	0.49
51:BR:26:LEU:HD21	51:BR:39:VAL:HG13	1.94	0.49
1:CA:300:A:P	22:CY:86:ARG:NH2	2.84	0.49
1:CA:819:A:C4	1:CA:1189:A:C2	3.00	0.49
1:CA:2171:A:H1'	1:CA:2172:U:C6	2.47	0.49
1:CA:2773:C:H5"	5:CE:164:ARG:HG2	1.93	0.49
1:CA:2849:U:H4'	1:CA:2868:A:C2	2.47	0.49
34:DA:1148:U:H2'	34:DA:1149:C:O4'	2.13	0.49
35:DB:178:ARG:HH21	41:DH:74:PRO:HB3	1.78	0.49
39:DF:87:ARG:HG3	39:DF:87:ARG:NH1	2.18	0.49
42:DI:3:GLN:CG	42:DI:20:ARG:HE	2.26	0.49
46:DM:70:LEU:O	46:DM:74:VAL:HG23	2.12	0.49
1:AA:1220:U:O3'	1:AA:1221:G:H4'	2.13	0.49
1:AA:2830:A:C8	5:AE:109:LYS:HE2	2.47	0.49
13:AP:84:ASN:HB3	13:AP:117:GLU:O	2.13	0.49
17:AT:15:VAL:HG13	17:AT:79:HIS:CE1	2.48	0.49
17:AT:77:PRO:HB2	17:AT:80:SER:HB2	1.94	0.49
23:AZ:73:GLN:HB3	23:AZ:87:ASP:HB2	1.95	0.49
34:BA:21:G:H2'	34:BA:22:G:C8	2.47	0.49
34:BA:92:C:H2'	34:BA:93:G:C8	2.48	0.49
34:BA:693:G:H2'	34:BA:694:A:C8	2.48	0.49
34:BA:903:G:OP1	65:BA:1910:HOH:O	2.19	0.49
34:BA:1342:C:O2'	42:BI:124:GLN:HG3	2.12	0.49
44:BK:73:MET:HG2	44:BK:103:LEU:HD21	1.94	0.49
46:BM:3:ARG:HG3	46:BM:4:ILE:H	1.77	0.49
59:BZ:140:ASP:HA	59:BZ:172:ASP:H	1.78	0.49
1:CA:1130:U:O2	5:CE:149:ARG:NH2	2.40	0.49
1:CA:1498:C:O4'	1:CA:1577:C:H4'	2.13	0.49
1:CA:2396:G:OP1	25:C1:25:LYS:NZ	2.29	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:CK:27:VAL:HA	9:CK:113:GLN:HA	1.95	0.49
34:DA:9:G:OP1	38:DE:122:GLU:HG3	2.13	0.49
34:DA:91:C:H2'	34:DA:92:C:C6	2.48	0.49
34:DA:1073:U:O2	35:DB:104:ASN:ND2	2.39	0.49
59:DZ:244:ALA:HA	59:DZ:247:ARG:HB3	1.94	0.49
59:DZ:302:HIS:HD2	59:DZ:303:PRO:HD2	1.77	0.49
1:AA:2096:U:H2'	1:AA:2097:U:C6	2.47	0.49
1:AA:2181:G:H2'	1:AA:2182:G:C8	2.48	0.49
1:AA:2660:C:H2'	1:AA:2661:U:C6	2.48	0.49
18:AU:36:ARG:HD2	18:AU:40:PHE:CZ	2.48	0.49
22:AY:86:ARG:HH11	22:AY:100:ALA:HA	1.76	0.49
34:BA:707:C:H2'	34:BA:708:C:C6	2.48	0.49
34:BA:757:U:H2'	34:BA:758:G:O4'	2.13	0.49
34:BA:1128:C:H4'	34:BA:1148:U:O2	2.13	0.49
53:BT:76:ALA:O	53:BT:80:ARG:HG2	2.13	0.49
1:CA:1169:G:H1	1:CA:1180:C:H42	1.61	0.49
1:CA:2405:G:OP1	13:CP:77:ARG:NH2	2.44	0.49
4:CD:24:ILE:HD13	4:CD:84:TYR:HB2	1.95	0.49
15:CR:30:THR:HG22	15:CR:31:HIS:CD2	2.48	0.49
15:CR:33:ARG:HG3	15:CR:115:GLU:HB3	1.95	0.49
18:CU:34:LYS:HE2	18:CU:34:LYS:HA	1.94	0.49
20:CW:19:LEU:HB3	29:C5:25:LEU:HD11	1.95	0.49
23:CZ:93:ASP:HA	23:CZ:131:ARG:NH2	2.28	0.49
34:DA:767:A:H2'	34:DA:768:A:O4'	2.12	0.49
34:DA:983:A:H3'	34:DA:983:A:N3	2.28	0.49
36:DC:120:VAL:HA	36:DC:123:GLN:HE21	1.78	0.49
51:DR:52:PRO:O	51:DR:56:THR:HG23	2.12	0.49
1:AA:239:G:P	32:A8:13:ARG:HH22	2.35	0.49
1:AA:346:A:H3'	6:AF:169:ASN:HD21	1.77	0.49
1:AA:868:A:H2'	1:AA:991:G:H5"	1.94	0.49
1:AA:1067:A:H8	1:AA:1067:A:H3'	1.76	0.49
1:AA:1468:G:H1'	1:AA:1542:A:N1	2.27	0.49
1:AA:1594:C:H2'	1:AA:1595:C:C6	2.47	0.49
1:AA:2250:G:N3	1:AA:2250:G:H2'	2.26	0.49
1:AA:2285:A:H2'	1:AA:2286:A:C8	2.48	0.49
3:AC:24:ASP:OD1	3:AC:24:ASP:C	2.55	0.49
34:BA:222:U:H2'	34:BA:223:U:C6	2.48	0.49
34:BA:443:C:H2'	34:BA:444:C:C6	2.48	0.49
34:BA:559:A:OP1	38:BE:126:ARG:NH2	2.45	0.49
34:BA:814:A:N7	34:BA:816:A:C4	2.81	0.49
35:BB:20:GLU:HA	35:BB:21:ARG:NH2	2.27	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:BB:98:LEU:HG	35:BB:101:MET:HE3	1.94	0.49
37:BD:107:ARG:HH12	37:BD:194:LEU:HD21	1.77	0.49
44:BK:48:ILE:O	44:BK:50:TYR:N	2.45	0.49
59:BZ:78:ARG:HH21	59:BZ:357:ARG:NH2	2.10	0.49
59:BZ:147:TRP:O	59:BZ:151:ARG:HB2	2.13	0.49
1:CA:500:G:N2	1:CA:502:A:H3'	2.28	0.49
1:CA:608:A:H2'	1:CA:609:A:C8	2.48	0.49
1:CA:613:G:N2	1:CA:614(C):A:O2'	2.46	0.49
1:CA:1031:G:H21	33:C9:36:GLN:NE2	2.06	0.49
2:CB:61:G:C6	2:CB:62:C:C4	3.01	0.49
34:DA:8:A:N6	37:DD:209:ARG:HB2	2.27	0.49
34:DA:522:C:OP2	45:DL:69:TYR:OH	2.22	0.49
34:DA:790:A:H2'	34:DA:791:G:C8	2.48	0.49
34:DA:909:A:H2'	34:DA:910:C:O4'	2.13	0.49
34:DA:1121:U:C2'	34:DA:1122:U:H5'	2.43	0.49
35:DB:96:ARG:HD2	35:DB:98:LEU:HD13	1.94	0.49
36:DC:32:LEU:HD12	36:DC:59:ARG:NH1	2.27	0.49
40:DG:26:PHE:O	40:DG:30:ILE:HG13	2.13	0.49
45:DL:102:ARG:HE	45:DL:102:ARG:HB3	1.49	0.49
1:AA:656:A:OP1	13:AP:65:ARG:NH1	2.44	0.49
1:AA:794:U:O2	1:AA:2036:A:H1'	2.12	0.49
1:AA:801:C:H2'	1:AA:802:C:C6	2.48	0.49
1:AA:1846:A:P	4:AD:54:ARG:HH22	2.36	0.49
3:AC:42:VAL:HA	3:AC:216:THR:O	2.13	0.49
4:AD:71:ASP:CB	4:AD:103:ARG:HH22	2.26	0.49
23:AZ:111:VAL:C	23:AZ:113:ALA:H	2.21	0.49
41:BH:29:SER:OG	41:BH:32:LYS:HG3	2.13	0.49
59:BZ:519:ARG:HH22	59:BZ:678:GLU:H	1.59	0.49
1:CA:647:G:O5'	1:CA:647:G:H8	1.96	0.49
3:CC:184:GLU:O	3:CC:188:ASP:OD2	2.31	0.49
4:CD:273:ARG:HG2	4:CD:274:ARG:N	2.28	0.49
13:CP:59:LEU:O	32:C8:13:ARG:HD2	2.13	0.49
13:CP:101:VAL:HA	13:CP:106:LEU:O	2.13	0.49
14:CQ:18:LYS:O	14:CQ:98:LYS:NZ	2.35	0.49
17:CT:6:LEU:O	17:CT:10:VAL:HG23	2.12	0.49
34:DA:707:C:H2'	34:DA:708:C:H6	1.78	0.49
34:DA:1101:A:H4'	34:DA:1102:A:O5'	2.12	0.49
34:DA:1251:A:H2'	34:DA:1252:A:C8	2.47	0.49
43:DJ:63:PHE:HE2	47:DN:45:ARG:HA	1.78	0.49
51:DR:33:ASP:OD2	51:DR:36:ASN:HB2	2.13	0.49
59:DZ:169:GLY:H	59:DZ:170:ARG:NH1	2.09	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:898:U:O2'	27:A3:42:ALA:O	2.29	0.48
1:AA:1890:A:N6	1:AA:1905:G:O2'	2.45	0.48
1:AA:2021:C:H4'	1:AA:2736:C:O2	2.13	0.48
7:AG:126:ASP:HB3	7:AG:130:ASN:H	1.78	0.48
15:AR:118:GLU:H	15:AR:118:GLU:CD	2.21	0.48
18:AU:61:TRP:CZ2	18:AU:93:LYS:HB2	2.48	0.48
34:BA:429:U:H3'	37:BD:9:CYS:SG	2.53	0.48
34:BA:674:G:H2'	34:BA:675:A:C8	2.48	0.48
37:BD:88:VAL:HG12	37:BD:91:SER:H	1.78	0.48
38:BE:36:ASP:OD2	38:BE:40:ARG:HB2	2.13	0.48
1:CA:272:G:H4'	1:CA:272(A):U:H5"	1.95	0.48
1:CA:1434:A:H61	1:CA:1558:A:N6	2.10	0.48
1:CA:1628:G:H2'	1:CA:1629:U:C6	2.48	0.48
1:CA:2365:G:N7	32:C8:39:LYS:NZ	2.54	0.48
2:CB:12:C:O5'	2:CB:12:C:H6	1.96	0.48
34:DA:687:A:N3	34:DA:688:G:H1'	2.28	0.48
35:DB:103:THR:HG23	35:DB:176:GLU:OE1	2.13	0.48
37:DD:98:GLU:OE1	37:DD:103:ASN:ND2	2.46	0.48
52:DS:11:VAL:O	52:DS:13:ASP:N	2.46	0.48
1:AA:311:C:H2'	1:AA:312:C:C6	2.48	0.48
1:AA:537:G:N7	65:AA:3901:HOH:O	2.34	0.48
1:AA:556:C:OP1	1:AA:584:G:N1	2.45	0.48
1:AA:1117:G:H1'	1:AA:1135:G:C8	2.48	0.48
1:AA:1425:A:H4'	1:AA:1426:G:OP2	2.12	0.48
1:AA:1492:C:H2'	1:AA:1493:C:H6	1.78	0.48
5:AE:120:TRP:CD2	5:AE:155:LYS:HG2	2.48	0.48
6:AF:53:THR:HG22	6:AF:56:GLU:HG3	1.95	0.48
10:AL:112:MET:HG2	10:AL:113:PRO:HD3	1.94	0.48
13:AP:83:VAL:HG13	13:AP:112:LEU:HD21	1.94	0.48
14:AQ:56:ARG:HH12	56:BW:52:G:H4'	1.78	0.48
15:AR:86:ARG:NH2	15:AR:87:TYR:OH	2.44	0.48
34:BA:1014:A:H4'	52:BS:14:HIS:CE1	2.48	0.48
35:BB:229:VAL:HG12	35:BB:230:VAL:H	1.77	0.48
58:BY:28:G:H2'	58:BY:29:G:H8	1.78	0.48
59:BZ:-29:LEU:H	59:BZ:-29:LEU:CD2	2.26	0.48
1:CA:1091:G:H2'	1:CA:1092:C:C6	2.49	0.48
4:CD:2:ALA:O	4:CD:3:VAL:HB	2.13	0.48
34:DA:1051:C:H2'	34:DA:1052:U:H6	1.78	0.48
35:DB:219:VAL:O	35:DB:222:ILE:HG12	2.13	0.48
36:DC:39:ILE:O	36:DC:43:LEU:HG	2.13	0.48
40:DG:93:PRO:HA	40:DG:96:GLN:HE21	1.78	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1068:G:N7	11:AN:66:LYS:HE2	2.28	0.48
1:AA:1098:C:H2'	1:AA:1099:C:C6	2.48	0.48
1:AA:1384:G:O2'	1:AA:1439:A:N1	2.42	0.48
1:AA:2331:G:C2	16:AS:3:ARG:HA	2.47	0.48
4:AD:35:LYS:HB2	4:AD:36:PRO:HD2	1.95	0.48
4:AD:124:PRO:O	4:AD:126:GLN:N	2.46	0.48
27:A3:23:LEU:HD13	27:A3:50:VAL:HG11	1.95	0.48
34:BA:91:C:H5'	34:BA:92:C:OP2	2.14	0.48
34:BA:1239:A:C4	34:BA:1298:C:N4	2.81	0.48
35:BB:27:LYS:O	35:BB:194:PRO:HG2	2.12	0.48
37:BD:98:GLU:OE1	37:BD:107:ARG:NH1	2.46	0.48
42:BI:93:ARG:NH1	42:BI:93:ARG:HB2	2.29	0.48
52:BS:51:VAL:O	52:BS:58:VAL:N	2.44	0.48
59:BZ:125:ALA:C	59:BZ:132:ARG:HH12	2.21	0.48
1:CA:1342:A:O2'	1:CA:1344:G:OP2	2.26	0.48
1:CA:2132:U:C4	3:CC:6:LYS:CE	2.94	0.48
1:CA:2356:C:H2'	1:CA:2357:U:O4'	2.14	0.48
1:CA:2364:C:H2'	1:CA:2365:G:O4'	2.13	0.48
1:CA:2522:U:O2'	1:CA:2647:U:OP1	2.24	0.48
3:CC:24:ASP:C	3:CC:24:ASP:OD1	2.55	0.48
11:CN:128:HIS:CE1	11:CN:135:PRO:HG2	2.48	0.48
20:CW:60:ASN:HD22	20:CW:60:ASN:N	2.11	0.48
32:C8:33:ASN:HA	32:C8:36:LYS:HD3	1.95	0.48
34:DA:363:A:C5	45:DL:31:PRO:HD2	2.47	0.48
34:DA:428:G:OP2	37:DD:10:ARG:NH1	2.47	0.48
34:DA:1355:G:H2'	34:DA:1356:G:H8	1.78	0.48
35:DB:111:ARG:HG2	35:DB:111:ARG:HH11	1.78	0.48
48:DO:24:SER:O	48:DO:28:GLN:HG3	2.12	0.48
59:DZ:103:GLY:H	59:DZ:130:VAL:HG23	1.77	0.48
1:AA:504:A:N1	1:AA:525:G:H4'	2.27	0.48
1:AA:662:A:H4'	1:AA:663:G:O5'	2.14	0.48
1:AA:2584:A:N7	5:AE:144:ARG:HD2	2.27	0.48
1:AA:2686:G:H5'	12:AO:26:LYS:HE2	1.95	0.48
2:AB:48:A:H4'	16:AS:95:HIS:HD2	1.79	0.48
6:AF:8:GLN:HE22	6:AF:21:ALA:HB2	1.78	0.48
14:AQ:54:MET:HG3	14:AQ:117:ALA:HB1	1.96	0.48
15:AR:38:VAL:HG22	15:AR:112:ALA:HB2	1.95	0.48
25:A1:5:CYS:SG	25:A1:62:VAL:HG23	2.53	0.48
25:A1:8:SER:OG	25:A1:10:LYS:HG3	2.13	0.48
34:BA:109:A:H4'	34:BA:110:C:OP2	2.13	0.48
34:BA:1325:C:H2'	34:BA:1326:C:C6	2.48	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:BB:178:ARG:HH22	41:BH:68:ARG:HH12	1.60	0.48
37:BD:98:GLU:OE1	37:BD:103:ASN:ND2	2.35	0.48
37:BD:187:ARG:HG2	37:BD:188:LEU:N	2.29	0.48
40:BG:50:ILE:HD11	40:BG:58:PRO:HA	1.95	0.48
40:BG:152:ALA:O	40:BG:155:ARG:HB3	2.13	0.48
44:BK:62:GLN:HB2	44:BK:93:GLN:HG3	1.95	0.48
59:BZ:150:ILE:O	59:BZ:154:GLN:HG3	2.13	0.48
1:CA:848:G:N9	1:CA:933:A:H8	2.11	0.48
1:CA:2163:C:C5	1:CA:2164:C:H1'	2.49	0.48
6:CF:51:THR:O	6:CF:93:LYS:HE2	2.13	0.48
12:CO:2:ILE:HD12	12:CO:6:THR:HG21	1.95	0.48
14:CQ:75:THR:HA	14:CQ:89:ASN:O	2.12	0.48
34:DA:769:G:O2'	34:DA:770:C:H5'	2.13	0.48
34:DA:1208:C:H2'	34:DA:1209:C:H6	1.79	0.48
35:DB:16:HIS:HD2	35:DB:204:ASN:HB3	1.79	0.48
47:DN:27:CYS:SG	47:DN:28:GLY:N	2.86	0.48
59:DZ:606:MET:O	59:DZ:646:PHE:HA	2.14	0.48
1:AA:268:G:HO2'	1:AA:269:G:H8	1.61	0.48
1:AA:746:A:H2'	1:AA:747:G:O4'	2.13	0.48
1:AA:908:A:C2	1:AA:963:A:C4	3.01	0.48
1:AA:945:A:O2'	1:AA:946:A:H8	1.96	0.48
1:AA:2372:A:H2'	1:AA:2373:A:O4'	2.14	0.48
4:AD:10:THR:OG1	4:AD:13:ARG:HB2	2.13	0.48
24:A0:32:ARG:H	24:A0:35:ASN:ND2	2.11	0.48
34:BA:153:C:N4	34:BA:168:G:H1	2.11	0.48
35:BB:189:ASP:OD1	35:BB:189:ASP:N	2.33	0.48
38:BE:84:PHE:HB3	38:BE:134:ALA:HB2	1.95	0.48
56:BW:9:A:H1'	56:BW:45:U:O2'	2.14	0.48
59:BZ:2:LYS:HA	59:BZ:5:LEU:HD12	1.95	0.48
59:BZ:221:ALA:HB2	59:BZ:227:ILE:HG22	1.95	0.48
1:CA:848:G:C4	1:CA:933:A:H8	2.32	0.48
1:CA:1274:A:N3	1:CA:1297:C:H1'	2.28	0.48
1:CA:2235:G:H2'	1:CA:2236:C:C6	2.48	0.48
1:CA:2695:C:H2'	1:CA:2696:U:C6	2.49	0.48
2:CB:3:C:H2'	2:CB:4:C:H6	1.78	0.48
3:CC:55:SER:C	3:CC:57:GLN:N	2.71	0.48
6:CF:120:GLU:HB2	6:CF:122:LYS:HG2	1.95	0.48
14:CQ:38:GLU:HA	14:CQ:99:PRO:HG3	1.96	0.48
34:DA:690:G:H2'	34:DA:691:G:C8	2.49	0.48
34:DA:1347:G:H5"	42:DI:107:ARG:HB3	1.94	0.48
35:DB:210:SER:OG	35:DB:211:ILE:N	2.46	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:DL:24:VAL:HG12	45:DL:27:LEU:HB2	1.95	0.48
52:DS:27:GLU:HB3	52:DS:28:LYS:HD3	1.96	0.48
59:DZ:149:VAL:O	59:DZ:153:MET:HB2	2.12	0.48
59:DZ:634:MET:HE3	59:DZ:643:ILE:HG12	1.95	0.48
1:AA:518:G:O6	65:AA:3927:HOH:O	2.18	0.48
1:AA:878:G:O2'	13:AP:38:GLN:NE2	2.47	0.48
4:AD:273:ARG:HG2	4:AD:274:ARG:H	1.79	0.48
5:AE:174:ASP:OD1	5:AE:175:VAL:N	2.47	0.48
6:AF:118:ALA:HB2	6:AF:123:LEU:HD23	1.95	0.48
14:AQ:31:ASP:HB2	14:AQ:32:TYR:CD2	2.49	0.48
25:A1:50:ARG:HG2	25:A1:59:THR:HB	1.95	0.48
34:BA:736:C:H2'	34:BA:737:A:H8	1.78	0.48
34:BA:1053:G:N7	34:BA:1200:C:H5"	2.28	0.48
34:BA:1233:G:H2'	34:BA:1234:C:C6	2.49	0.48
35:BB:101:MET:HA	35:BB:108:ILE:HD12	1.94	0.48
46:BM:86:CYS:HB2	52:BS:73:GLU:HB3	1.96	0.48
57:BX:19:G:H5"	57:BX:60:U:O4	2.12	0.48
1:CA:65:C:H2'	1:CA:66:C:H6	1.79	0.48
1:CA:1025:G:C4	1:CA:1135:C:H1'	2.48	0.48
1:CA:1860:G:H5'	3:CC:206:LYS:HE2	1.87	0.48
1:CA:2107:C:H42	1:CA:2182:G:H1	1.61	0.48
1:CA:2163:C:H5	1:CA:2164:C:H1'	1.78	0.48
1:CA:2359:C:H2'	1:CA:2360:A:O4'	2.13	0.48
4:CD:94:LEU:HD22	4:CD:95:LEU:H	1.79	0.48
9:CK:118:THR:N	9:CK:121:ASP:O	2.47	0.48
28:C4:62:ARG:H	28:C4:62:ARG:NE	2.11	0.48
34:DA:448:A:P	34:DA:485:G:H22	2.36	0.48
34:DA:586:C:O2'	34:DA:878:G:H4'	2.12	0.48
53:DT:54:LYS:HA	53:DT:57:ARG:CZ	2.44	0.48
59:DZ:169:GLY:N	59:DZ:170:ARG:NH1	2.61	0.48
1:AA:908:A:H2'	1:AA:909:G:O4'	2.14	0.48
7:AG:48:GLU:HA	7:AG:51:ARG:NE	2.27	0.48
23:AZ:41:LEU:O	23:AZ:41:LEU:HD22	2.13	0.48
23:AZ:152:ALA:O	23:AZ:155:LEU:HB2	2.14	0.48
34:BA:1144:G:N2	34:BA:1146:A:H62	2.12	0.48
34:BA:1205:U:O2'	36:BC:195:VAL:HG23	2.14	0.48
41:BH:114:THR:HG22	41:BH:130:GLY:O	2.13	0.48
44:BK:20:TYR:HB2	44:BK:31:THR:HG23	1.94	0.48
1:CA:697:C:H2'	1:CA:698:C:C6	2.48	0.48
1:CA:919:G:N2	1:CA:2269:A:OP2	2.47	0.48
1:CA:1005:C:H2'	1:CA:1006:C:C6	2.49	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:2507:C:H2'	1:CA:2508:G:O4'	2.14	0.48
6:CF:192:LEU:HD22	6:CF:194:MET:HG3	1.96	0.48
15:CR:97:VAL:HG22	15:CR:114:VAL:HG13	1.96	0.48
34:DA:1238:A:N3	34:DA:1241:G:O2'	2.42	0.48
34:DA:1318:A:H5"	52:DS:3:ARG:NH2	2.29	0.48
34:DA:1499:A:H1'	34:DA:1520:G:H5'	1.95	0.48
35:DB:121:LEU:H	35:DB:125:PRO:HG2	1.78	0.48
37:DD:8:VAL:HG23	37:DD:11:LEU:HD22	1.96	0.48
41:DH:20:TYR:HD2	41:DH:65:TYR:CD2	2.32	0.48
43:DJ:5:ARG:N	43:DJ:73:ASP:HA	2.29	0.48
59:DZ:556:ILE:HD13	59:DZ:558:PHE:HD2	1.78	0.48
1:AA:311:C:H2'	1:AA:312:C:H6	1.78	0.48
1:AA:313:A:H61	1:AA:375:G:H1'	1.79	0.48
1:AA:997:G:OP1	14:AQ:16:ARG:NH2	2.47	0.48
1:AA:1071:G:C4	1:AA:1180:C:H1'	2.49	0.48
1:AA:1210:G:H2'	1:AA:1211:U:C6	2.49	0.48
1:AA:1769:G:H2'	1:AA:1770:A:H8	1.79	0.48
1:AA:2181:G:H2'	1:AA:2182:G:H8	1.78	0.48
11:AN:112:LEU:HD12	11:AN:112:LEU:O	2.14	0.48
34:BA:437:U:O2'	37:BD:123:HIS:HD2	1.97	0.48
34:BA:1299:A:N3	34:BA:1299:A:H5"	2.29	0.48
36:BC:8:ILE:HD13	36:BC:184:TYR:HB3	1.94	0.48
39:BF:82:ARG:HB3	39:BF:85:VAL:HG23	1.96	0.48
43:BJ:44:VAL:HG13	43:BJ:66:ARG:HG2	1.95	0.48
1:CA:38:A:H2'	1:CA:39:C:C6	2.49	0.48
1:CA:1142(A):A:C4	1:CA:1144:G:C8	3.02	0.48
1:CA:1384:A:N3	1:CA:1405:U:H1'	2.29	0.48
3:CC:55:SER:C	3:CC:57:GLN:H	2.19	0.48
8:CH:164:TYR:HB2	8:CH:167:GLU:HB2	1.96	0.48
38:DE:16:THR:OG1	38:DE:17:ALA:N	2.45	0.48
40:DG:94:ARG:O	40:DG:97:GLN:HB3	2.14	0.48
59:DZ:514:VAL:HA	59:DZ:564:LYS:O	2.13	0.48
1:AA:116:A:C8	1:AA:117:A:C8	3.02	0.48
1:AA:2567:U:H5"	1:AA:2568:C:OP2	2.14	0.48
21:AX:31:HIS:CD2	21:AX:32:PRO:HD2	2.48	0.48
23:AZ:120:ILE:HG13	23:AZ:171:ILE:C	2.39	0.48
34:BA:49:U:C2	34:BA:361:G:N2	2.82	0.48
34:BA:1189:C:H5"	34:BA:1190:G:OP2	2.14	0.48
34:BA:1279:A:H5"	34:BA:1280:A:OP1	2.14	0.48
37:BD:31:CYS:SG	37:BD:33:MET:N	2.87	0.48
52:BS:15:LEU:O	52:BS:19:VAL:HG23	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:BY:58:A:C2	58:BY:60:U:H2'	2.48	0.48
59:BZ:21:ILE:HD11	59:BZ:117:GLN:NE2	2.29	0.48
59:BZ:75:LYS:HA	59:BZ:75:LYS:HZ2	1.78	0.48
59:BZ:132:ARG:N	59:BZ:132:ARG:HD3	2.28	0.48
12:CO:102:VAL:HB	12:CO:106:LEU:HD12	1.94	0.48
34:DA:70:G:H1	34:DA:99:U:H3	1.60	0.48
38:DE:92:LYS:HB3	38:DE:119:LEU:HB2	1.96	0.48
50:DQ:95:TYR:HA	50:DQ:98:LEU:HD12	1.96	0.48
57:DX:49:G:N2	57:DX:66:C:C2	2.82	0.48
1:AA:1566:U:H2'	1:AA:1567:G:O4'	2.14	0.48
1:AA:2339:A:H2'	1:AA:2340:A:C8	2.48	0.48
4:AD:108:PRO:HB3	4:AD:143:HIS:CE1	2.49	0.48
14:AQ:57:HIS:CE1	14:AQ:116:GLU:HG2	2.49	0.48
23:AZ:29:TYR:HB3	23:AZ:34:ASN:ND2	2.17	0.48
28:A4:61:ARG:HH21	52:BS:42:PRO:CD	2.26	0.48
34:BA:1226:C:H4'	52:BS:80:TYR:CZ	2.49	0.48
58:BY:9:A:H1'	58:BY:45:U:H2'	1.96	0.48
59:BZ:637:ARG:C	59:BZ:639:ASN:H	2.21	0.48
1:CA:660:G:O3'	6:CF:38:ARG:NH2	2.47	0.48
1:CA:1220:A:OP2	18:CU:19:LYS:NZ	2.47	0.48
1:CA:1830:C:OP2	65:CA:3733:HOH:O	2.20	0.48
1:CA:1837:C:O2'	1:CA:1927:A:N3	2.42	0.48
4:CD:134:ARG:NH1	4:CD:188:GLU:OE2	2.47	0.48
15:CR:17:ARG:O	15:CR:20:LEU:HB3	2.14	0.48
18:CU:32:PHE:HZ	18:CU:36:ARG:HH21	1.61	0.48
30:C6:25:LYS:HE3	30:C6:30:THR:O	2.13	0.48
34:DA:300:A:H2'	34:DA:301:G:O4'	2.14	0.48
34:DA:392:G:H2'	34:DA:393:A:C8	2.49	0.48
34:DA:689:C:P	44:DK:46:GLY:HA3	2.54	0.48
35:DB:76:GLN:NE2	35:DB:206:ASP:O	2.47	0.48
38:DE:10:MET:HB3	38:DE:13:ILE:HD11	1.96	0.48
50:DQ:5:VAL:O	50:DQ:6:LEU:HD13	2.14	0.48
59:DZ:170:ARG:HD3	59:DZ:170:ARG:HA	1.62	0.48
59:DZ:328:ILE:HD12	59:DZ:377:VAL:HG12	1.96	0.48
4:AD:146:GLU:HB2	4:AD:189:CYS:HB3	1.96	0.47
5:AE:141:ILE:HD12	5:AE:150:VAL:HG21	1.96	0.47
5:AE:178:GLU:H	5:AE:178:GLU:CD	2.21	0.47
19:AV:5:VAL:HG21	19:AV:35:LEU:HD23	1.96	0.47
34:BA:110:C:O2'	49:BP:25:ARG:O	2.26	0.47
34:BA:411:A:C8	34:BA:413:G:C8	3.01	0.47
35:BB:20:GLU:HB3	35:BB:190:THR:OG1	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:BE:10:MET:HA	38:BE:32:VAL:HG22	1.95	0.47
40:BG:8:GLU:H	40:BG:8:GLU:CD	2.21	0.47
53:BT:21:LYS:O	53:BT:25:ARG:HG3	2.15	0.47
1:CA:218:A:C2	1:CA:235:U:H4'	2.49	0.47
1:CA:1514:U:H2'	1:CA:1515:G:C8	2.49	0.47
1:CA:2395:C:O2'	25:C1:30:VAL:HG22	2.14	0.47
1:CA:2712(A):A:H5"	1:CA:2713:A:OP2	2.13	0.47
7:CG:18:GLU:HG3	7:CG:18:GLU:O	2.12	0.47
8:CH:54:ARG:HD3	8:CH:65:HIS:ND1	2.29	0.47
22:CY:13:VAL:HB	22:CY:72:VAL:HG13	1.95	0.47
23:CZ:45:ASP:CG	23:CZ:49:ARG:HH11	2.22	0.47
24:C0:23:VAL:HG22	24:C0:38:VAL:HG22	1.96	0.47
28:C4:59:PHE:HA	28:C4:60:GLN:C	2.39	0.47
34:DA:563:A:H2'	34:DA:567:G:C8	2.49	0.47
34:DA:1273:G:H3'	34:DA:1274:G:C8	2.48	0.47
34:DA:1342:C:H4'	42:DI:125:TYR:HB3	1.95	0.47
34:DA:1375:A:O2'	40:DG:29:LYS:NZ	2.47	0.47
39:DF:30:LEU:HD23	39:DF:75:LEU:HD21	1.96	0.47
1:AA:354:A:H2	1:AA:1255:A:C2'	2.26	0.47
1:AA:2317:A:H5"	7:AG:134:GLY:HA3	1.96	0.47
6:AF:161:GLU:HG2	6:AF:164:ARG:NH2	2.29	0.47
34:BA:708:C:H2'	34:BA:709:G:H8	1.79	0.47
34:BA:814:A:H2'	34:BA:816:A:H5"	1.96	0.47
35:BB:170:GLU:O	35:BB:174:VAL:HG23	2.14	0.47
39:BF:89:MET:HE2	39:BF:91:VAL:HG22	1.96	0.47
49:BP:22:THR:HA	49:BP:33:ILE:HG12	1.96	0.47
59:BZ:146:LEU:HD12	59:BZ:167:PRO:CD	2.44	0.47
59:BZ:168:ILE:HD11	59:BZ:178:ILE:HG13	1.96	0.47
59:BZ:348:ARG:HG2	59:BZ:348:ARG:NH1	2.29	0.47
59:BZ:416:LYS:HB2	59:BZ:474:ALA:HA	1.96	0.47
1:CA:930:U:H4'	1:CA:931:G:O5'	2.14	0.47
1:CA:1641:A:H2'	1:CA:1642:G:O4'	2.14	0.47
1:CA:2611:U:OP2	1:CA:2611:U:H3'	2.14	0.47
1:CA:2693:A:H2'	1:CA:2694:G:H8	1.78	0.47
22:CY:37:VAL:HG21	22:CY:72:VAL:HG21	1.95	0.47
34:DA:149:A:H2'	34:DA:150:C:C6	2.49	0.47
34:DA:714:G:H2'	34:DA:715:A:C8	2.49	0.47
34:DA:920:U:C2	34:DA:921:U:C5	3.02	0.47
34:DA:927:G:OP2	34:DA:927:G:H4'	2.12	0.47
34:DA:1239:A:N6	34:DA:1299:A:H62	2.11	0.47
35:DB:82:ARG:HG3	35:DB:92:TYR:OH	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:DB:141:GLU:HG2	35:DB:145:LEU:HD12	1.97	0.47
51:DR:26:LEU:HD21	51:DR:42:ARG:HE	1.79	0.47
1:AA:142:G:H1'	21:AX:37:THR:HG21	1.96	0.47
1:AA:1358:U:H4'	1:AA:1359:U:O5'	2.14	0.47
1:AA:2074:G:H4'	5:AE:143:ASN:O	2.14	0.47
8:AH:89:ILE:HD12	8:AH:96:ALA:HB2	1.95	0.47
12:AO:87:ILE:HD12	12:AO:91:LEU:HA	1.96	0.47
34:BA:164:U:H2'	34:BA:165:C:C6	2.49	0.47
34:BA:927:G:H4'	34:BA:927:G:OP2	2.13	0.47
34:BA:1020:U:H2'	34:BA:1021:G:C8	2.49	0.47
34:BA:1229:A:OP2	46:BM:114:ARG:HD3	2.14	0.47
36:BC:22:TRP:CH2	36:BC:32:LEU:HB2	2.49	0.47
36:BC:52:LEU:HD23	36:BC:54:ARG:H	1.79	0.47
49:BP:8:ARG:C	49:BP:9:PHE:HD1	2.22	0.47
52:BS:52:TYR:HA	52:BS:56:GLN:O	2.14	0.47
59:BZ:534:ILE:HD11	59:BZ:570:GLY:HA3	1.96	0.47
1:CA:185:U:H4'	1:CA:218:A:H4'	1.95	0.47
1:CA:500:G:N1	1:CA:503:A:OP2	2.47	0.47
34:DA:429:U:H3'	37:DD:9:CYS:SG	2.54	0.47
34:DA:636:U:H2'	34:DA:637:G:C8	2.49	0.47
34:DA:1041:A:C6	34:DA:1042:G:C6	3.02	0.47
34:DA:1301:U:O2'	34:DA:1302:U:H5'	2.14	0.47
34:DA:1338:G:C6	34:DA:1339:A:C6	3.02	0.47
37:DD:68:TYR:CE1	37:DD:97:LEU:HB3	2.49	0.47
1:AA:225:C:H2'	1:AA:226:C:H6	1.78	0.47
1:AA:826:U:P	4:AD:49:ILE:HD12	2.55	0.47
1:AA:955:A:H2'	1:AA:958:C:C5	2.49	0.47
16:AS:83:LYS:HE2	16:AS:83:LYS:HB2	1.60	0.47
34:BA:354:G:C2'	34:BA:355:C:H5'	2.44	0.47
34:BA:436:C:H2'	34:BA:437:U:C6	2.49	0.47
34:BA:1255:G:N7	43:BJ:43:ARG:NH2	2.62	0.47
35:BB:212:GLN:NE2	35:BB:234:PRO:O	2.47	0.47
59:BZ:217:VAL:HG13	59:BZ:242:LEU:HD21	1.95	0.47
59:BZ:542:VAL:HG23	59:BZ:582:PHE:O	2.14	0.47
1:CA:1266:G:O4'	20:CW:15:ARG:NH2	2.47	0.47
1:CA:2203:U:O4'	4:CD:151:LYS:HE2	2.14	0.47
1:CA:2356:C:O3'	24:C0:20:ARG:HD3	2.14	0.47
1:CA:2391:G:OP2	32:C8:32:LEU:HD23	2.13	0.47
10:CL:103:GLN:HA	10:CL:106:GLU:HG2	1.96	0.47
32:C8:10:ALA:CB	32:C8:62:LEU:HD21	2.43	0.47
34:DA:194:C:H2'	34:DA:195:A:H5"	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:DA:374:A:C6	34:DA:375:U:C4	3.02	0.47
34:DA:1342:C:H1'	42:DI:124:GLN:HE21	1.79	0.47
35:DB:134:GLU:O	35:DB:138:LEU:HG	2.15	0.47
42:DI:17:VAL:HG11	42:DI:80:GLY:C	2.38	0.47
1:AA:1105:G:H1	1:AA:1125:C:H42	1.61	0.47
3:AC:30:VAL:CG2	3:AC:31:LYS:H	2.27	0.47
3:AC:184:GLU:O	3:AC:188:ASP:OD2	2.31	0.47
14:AQ:7:MET:HE2	14:AQ:7:MET:HB2	1.63	0.47
34:BA:586:C:O2'	34:BA:878:G:H4'	2.14	0.47
49:BP:74:LEU:O	49:BP:79:VAL:HG23	2.13	0.47
52:BS:36:ARG:HB3	52:BS:72:GLY:CA	2.44	0.47
52:BS:65:ASN:HD22	52:BS:65:ASN:N	2.12	0.47
58:BY:19:G:H4'	58:BY:20:U:OP2	2.12	0.47
1:CA:757:U:H2'	1:CA:758:C:O4'	2.15	0.47
1:CA:870:A:C2	1:CA:908:C:C2	3.02	0.47
1:CA:1486:A:O2'	1:CA:1487:G:H5'	2.14	0.47
1:CA:1847:A:H3'	1:CA:1848:A:H5'	1.97	0.47
1:CA:2166:G:N7	1:CA:2168:G:N2	2.62	0.47
1:CA:2171:A:N3	1:CA:2172:U:N3	2.62	0.47
1:CA:2440:C:OP2	65:CA:3732:HOH:O	2.20	0.47
3:CC:180:SER:O	3:CC:181:PHE:O	2.33	0.47
6:CF:30:PRO:HB3	13:CP:1:MET:HE1	1.95	0.47
14:CQ:24:GLY:HA2	14:CQ:67:ARG:NH2	2.29	0.47
19:CV:29:PRO:HA	19:CV:61:VAL:HG22	1.95	0.47
34:DA:321:A:N7	34:DA:328:C:O2'	2.35	0.47
1:AA:354:A:O2'	1:AA:355:A:H8	1.96	0.47
1:AA:592:U:C4	1:AA:593:G:C6	3.03	0.47
6:AF:150:GLY:HA2	6:AF:172:TRP:CD2	2.49	0.47
12:AO:17:ARG:HD2	12:AO:17:ARG:HA	1.62	0.47
12:AO:35:VAL:HG11	12:AO:103:ALA:CB	2.44	0.47
13:AP:134:ALA:O	13:AP:138:LEU:HB2	2.14	0.47
23:AZ:153:SER:HB3	23:AZ:167:PRO:HB3	1.97	0.47
33:A9:27:CYS:SG	33:A9:28:GLU:N	2.87	0.47
48:BO:29:VAL:HG11	48:BO:81:LEU:HD21	1.97	0.47
59:BZ:286:ILE:HD13	59:BZ:286:ILE:H	1.79	0.47
59:BZ:325:LEU:HD23	59:BZ:325:LEU:HA	1.75	0.47
1:CA:839:U:H2'	1:CA:840:C:C6	2.50	0.47
1:CA:1054:A:N6	1:CA:1055:G:C6	2.82	0.47
1:CA:1319:G:C6	1:CA:1320:C:N4	2.82	0.47
1:CA:1477:A:H2'	1:CA:1478:G:O4'	2.13	0.47
1:CA:2469:A:H2'	1:CA:2470:G:O4'	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:CN:102:ALA:O	11:CN:106:MET:HG3	2.15	0.47
16:CS:61:ASN:O	16:CS:65:VAL:HG23	2.14	0.47
23:CZ:105:VAL:N	23:CZ:139:VAL:O	2.48	0.47
34:DA:633:G:H2'	34:DA:634:C:C6	2.50	0.47
34:DA:1264:C:H2'	34:DA:1265:G:C8	2.49	0.47
36:DC:56:ASP:C	36:DC:57:ILE:HD12	2.40	0.47
36:DC:123:GLN:O	36:DC:128:PHE:HB2	2.15	0.47
40:DG:50:ILE:HD11	40:DG:58:PRO:HB3	1.95	0.47
40:DG:75:VAL:HA	40:DG:87:VAL:O	2.15	0.47
1:AA:762:G:C2	48:BO:56:LEU:HD21	2.49	0.47
1:AA:821:A:H2'	1:AA:821:A:N3	2.29	0.47
1:AA:1109:G:N2	1:AA:1122:C:O2	2.48	0.47
1:AA:1525:G:H2'	1:AA:1526:G:H8	1.78	0.47
1:AA:2228:G:H2'	1:AA:2229:A:C2	2.50	0.47
3:AC:180:SER:O	3:AC:181:PHE:O	2.32	0.47
4:AD:206:LEU:HD23	4:AD:206:LEU:HA	1.69	0.47
6:AF:101:LEU:HD12	6:AF:102:PRO:HD2	1.96	0.47
7:AG:21:ARG:O	7:AG:21:ARG:HG2	2.13	0.47
7:AG:63:ILE:HD13	7:AG:141:PHE:CG	2.50	0.47
22:AY:38:ILE:HD11	22:AY:66:PRO:HG3	1.97	0.47
34:BA:28:G:O2'	34:BA:296:U:OP1	2.30	0.47
34:BA:1233:G:H2'	34:BA:1234:C:H6	1.80	0.47
34:BA:1316:G:N2	34:BA:1318:A:H3'	2.30	0.47
36:BC:6:HIS:CD2	36:BC:7:PRO:HD2	2.49	0.47
37:BD:173:TRP:CD1	37:BD:173:TRP:H	2.33	0.47
39:BF:15:ASP:OD1	39:BF:18:GLN:N	2.39	0.47
47:BN:3:ARG:HB3	47:BN:3:ARG:HH21	1.79	0.47
51:BR:51:LEU:HD23	51:BR:52:PRO:HD2	1.96	0.47
59:BZ:20:HIS:CE1	59:BZ:115:GLU:HB3	2.49	0.47
59:BZ:359:HIS:ND1	59:BZ:362:HIS:CE1	2.83	0.47
59:BZ:386:GLY:O	59:BZ:401:SER:OG	2.31	0.47
59:BZ:399:LEU:O	59:BZ:401:SER:N	2.48	0.47
59:BZ:484:ARG:NH1	59:BZ:559:PRO:HG2	2.30	0.47
1:CA:479:A:N3	1:CA:481:G:H5"	2.29	0.47
1:CA:674:G:H1'	6:CF:74:ARG:HD3	1.96	0.47
1:CA:747:U:O2	1:CA:2014:A:H1'	2.15	0.47
1:CA:750:A:H2'	1:CA:751:A:H5"	1.97	0.47
1:CA:2108:C:H2'	1:CA:2109:U:C6	2.50	0.47
1:CA:2126:A:H61	1:CA:2172:U:H5'	1.80	0.47
2:CB:66:A:H61	2:CB:109:C:H5"	1.79	0.47
3:CC:42:VAL:HA	3:CC:216:THR:O	2.13	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:CD:72:LYS:HG3	4:CD:103:ARG:NH2	2.30	0.47
7:CG:23:PHE:HB2	7:CG:25:TYR:CE1	2.50	0.47
9:CK:70:GLU:O	9:CK:72:ASP:N	2.48	0.47
14:CQ:11:LYS:NZ	14:CQ:88:GLY:O	2.32	0.47
20:CW:29:LEU:O	20:CW:33:ARG:HG3	2.15	0.47
29:C5:35:GLU:HG2	29:C5:51:TYR:CG	2.49	0.47
31:C7:1:MET:HB2	31:C7:1:MET:HE3	1.67	0.47
34:DA:518:C:H5"	34:DA:519:C:C6	2.49	0.47
34:DA:1030(A):G:H2'	34:DA:1030(B):C:H5"	1.97	0.47
34:DA:1076:C:C2	34:DA:1082:G:N2	2.82	0.47
34:DA:1203:C:H2'	34:DA:1204:A:H8	1.80	0.47
34:DA:1278:U:H5'	34:DA:1279:A:C5'	2.44	0.47
34:DA:1305:G:O2'	34:DA:1331:G:N2	2.47	0.47
36:DC:129:ALA:O	36:DC:133:ALA:N	2.41	0.47
38:DE:101:ILE:HG13	38:DE:119:LEU:HD23	1.96	0.47
41:DH:109:ILE:HB	41:DH:120:THR:HG22	1.97	0.47
42:DI:23:ASN:OD1	42:DI:25:LYS:HE2	2.15	0.47
43:DJ:49:VAL:HG12	43:DJ:61:GLU:O	2.14	0.47
47:DN:32:SER:O	47:DN:40:CYS:HA	2.15	0.47
57:DX:23:C:H2'	57:DX:24:U:C6	2.50	0.47
57:DX:67:C:C2'	57:DX:68:C:H5'	2.44	0.47
59:DZ:15:ILE:HA	59:DZ:103:GLY:O	2.14	0.47
59:DZ:272:LEU:O	59:DZ:276:VAL:HG23	2.14	0.47
59:DZ:490:PRO:HG3	59:DZ:516:PRO:HD2	1.96	0.47
1:AA:440:C:OP2	65:AA:3933:HOH:O	2.21	0.47
1:AA:894:U:H5	1:AA:978:A:H62	1.58	0.47
1:AA:2147:G:OP1	3:AC:71:LYS:HE2	2.15	0.47
1:AA:2623:U:H6	1:AA:2623:U:H5'	1.80	0.47
3:AC:68:GLY:N	3:AC:189:ASN:ND2	2.62	0.47
5:AE:12:THR:HG22	5:AE:13:ARG:H	1.80	0.47
18:AU:74:LEU:HD12	18:AU:74:LEU:H	1.79	0.47
34:BA:1070:U:H2'	34:BA:1071:C:H6	1.80	0.47
52:BS:27:GLU:HG2	52:BS:47:HIS:NE2	2.29	0.47
57:BX:31:G:C8	57:BX:32:5MC:HM53	2.49	0.47
59:BZ:114:VAL:O	59:BZ:115:GLU:HB2	2.15	0.47
59:BZ:405:PRO:CB	59:BZ:406:GLU:HA	2.45	0.47
1:CA:196:A:H2'	1:CA:196:A:N3	2.30	0.47
1:CA:1059:G:H5'	1:CA:1060:U:O5'	2.15	0.47
1:CA:1891:G:O6	65:CA:3730:HOH:O	2.20	0.47
3:CC:6:LYS:HA	3:CC:9:ARG:NH1	2.30	0.47
3:CC:206:LYS:HB3	3:CC:206:LYS:HZ2	1.80	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:CE:52:LEU:O	5:CE:76:ARG:N	2.38	0.47
6:CF:150:GLY:HA2	6:CF:172:TRP:CE3	2.49	0.47
20:CW:14:PRO:HG2	20:CW:78:GLU:HG2	1.96	0.47
21:CX:44:GLU:OE2	21:CX:51:VAL:N	2.48	0.47
28:C4:48:ARG:HA	28:C4:48:ARG:HD3	1.76	0.47
34:DA:364:A:H2'	34:DA:365:U:C6	2.50	0.47
34:DA:404:U:H2'	34:DA:405:U:H6	1.80	0.47
34:DA:713:G:H2'	34:DA:714:G:C8	2.50	0.47
34:DA:1059:C:OP2	36:DC:199:LYS:NZ	2.43	0.47
34:DA:1121:U:H2'	34:DA:1122:U:H5'	1.97	0.47
45:DL:7:ILE:HD13	45:DL:7:ILE:HA	1.78	0.47
49:DP:60:LEU:HD13	49:DP:60:LEU:HA	1.70	0.47
59:DZ:408:VAL:O	59:DZ:482:ALA:HB3	2.15	0.47
1:AA:2720:G:H1'	15:AR:71:GLN:HE22	1.79	0.47
28:A4:36:CYS:SG	28:A4:37:SER:N	2.88	0.47
28:A4:57:GLU:HB2	28:A4:58:ARG:HE	1.80	0.47
34:BA:189(D):C:O2	34:BA:189(H):G:C6	2.68	0.47
34:BA:974:A:P	47:BN:29:ARG:HH21	2.37	0.47
34:BA:1037:C:H2'	34:BA:1038:C:C6	2.50	0.47
36:BC:6:HIS:CD2	36:BC:8:ILE:H	2.32	0.47
38:BE:32:VAL:O	38:BE:43:LEU:HD12	2.15	0.47
39:BF:37:VAL:HG12	39:BF:38:GLU:O	2.15	0.47
1:CA:193:U:OP2	65:CA:3734:HOH:O	2.20	0.47
1:CA:660:G:H5'	6:CF:99:TYR:CE2	2.50	0.47
1:CA:1312:U:OP2	21:CX:63:LYS:NZ	2.36	0.47
1:CA:1590:U:H2'	1:CA:1591:G:C8	2.49	0.47
1:CA:2119:A:H2	1:CA:2171:A:H5'	1.79	0.47
1:CA:2427:C:H5"	1:CA:2428:G:OP1	2.14	0.47
3:CC:17:PRO:HG2	3:CC:18:ASN:H	1.79	0.47
3:CC:42:VAL:CG1	3:CC:43:GLU:H	2.28	0.47
7:CG:121:ASN:O	7:CG:124:SER:HB3	2.15	0.47
11:CN:67:LEU:HD13	11:CN:87:LEU:HD13	1.97	0.47
34:DA:1049:U:C5	34:DA:1201:A:H5'	2.50	0.47
34:DA:1126:U:C4'	34:DA:1281:U:H1'	2.44	0.47
35:DB:167:PRO:HD3	35:DB:187:LEU:O	2.15	0.47
36:DC:50:ALA:HB1	36:DC:70:VAL:HG21	1.96	0.47
36:DC:137:ALA:HA	36:DC:140:ARG:NH1	2.30	0.47
53:DT:50:GLU:H	53:DT:99:LEU:HD12	1.79	0.47
59:DZ:182:ARG:O	59:DZ:184:LYS:N	2.48	0.47
59:DZ:262:SER:HB3	59:DZ:267:LYS:HB2	1.96	0.47
1:AA:1095:C:C2'	1:AA:1096:A:H5'	2.45	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:46:ALA:O	3:AC:47:LYS:HB2	2.15	0.47
4:AD:52:ARG:HB2	4:AD:53:PHE:CD2	2.50	0.47
9:AK:54:ALA:HB1	9:AK:83:TYR:O	2.14	0.47
27:A3:18:ASP:OD1	27:A3:18:ASP:N	2.48	0.47
27:A3:43:ILE:O	27:A3:47:VAL:HG23	2.15	0.47
34:BA:696:A:N1	34:BA:797:C:O2'	2.39	0.47
34:BA:738:C:H2'	34:BA:739:C:C6	2.50	0.47
34:BA:1391:U:H2'	34:BA:1392:G:C8	2.50	0.47
34:BA:1456:G:H1'	53:BT:39:LYS:NZ	2.30	0.47
42:BI:53:VAL:O	42:BI:55:ALA:N	2.48	0.47
46:BM:33:ALA:HB2	46:BM:64:TRP:HH2	1.80	0.47
53:BT:56:MET:HE3	53:BT:56:MET:HB2	1.82	0.47
59:BZ:226:ASN:HB3	59:BZ:241:GLU:OE2	2.15	0.47
1:CA:328:U:H4'	22:CY:68:HIS:CE1	2.50	0.47
1:CA:1713:U:H2'	1:CA:1714:G:H8	1.80	0.47
1:CA:2167:U:OP1	1:CA:2167:U:H4'	2.15	0.47
5:CE:111:ARG:HD3	15:CR:1:MET:HE1	1.97	0.47
8:CH:7:LEU:HA	8:CH:8:PRO:HD3	1.80	0.47
13:CP:97:PRO:HD3	13:CP:126:VAL:O	2.15	0.47
20:CW:58:ALA:HB1	20:CW:64:MET:HB2	1.96	0.47
34:DA:828:A:N6	34:DA:858:G:O2'	2.47	0.47
34:DA:936:C:H2'	34:DA:937:A:O4'	2.15	0.47
47:DN:24:CYS:HB3	47:DN:27:CYS:SG	2.55	0.47
49:DP:57:ARG:NH2	49:DP:79:VAL:O	2.48	0.47
3:AC:17:PRO:HG2	3:AC:18:ASN:H	1.79	0.46
4:AD:242:ARG:N	4:AD:242:ARG:HD3	2.29	0.46
6:AF:29:ASN:HB3	6:AF:112:MET:HE1	1.97	0.46
22:AY:23:ARG:HG2	22:AY:42:VAL:HG22	1.96	0.46
34:BA:1284:C:H3'	34:BA:1285:A:H8	1.80	0.46
34:BA:1346:A:N1	34:BA:1374:A:H5"	2.30	0.46
49:BP:20:VAL:HG21	49:BP:32:TYR:CG	2.50	0.46
58:BY:72:C:H2'	58:BY:73:A:O4'	2.15	0.46
1:CA:620:G:H5'	1:CA:620:G:N3	2.30	0.46
1:CA:882:G:H2'	1:CA:883:G:C8	2.46	0.46
9:CK:23:SER:HA	9:CK:117:LEU:O	2.15	0.46
19:CV:71:LEU:HD23	19:CV:71:LEU:HA	1.72	0.46
27:C3:6:VAL:HG13	27:C3:56:VAL:HG22	1.97	0.46
34:DA:900:A:H2'	34:DA:901:A:C8	2.50	0.46
34:DA:1289:A:C8	34:DA:1290:G:C8	3.03	0.46
36:DC:114:PRO:HA	36:DC:185:GLY:HA3	1.96	0.46
43:DJ:35:SER:HB3	43:DJ:73:ASP:HB2	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:DX:55:PSU:O2'	57:DX:57:A:N7	2.31	0.46
1:AA:1907:A:H2'	1:AA:1908:C:O4'	2.14	0.46
7:AG:126:ASP:CG	7:AG:130:ASN:HD22	2.23	0.46
8:AH:40:GLU:OE2	8:AH:60:ARG:NH1	2.47	0.46
11:AN:75:TYR:CE2	11:AN:77:GLY:HA2	2.50	0.46
12:AO:2:ILE:HB	12:AO:33:ALA:HB3	1.97	0.46
20:AW:14:PRO:HG2	20:AW:78:GLU:CG	2.44	0.46
32:A8:39:LYS:O	32:A8:43:GLN:HG3	2.14	0.46
57:BX:55:PSU:O2'	57:BX:57:A:N7	2.37	0.46
59:BZ:233:GLU:HB3	59:BZ:234:GLY:H	1.54	0.46
1:CA:579:G:H2'	1:CA:580:C:C6	2.50	0.46
1:CA:740:U:H2'	1:CA:741:G:C8	2.51	0.46
1:CA:993:G:N2	19:CV:23:GLU:OE2	2.45	0.46
1:CA:2014:A:H2'	1:CA:2015:A:C8	2.50	0.46
1:CA:2336:A:H61	24:C0:43:THR:HG21	1.79	0.46
1:CA:2615:U:H2'	1:CA:2616:C:H6	1.80	0.46
3:CC:176:VAL:O	3:CC:176:VAL:HG12	2.15	0.46
4:CD:175:LEU:HD12	4:CD:185:VAL:HG21	1.97	0.46
7:CG:136:ARG:HD2	7:CG:136:ARG:C	2.40	0.46
8:CH:113:VAL:HG11	8:CH:151:ILE:HD13	1.96	0.46
10:CL:78:ILE:O	10:CL:78:ILE:HG12	2.15	0.46
15:CR:29:LEU:HD12	15:CR:29:LEU:HA	1.83	0.46
19:CV:6:LYS:HB2	19:CV:38:LEU:HD21	1.97	0.46
26:C2:9:GLN:OE1	26:C2:56:GLN:HG2	2.15	0.46
34:DA:543:C:O2'	34:DA:544:G:H5'	2.14	0.46
34:DA:1159:U:O4'	34:DA:1182:G:N2	2.47	0.46
34:DA:1347:G:N2	34:DA:1373:G:H2'	2.29	0.46
1:AA:397:G:H4'	1:AA:398:A:OP2	2.15	0.46
1:AA:1769:G:H2'	1:AA:1770:A:C8	2.51	0.46
3:AC:223:VAL:HG23	3:AC:223:VAL:O	2.15	0.46
5:AE:9:VAL:HB	17:AT:3:ARG:HG2	1.97	0.46
14:AQ:48:GLU:HB2	65:AQ:3102:HOH:O	2.14	0.46
18:AU:112:ARG:HH11	18:AU:112:ARG:CG	2.28	0.46
34:BA:576:G:O6	34:BA:880:C:O2'	2.27	0.46
41:BH:20:TYR:HD2	41:BH:65:TYR:CE2	2.32	0.46
43:BJ:16:LEU:HD21	43:BJ:70:ARG:HG2	1.97	0.46
46:BM:84:ILE:HG13	46:BM:86:CYS:N	2.29	0.46
1:CA:32:C:O2'	1:CA:33:U:H5'	2.16	0.46
1:CA:861:A:C2	1:CA:917:A:C4	3.03	0.46
1:CA:1042:G:H1	1:CA:1113:U:H3	1.63	0.46
1:CA:2178:C:O2'	3:CC:169:THR:CB	2.56	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:2454:G:H1'	65:CA:3844:HOH:O	2.15	0.46
13:CP:59:LEU:HD12	13:CP:60:MET:HE2	1.98	0.46
14:CQ:21:THR:CG2	14:CQ:101:ARG:HH11	2.28	0.46
34:DA:147:G:H1	34:DA:175:C:H42	1.64	0.46
34:DA:179:A:H2'	34:DA:180:U:C6	2.50	0.46
34:DA:364:A:H2'	34:DA:365:U:H6	1.80	0.46
34:DA:724:G:C2	34:DA:725:G:C8	3.03	0.46
58:DY:25:C:H2'	58:DY:26:A:H8	1.80	0.46
59:DZ:620:VAL:O	59:DZ:624:LEU:HB2	2.16	0.46
1:AA:1913:G:C6	1:AA:1914:C:C4	3.03	0.46
1:AA:2332:A:H2'	1:AA:2332:A:N3	2.31	0.46
1:AA:2430:A:H2'	1:AA:2431:U:C6	2.50	0.46
65:AA:4595:HOH:O	5:AE:147:PRO:HD2	2.15	0.46
3:AC:6:LYS:HA	3:AC:9:ARG:NH1	2.30	0.46
3:AC:42:VAL:O	3:AC:216:THR:C	2.59	0.46
26:A2:35:LEU:HD23	26:A2:35:LEU:HA	1.63	0.46
34:BA:160:A:H2'	34:BA:160:A:N3	2.31	0.46
34:BA:487:A:H2'	34:BA:488:C:O4'	2.16	0.46
34:BA:923:A:OP1	38:BE:21:ALA:HB2	2.14	0.46
34:BA:1148:U:O3'	42:BI:14:VAL:HG11	2.15	0.46
35:BB:18:GLY:O	35:BB:19:HIS:HB3	2.16	0.46
44:BK:27:ASN:OD1	44:BK:55:LYS:HB3	2.15	0.46
51:BR:33:ASP:OD2	51:BR:36:ASN:HB2	2.16	0.46
59:BZ:19:ALA:HB1	59:BZ:23:ALA:HB3	1.97	0.46
59:BZ:165:GLN:HA	59:BZ:180:VAL:HG13	1.95	0.46
59:BZ:414:GLU:C	59:BZ:416:LYS:H	2.22	0.46
1:CA:580:C:H2'	1:CA:581:C:C6	2.51	0.46
1:CA:1001:A:H2'	1:CA:1002:G:O4'	2.14	0.46
1:CA:2261:C:O2'	1:CA:2262:U:H5'	2.15	0.46
1:CA:2430:A:OP2	65:CA:3703:HOH:O	2.20	0.46
1:CA:2483:C:OP1	56:DW:64:A:H4'	2.16	0.46
1:CA:2493:U:H2'	1:CA:2494:G:O4'	2.15	0.46
1:CA:2685:G:N7	65:CA:3790:HOH:O	2.36	0.46
7:CG:39:ILE:N	7:CG:39:ILE:HD12	2.31	0.46
8:CH:13:LYS:HA	8:CH:14:GLY:HA2	1.70	0.46
8:CH:139:GLN:HG3	8:CH:140:LYS:N	2.30	0.46
8:CH:147:ASN:N	8:CH:147:ASN:OD1	2.47	0.46
10:CL:76:TYR:CD2	10:CL:77:LEU:HD23	2.50	0.46
12:CO:1:MET:HG2	12:CO:67:LYS:HG2	1.96	0.46
33:C9:25:VAL:HB	33:C9:34:GLN:HB2	1.97	0.46
34:DA:186:C:H2'	34:DA:187:C:H6	1.80	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:DA:426:G:OP1	37:DD:36:ARG:HD2	2.16	0.46
34:DA:509:A:C8	34:DA:509:A:H3'	2.50	0.46
35:DB:167:PRO:HG3	35:DB:188:ALA:HB2	1.98	0.46
35:DB:218:ALA:O	35:DB:222:ILE:HG23	2.16	0.46
38:DE:68:GLU:OE1	38:DE:70:PRO:HG3	2.15	0.46
1:AA:449:A:H2'	1:AA:450:A:C8	2.50	0.46
1:AA:1343:C:OP1	1:AA:2722:C:H4'	2.16	0.46
3:AC:42:VAL:CG1	3:AC:43:GLU:H	2.27	0.46
7:AG:72:ARG:NH1	7:AG:87:PRO:HG3	2.31	0.46
7:AG:83:ARG:O	7:AG:86:MET:HB2	2.16	0.46
12:AO:23:ARG:HG3	12:AO:24:VAL:N	2.29	0.46
34:BA:52:G:H2'	34:BA:53:A:C8	2.50	0.46
38:BE:148:VAL:HG21	41:BH:107:LEU:HB3	1.98	0.46
40:BG:26:PHE:CE2	40:BG:30:ILE:HD11	2.50	0.46
46:BM:80:ARG:NH2	52:BS:69:HIS:HE1	2.14	0.46
53:BT:57:ARG:HH12	53:BT:100:ILE:HG13	1.79	0.46
59:BZ:145:ASP:HB3	59:BZ:148:LEU:HB3	1.98	0.46
59:BZ:670:VAL:HB	59:BZ:672:PHE:CZ	2.51	0.46
59:BZ:687:LEU:O	59:BZ:689:LYS:N	2.49	0.46
1:CA:621:A:OP2	13:CP:108:LYS:NZ	2.43	0.46
1:CA:908:C:O2'	1:CA:909:A:H5'	2.16	0.46
1:CA:1075:C:H5'	14:CQ:59:ARG:HH21	1.79	0.46
1:CA:1232:G:C6	1:CA:1233:C:C4	3.03	0.46
1:CA:1300:U:H4'	1:CA:1301:A:H5"	1.96	0.46
5:CE:12:THR:HG22	17:CT:58:ASN:HD21	1.81	0.46
6:CF:184:TYR:HE1	13:CP:3:LEU:HD21	1.80	0.46
14:CQ:135:ASP:HB3	14:CQ:137:TYR:H	1.79	0.46
34:DA:165:C:H2'	34:DA:166:G:C8	2.50	0.46
34:DA:1288:A:N1	34:DA:1371:G:H1'	2.30	0.46
36:DC:5:ILE:HD11	47:DN:49:HIS:HE1	1.79	0.46
43:DJ:65:LEU:HD13	47:DN:56:VAL:HG22	1.97	0.46
51:DR:32:ARG:HD2	51:DR:65:ILE:CG2	2.45	0.46
59:DZ:183:MET:SD	59:DZ:213:HIS:HB2	2.56	0.46
1:AA:2086:C:H2'	1:AA:2087:C:C6	2.50	0.46
1:AA:2274:U:H4'	1:AA:2340:A:C2	2.50	0.46
2:AB:13:A:N1	2:AB:69:G:O2'	2.46	0.46
2:AB:66:A:H61	2:AB:108:U:H2'	1.79	0.46
3:AC:176:VAL:O	3:AC:176:VAL:HG12	2.15	0.46
5:AE:176:ILE:HB	5:AE:181:LEU:HB2	1.97	0.46
7:AG:79:ASN:OD1	7:AG:79:ASN:N	2.48	0.46
7:AG:171:ALA:O	7:AG:175:LEU:HD22	2.14	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:AT:96:ARG:CZ	17:AT:96:ARG:HB3	2.46	0.46
34:BA:836:G:C6	34:BA:851:G:C6	3.04	0.46
34:BA:954:G:H2'	34:BA:955:U:C6	2.51	0.46
34:BA:1036:G:H3'	34:BA:1037:C:H6	1.81	0.46
37:BD:97:LEU:HD23	37:BD:97:LEU:HA	1.70	0.46
38:BE:83:GLU:HG2	38:BE:88:LYS:HD2	1.98	0.46
56:BW:18:G:O2'	56:BW:57:G:N2	2.44	0.46
59:BZ:20:HIS:HA	59:BZ:117:GLN:CB	2.45	0.46
1:CA:125:G:OP1	31:C7:14:LYS:HE2	2.15	0.46
1:CA:996:A:C2	1:CA:997:G:C8	3.03	0.46
1:CA:1063:G:O2'	10:CL:89:HIS:O	2.33	0.46
1:CA:1449:A:H5'	1:CA:1450:G:OP2	2.15	0.46
1:CA:1889:A:H2'	1:CA:1890:A:C8	2.51	0.46
1:CA:2061:G:H5"	1:CA:2503:A:C2	2.51	0.46
3:CC:42:VAL:O	3:CC:216:THR:C	2.59	0.46
19:CV:43:GLU:N	19:CV:43:GLU:OE2	2.49	0.46
34:DA:622:A:C8	34:DA:623:C:C6	3.04	0.46
38:DE:139:LEU:C	38:DE:141:GLN:N	2.72	0.46
59:DZ:350:GLU:OE2	59:DZ:383:THR:OG1	2.31	0.46
59:DZ:409:ILE:HG12	59:DZ:459:LEU:HD12	1.97	0.46
1:AA:1057:G:OP1	18:AU:77:SER:OG	2.33	0.46
1:AA:1451:U:H2'	1:AA:1452:U:C6	2.51	0.46
1:AA:1817:A:H8	65:AA:4310:HOH:O	1.98	0.46
3:AC:20:VAL:O	3:AC:224:ARG:O	2.34	0.46
3:AC:211:ARG:HG2	3:AC:211:ARG:HH11	1.81	0.46
4:AD:145:VAL:HG12	4:AD:146:GLU:O	2.15	0.46
15:AR:56:LYS:HE3	15:AR:87:TYR:O	2.16	0.46
26:A2:41:ILE:HG13	26:A2:43:GLN:HG3	1.97	0.46
34:BA:452:A:O2'	34:BA:453:A:OP2	2.28	0.46
34:BA:1318:A:OP1	52:BS:3:ARG:NH2	2.49	0.46
36:BC:181:ASN:ND2	36:BC:204:LEU:HD12	2.30	0.46
37:BD:8:VAL:O	37:BD:11:LEU:HB2	2.15	0.46
40:BG:18:TYR:CD2	40:BG:59:LEU:HD13	2.51	0.46
41:BH:132:GLU:O	41:BH:134:ILE:N	2.48	0.46
59:BZ:9:LEU:HD22	59:BZ:284:LEU:HD13	1.96	0.46
59:BZ:280:LEU:HA	59:BZ:281:PRO:HD3	1.76	0.46
59:BZ:342:TYR:N	59:BZ:390:VAL:O	2.47	0.46
1:CA:491:G:H2'	1:CA:492:A:H8	1.81	0.46
1:CA:1210:A:H5"	1:CA:1212:G:O4'	2.16	0.46
1:CA:2079:U:O3'	25:C1:35:THR:OG1	2.32	0.46
1:CA:2113:U:H3	1:CA:2170:A:N6	2.13	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:2173:A:H2'	1:CA:2174:C:O4'	2.16	0.46
1:CA:2422:A:H5'	58:DY:76:A:H62	1.80	0.46
7:CG:103:LEU:HD23	7:CG:106:LEU:HD23	1.98	0.46
7:CG:109:VAL:HG21	28:C4:14:ILE:HD13	1.96	0.46
8:CH:90:LYS:HD2	8:CH:163:TYR:CD1	2.51	0.46
12:CO:64:ARG:HG2	12:CO:79:PHE:CD1	2.50	0.46
17:CT:106:SER:O	17:CT:110:ILE:HG13	2.15	0.46
34:DA:109:A:H2'	34:DA:326:G:N2	2.29	0.46
34:DA:921:U:H2'	34:DA:922:G:O4'	2.16	0.46
34:DA:1241:G:H2'	34:DA:1242:C:C6	2.51	0.46
34:DA:1318:A:H5"	52:DS:3:ARG:HH22	1.80	0.46
35:DB:90:MET:SD	35:DB:222:ILE:HD12	2.55	0.46
36:DC:77:ILE:HG13	36:DC:78:GLY:H	1.79	0.46
38:DE:5:ASP:OD1	38:DE:5:ASP:N	2.49	0.46
39:DF:30:LEU:HB3	39:DF:35:ALA:HB3	1.98	0.46
56:DW:44:G:H2'	56:DW:45:U:H5'	1.97	0.46
59:DZ:606:MET:HE2	59:DZ:671:MET:HE3	1.97	0.46
1:AA:553:A:C2	1:AA:2065:C:H4'	2.49	0.46
1:AA:834:U:H5"	1:AA:835:A:H5'	1.98	0.46
1:AA:1993:A:OP1	65:AA:3932:HOH:O	2.20	0.46
23:AZ:128:VAL:HG23	23:AZ:161:VAL:HA	1.97	0.46
34:BA:1104:G:H2'	34:BA:1105:A:H8	1.81	0.46
34:BA:1260:C:O5'	34:BA:1284:C:H4'	2.16	0.46
59:BZ:87:HIS:O	59:BZ:90:PHE:N	2.45	0.46
59:BZ:520:GLY:H	59:BZ:562:ASP:CG	2.23	0.46
1:CA:27:G:C2	1:CA:512:G:N3	2.83	0.46
1:CA:271(O):C:H2'	1:CA:271(P):C:C6	2.51	0.46
1:CA:1584:C:H2'	1:CA:1586:A:H5'	1.97	0.46
1:CA:2395:C:H2'	1:CA:2396:G:O4'	2.15	0.46
3:CC:48:LEU:HD23	3:CC:59:VAL:HG21	1.98	0.46
3:CC:211:ARG:HG2	3:CC:211:ARG:HH11	1.81	0.46
5:CE:60:ASN:CG	5:CE:62:PRO:HD2	2.41	0.46
5:CE:176:ILE:HB	5:CE:181:LEU:HB2	1.97	0.46
12:CO:111:PHE:O	12:CO:115:VAL:HG23	2.15	0.46
15:CR:33:ARG:HE	15:CR:113:LEU:HD22	1.80	0.46
20:CW:1:MET:HE3	20:CW:2:GLU:H	1.81	0.46
22:CY:9:LYS:HA	22:CY:10:GLY:HA2	1.59	0.46
22:CY:44:ILE:HA	22:CY:63:LYS:O	2.16	0.46
34:DA:955:U:H2'	34:DA:956:U:O4'	2.16	0.46
34:DA:1305:G:H5'	54:DU:4:GLY:HA3	1.97	0.46
40:DG:113:GLU:HB2	40:DG:119:ARG:HG2	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:DL:85:ILE:HG22	45:DL:100:ILE:HG12	1.97	0.46
1:AA:1550:C:H2'	1:AA:1551:C:C6	2.51	0.46
15:AR:44:LEU:HD22	15:AR:48:VAL:HG23	1.98	0.46
23:AZ:139:VAL:HG22	23:AZ:155:LEU:HD11	1.96	0.46
34:BA:189(B):C:N3	34:BA:189(J):G:C2	2.84	0.46
34:BA:1161:C:H2'	34:BA:1162:C:C6	2.51	0.46
43:BJ:31:GLY:HA2	43:BJ:32:ALA:HA	1.44	0.46
59:BZ:177:ILE:HD12	59:BZ:188:TYR:HE2	1.80	0.46
59:BZ:617:MET:HG2	59:BZ:643:ILE:HD11	1.96	0.46
1:CA:1902:C:H5'	4:CD:246:PRO:HD3	1.98	0.46
1:CA:2726:U:H4'	12:CO:1:MET:HE1	1.98	0.46
2:CB:76:G:H2'	2:CB:77:U:O4'	2.16	0.46
3:CC:46:ALA:O	3:CC:47:LYS:HB2	2.15	0.46
5:CE:108:SER:HB3	5:CE:165:VAL:HG21	1.97	0.46
18:CU:104:GLN:H	18:CU:104:GLN:CD	2.21	0.46
34:DA:1095:U:H2'	34:DA:1096:C:O4'	2.16	0.46
34:DA:1216:G:H5"	47:DN:5:ALA:HB2	1.97	0.46
36:DC:54:ARG:HB3	36:DC:54:ARG:NH1	2.30	0.46
48:DO:25:THR:HG21	48:DO:70:LEU:HB2	1.98	0.46
59:DZ:236:GLU:H	59:DZ:236:GLU:HG3	1.40	0.46
1:AA:801:C:H2'	1:AA:802:C:H6	1.81	0.46
1:AA:1067:A:H62	1:AA:1186:U:H3	1.63	0.46
1:AA:2087:C:H2'	1:AA:2088:C:C6	2.51	0.46
1:AA:2365:G:H1'	24:A0:34:GLY:HA3	1.97	0.46
2:AB:7:G:H5'	16:AS:29:PHE:CE2	2.51	0.46
32:A8:29:LYS:HB2	32:A8:33:ASN:HD21	1.81	0.46
34:BA:973:G:H3'	34:BA:974:A:H5"	1.98	0.46
34:BA:1350:A:C6	34:BA:1351:U:N3	2.84	0.46
37:BD:120:LEU:HB3	37:BD:126:ILE:HD11	1.97	0.46
40:BG:104:LEU:HD13	40:BG:104:LEU:HA	1.55	0.46
46:BM:65:LYS:O	46:BM:70:LEU:HG	2.16	0.46
57:BX:23:C:H2'	57:BX:24:U:C6	2.51	0.46
59:BZ:-38:TYR:CD2	59:BZ:-37:LEU:HD23	2.51	0.46
59:BZ:171:GLU:C	59:BZ:173:THR:H	2.23	0.46
1:CA:577:G:O2'	1:CA:1254:A:OP1	2.29	0.46
1:CA:1053:C:H2'	1:CA:1054:A:O5'	2.16	0.46
1:CA:1545:A:H2'	1:CA:1546:C:O4'	2.16	0.46
1:CA:1589:C:H2'	1:CA:1590:U:H6	1.78	0.46
1:CA:2630:G:H2'	1:CA:2631:G:C8	2.50	0.46
1:CA:2677:G:H2'	1:CA:2678:C:C6	2.51	0.46
1:CA:2741:A:H2'	1:CA:2742:C:O4'	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:C7:24:THR:O	31:C7:28:ARG:HG3	2.16	0.46
35:DB:96:ARG:O	35:DB:98:LEU:N	2.49	0.46
37:DD:4:TYR:O	37:DD:5:ILE:HG22	2.16	0.46
39:DF:10:LEU:HD12	39:DF:85:VAL:HA	1.98	0.46
59:DZ:-41:ALA:O	59:DZ:-36:LEU:HB2	2.16	0.46
59:DZ:546:ILE:HD13	59:DZ:565:VAL:HG11	1.98	0.46
1:AA:1153:G:H4'	9:AK:81:VAL:HA	1.98	0.45
1:AA:1179:U:O2'	1:AA:1182:G:OP1	2.31	0.45
1:AA:1314:A:H2'	1:AA:1315:A:O4'	2.16	0.45
1:AA:1345:G:H5'	1:AA:1347:A:O4'	2.16	0.45
1:AA:1462:G:O2'	1:AA:1463:C:H5	1.99	0.45
1:AA:1529:G:C6	1:AA:1553:A:C6	3.04	0.45
1:AA:2128:G:H1	1:AA:2205:C:N4	2.05	0.45
2:AB:7:G:H5'	16:AS:29:PHE:CD2	2.51	0.45
8:AH:90:LYS:HD2	8:AH:163:TYR:CD1	2.52	0.45
12:AO:115:VAL:HG13	12:AO:121:VAL:HG21	1.98	0.45
14:AQ:2:LEU:HB2	14:AQ:70:PRO:CG	2.46	0.45
21:AX:13:LEU:HD11	26:A2:41:ILE:HG22	1.97	0.45
34:BA:228:A:H2'	34:BA:229:U:O4'	2.16	0.45
34:BA:236:G:OP1	50:BQ:40:LYS:NZ	2.49	0.45
34:BA:1298:C:H4'	34:BA:1299:A:C4	2.51	0.45
35:BB:21:ARG:H	35:BB:21:ARG:HH21	1.65	0.45
46:BM:94:ARG:NH1	52:BS:80:TYR:HD2	2.14	0.45
1:CA:784:A:H5'	1:CA:785:G:OP1	2.16	0.45
1:CA:1063:G:H2'	1:CA:1064:C:C6	2.50	0.45
3:CC:37:LYS:O	3:CC:38:PHE:HB3	2.17	0.45
5:CE:21:VAL:HA	5:CE:22:PRO:HD3	1.72	0.45
34:DA:242:C:H2'	34:DA:243:A:H5'	1.96	0.45
34:DA:860:A:N6	34:DA:861:G:C2	2.84	0.45
34:DA:1023:G:H3'	34:DA:1024:G:H8	1.81	0.45
34:DA:1254:C:O5'	34:DA:1254:C:H6	1.99	0.45
34:DA:1431:C:H2'	34:DA:1432:G:O4'	2.16	0.45
36:DC:18:TRP:NE1	47:DN:55:GLY:H	2.14	0.45
41:DH:127:LEU:HA	41:DH:127:LEU:HD13	1.73	0.45
45:DL:6:THR:HG23	45:DL:9:GLN:OE1	2.16	0.45
46:DM:20:THR:C	46:DM:22:ILE:H	2.24	0.45
49:DP:74:LEU:HG	49:DP:79:VAL:HG21	1.97	0.45
59:DZ:75:LYS:HA	59:DZ:75:LYS:NZ	2.31	0.45
1:AA:67:G:H2'	1:AA:68:C:O4'	2.16	0.45
1:AA:669:A:H4'	1:AA:670:C:H5	1.81	0.45
1:AA:1097:G:H1	1:AA:1154:U:H5	1.64	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1261:G:OP2	18:AU:12:ARG:NH2	2.42	0.45
1:AA:2299:A:N6	1:AA:2356:U:H3	2.05	0.45
1:AA:2451:A:C5'	1:AA:2451:A:C8	3.00	0.45
1:AA:2812:A:H1'	1:AA:2904:U:H1'	1.97	0.45
5:AE:167:VAL:HG23	5:AE:170:LEU:HD11	1.98	0.45
21:AX:43:VAL:HG13	21:AX:47:PHE:HD2	1.81	0.45
28:A4:14:ILE:HB	28:A4:22:ILE:HB	1.97	0.45
33:A9:3:VAL:C	33:A9:4:ARG:HG3	2.40	0.45
36:BC:45:LYS:HE3	36:BC:45:LYS:HB2	1.78	0.45
40:BG:78:ARG:NH1	40:BG:79:ARG:HD2	2.31	0.45
44:BK:120:ARG:HA	44:BK:121:PRO:HD3	1.79	0.45
58:BY:40:C:H2'	58:BY:41:C:H6	1.82	0.45
1:CA:1022:G:C5	1:CA:1140:C:C4	3.04	0.45
1:CA:1406:U:H2'	1:CA:1407:C:C6	2.50	0.45
1:CA:1477:A:C2	1:CA:1515:G:C2	3.05	0.45
1:CA:1803:A:H4'	4:CD:259:THR:HG23	1.99	0.45
1:CA:2123:G:H2'	1:CA:2124:G:C8	2.51	0.45
1:CA:2722:G:H2'	1:CA:2723:C:C6	2.51	0.45
2:CB:21:G:H2'	2:CB:22:U:O4'	2.16	0.45
8:CH:144:VAL:O	8:CH:148:ILE:HG12	2.16	0.45
28:C4:33:VAL:HG12	28:C4:35:VAL:H	1.81	0.45
34:DA:160:A:H2'	34:DA:161:A:O4'	2.16	0.45
34:DA:601:C:H2'	34:DA:602:A:C8	2.51	0.45
34:DA:731:G:H5'	34:DA:766:A:H4'	1.97	0.45
34:DA:980:C:HO2'	47:DN:21:TYR:HE2	1.64	0.45
35:DB:44:LEU:HD22	35:DB:44:LEU:H	1.81	0.45
37:DD:135:LEU:C	37:DD:137:SER:H	2.23	0.45
37:DD:153:ARG:HB2	37:DD:181:MET:SD	2.57	0.45
46:DM:90:LEU:HD22	46:DM:93:ARG:HE	1.81	0.45
53:DT:36:LEU:HD12	53:DT:55:ILE:HG23	1.97	0.45
57:DX:72:A:C6	57:DX:73:A:C6	3.04	0.45
58:DY:30:G:H2'	58:DY:31:A:H8	1.81	0.45
59:DZ:166:LEU:O	59:DZ:178:ILE:N	2.41	0.45
59:DZ:609:GLU:O	59:DZ:669:PHE:HA	2.15	0.45
1:AA:354:A:H2	1:AA:1255:A:O2'	1.99	0.45
1:AA:2199:C:O2	3:AC:173:HIS:HE1	1.99	0.45
1:AA:2500:A:H2'	1:AA:2501:G:O4'	2.16	0.45
4:AD:85:ASP:OD2	4:AD:88:ARG:HD2	2.15	0.45
4:AD:106:ILE:O	4:AD:108:PRO:HD3	2.16	0.45
11:AN:4:TYR:CD2	18:AU:100:VAL:HG11	2.52	0.45
21:AX:61:GLY:HA3	21:AX:73:ARG:O	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:BA:13:U:OP1	65:BA:1911:HOH:O	2.21	0.45
34:BA:255:G:H2'	34:BA:256:U:C6	2.52	0.45
34:BA:1417:G:N2	34:BA:1482:G:H2'	2.32	0.45
37:BD:194:LEU:HD12	37:BD:195:ALA:H	1.81	0.45
44:BK:20:TYR:HB2	44:BK:31:THR:CG2	2.46	0.45
44:BK:59:TYR:CE2	44:BK:63:LEU:HD12	2.51	0.45
49:BP:40:ASP:HA	49:BP:41:PRO:HD2	1.76	0.45
53:BT:42:GLN:HG3	53:BT:43:LEU:HD23	1.99	0.45
57:BX:67:C:C2'	57:BX:68:C:H5'	2.46	0.45
59:BZ:10:LYS:O	59:BZ:282:SER:HB2	2.16	0.45
59:BZ:264:LEU:HD12	64:BZ:702:GDP:N3	2.31	0.45
59:BZ:634:MET:HE3	59:BZ:634:MET:HB3	1.81	0.45
1:CA:602:G:O2'	1:CA:655:A:N6	2.49	0.45
1:CA:2029:G:H2'	1:CA:2031:A:OP1	2.16	0.45
1:CA:2135:A:H2'	1:CA:2136:C:C6	2.51	0.45
22:CY:83:THR:OG1	22:CY:84:ARG:N	2.50	0.45
23:CZ:45:ASP:O	23:CZ:49:ARG:HG3	2.16	0.45
34:DA:302:G:N3	34:DA:556:C:H4'	2.30	0.45
34:DA:369:C:OP2	34:DA:388:G:N2	2.37	0.45
34:DA:757:U:H2'	34:DA:758:G:O4'	2.15	0.45
34:DA:1024:G:C2'	34:DA:1025:U:H5"	2.45	0.45
34:DA:1104:G:C4	34:DA:1105:A:C8	3.04	0.45
34:DA:1205:U:H4'	36:DC:195:VAL:HG23	1.97	0.45
34:DA:1216:G:H5"	47:DN:5:ALA:CB	2.46	0.45
36:DC:104:GLN:HE21	36:DC:105:GLU:N	2.13	0.45
54:DU:2:GLY:O	54:DU:4:GLY:N	2.49	0.45
59:DZ:560:VAL:HG11	59:DZ:594:VAL:HG11	1.99	0.45
1:AA:611:U:O4	1:AA:717:A:H1'	2.15	0.45
1:AA:2804:C:H2'	1:AA:2805:G:H8	1.82	0.45
7:AG:120:LEU:HD12	7:AG:179:PRO:HD2	1.99	0.45
7:AG:125:PHE:HB3	7:AG:166:ASP:CG	2.41	0.45
8:AH:41:MET:CE	8:AH:65:HIS:HA	2.46	0.45
28:A4:59:PHE:HA	28:A4:61:ARG:HG2	1.98	0.45
34:BA:435:C:H2'	34:BA:436:C:C6	2.51	0.45
34:BA:580:U:H2'	34:BA:581:G:O4'	2.16	0.45
34:BA:695:A:H2'	34:BA:696:A:O4'	2.17	0.45
34:BA:718:G:C8	44:BK:116:HIS:HB3	2.51	0.45
43:BJ:64:GLU:HB3	47:BN:59:ALA:HB2	1.99	0.45
43:BJ:67:THR:O	43:BJ:67:THR:OG1	2.34	0.45
47:BN:23:ARG:HD2	47:BN:28:GLY:O	2.16	0.45
59:BZ:14:ASN:OD1	59:BZ:80:ASN:HB2	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:1364:G:P	25:C1:3:LYS:HG3	2.56	0.45
1:CA:1488:G:C6	1:CA:1489:U:N3	2.85	0.45
1:CA:1773:A:H5"	65:CA:4070:HOH:O	2.15	0.45
1:CA:2135:A:OP1	1:CA:2160:G:H1'	2.16	0.45
1:CA:2881:C:H2'	1:CA:2882:A:O4'	2.16	0.45
4:CD:71:ASP:HB3	4:CD:103:ARG:NH2	2.32	0.45
6:CF:184:TYR:O	6:CF:188:ARG:HG3	2.15	0.45
28:C4:16:CYS:SG	28:C4:36:CYS:HB3	2.57	0.45
34:DA:604:G:H2'	34:DA:605:U:O4'	2.16	0.45
34:DA:641:U:O2	34:DA:642:A:N6	2.25	0.45
49:DP:22:THR:HA	49:DP:33:ILE:HG13	1.99	0.45
59:DZ:74:TRP:HA	59:DZ:74:TRP:CE3	2.49	0.45
59:DZ:215:LYS:O	59:DZ:219:VAL:HG23	2.16	0.45
1:AA:303:C:H42	1:AA:385:G:H1	1.63	0.45
1:AA:386:U:O2'	1:AA:387:G:H5"	2.16	0.45
1:AA:555:G:C5	1:AA:2044:U:H5"	2.51	0.45
1:AA:1336:C:H2'	1:AA:1337:C:C6	2.52	0.45
1:AA:1848:G:H2'	1:AA:1849:U:H5'	1.98	0.45
1:AA:2556:G:H1'	1:AA:2658:C:H4'	1.99	0.45
1:AA:2702:C:OP2	1:AA:2702:C:H6	1.99	0.45
1:AA:2891:C:H2'	1:AA:2892:A:O4'	2.17	0.45
2:AB:32:C:C2	2:AB:51:G:N2	2.85	0.45
3:AC:37:LYS:O	3:AC:38:PHE:HB3	2.17	0.45
3:AC:48:LEU:HD23	3:AC:59:VAL:HG21	1.98	0.45
23:AZ:28:MET:HA	23:AZ:88:PHE:O	2.17	0.45
28:A4:40:HIS:CE1	28:A4:42:PHE:HB3	2.52	0.45
34:BA:1118:C:OP1	42:BI:104:ARG:NH1	2.49	0.45
34:BA:1392:G:H21	34:BA:1502:A:H8	1.63	0.45
35:BB:16:HIS:CD2	35:BB:17:PHE:N	2.85	0.45
35:BB:208:ILE:H	35:BB:208:ILE:HD12	1.82	0.45
37:BD:65:ARG:HG2	37:BD:75:PHE:CD1	2.52	0.45
37:BD:126:ILE:HG22	37:BD:127:THR:H	1.82	0.45
40:BG:12:LEU:H	40:BG:12:LEU:HD12	1.80	0.45
48:BO:25:THR:HG21	48:BO:70:LEU:HB2	1.96	0.45
59:BZ:660:ARG:HE	59:BZ:665:GLY:HA2	1.82	0.45
1:CA:72:U:OP2	26:C2:29:LYS:NZ	2.44	0.45
1:CA:271(H):G:O2'	1:CA:271(I):G:H8	2.00	0.45
1:CA:1109:C:H2'	1:CA:1110:G:N7	2.31	0.45
1:CA:2275:C:H5'	1:CA:2275:C:C6	2.51	0.45
3:CC:20:VAL:O	3:CC:224:ARG:O	2.34	0.45
8:CH:3:ARG:NH2	8:CH:5:GLY:H	2.14	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:CN:4:TYR:CD2	18:CU:100:VAL:HG11	2.51	0.45
16:CS:3:ARG:HE	16:CS:4:LEU:N	2.14	0.45
18:CU:27:LEU:HB3	18:CU:31:SER:HB3	1.98	0.45
34:DA:97:G:O2'	34:DA:98:G:H5"	2.16	0.45
34:DA:545:C:O2'	34:DA:549:C:OP1	2.31	0.45
34:DA:1244:C:O2	34:DA:1294:G:N2	2.49	0.45
52:DS:15:LEU:HD12	52:DS:18:LYS:HD2	1.98	0.45
59:DZ:20:HIS:CE1	59:DZ:117:GLN:HG3	2.52	0.45
59:DZ:552:SER:HB3	59:DZ:591:LYS:HZ2	1.80	0.45
1:AA:517:A:H2'	1:AA:518:G:O4'	2.17	0.45
1:AA:2051:G:H2'	1:AA:2053:A:OP1	2.16	0.45
1:AA:2564:U:O2	1:AA:2566:U:H5'	2.17	0.45
1:AA:2792:U:H5'	1:AA:2794:A:O4'	2.16	0.45
13:AP:63:PRO:HG2	32:A8:25:MET:HB2	1.97	0.45
20:AW:10:VAL:HG21	20:AW:103:ILE:HD12	1.98	0.45
22:AY:92:ASN:HD22	22:AY:92:ASN:N	2.07	0.45
25:A1:94:LEU:HD23	25:A1:94:LEU:HA	1.72	0.45
32:A8:54:GLU:OE1	32:A8:54:GLU:HA	2.17	0.45
33:A9:7:VAL:HG12	33:A9:34:GLN:HB3	1.97	0.45
34:BA:262:A:C6	34:BA:263:A:C6	3.04	0.45
34:BA:667:G:H4'	48:BO:51:HIS:ND1	2.32	0.45
34:BA:865:A:H2'	34:BA:866:C:C6	2.52	0.45
37:BD:108:LEU:HB3	37:BD:110:PHE:CE1	2.52	0.45
40:BG:91:VAL:HB	40:BG:96:GLN:HG2	1.99	0.45
42:BI:46:ALA:HB1	42:BI:77:ILE:HG22	1.98	0.45
50:BQ:32:TYR:O	50:BQ:34:LYS:N	2.41	0.45
59:BZ:-9:LEU:HD12	59:BZ:-9:LEU:HA	1.71	0.45
59:BZ:93:GLU:HA	59:BZ:96:ARG:HG3	1.99	0.45
59:BZ:182:ARG:O	59:BZ:184:LYS:N	2.50	0.45
1:CA:1064:C:H3'	1:CA:1065:U:C6	2.51	0.45
1:CA:2318:G:N3	1:CA:2318:G:O2'	2.48	0.45
1:CA:2631:G:O2'	1:CA:2810:A:N1	2.42	0.45
3:CC:194:ILE:HD11	3:CC:227:PRO:HB2	1.99	0.45
3:CC:223:VAL:HG23	3:CC:223:VAL:O	2.15	0.45
16:CS:94:TYR:CE1	16:CS:99:LYS:HG3	2.52	0.45
26:C2:37:PHE:O	26:C2:40:SER:OG	2.31	0.45
29:C5:20:ARG:HG2	29:C5:23:HIS:CE1	2.51	0.45
34:DA:503:C:H2'	34:DA:504:C:H6	1.81	0.45
35:DB:51:LEU:O	35:DB:55:PHE:N	2.25	0.45
36:DC:105:GLU:OE1	36:DC:107:GLN:N	2.50	0.45
37:DD:31:CYS:O	37:DD:35:ARG:HG3	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:DD:163:GLU:O	37:DD:166:LYS:HG3	2.16	0.45
39:DF:2:ARG:HE	39:DF:69:GLU:HG2	1.80	0.45
59:DZ:357:ARG:NH1	59:DZ:373:ASP:OD1	2.49	0.45
1:AA:269:G:N7	1:AA:270:C:N4	2.65	0.45
1:AA:471:C:H2'	1:AA:472:G:O4'	2.16	0.45
1:AA:1817:A:H1'	1:AA:1960:A:N6	2.32	0.45
1:AA:2105:G:O5'	1:AA:2105:G:H8	2.00	0.45
1:AA:2343:G:O2'	24:A0:43:THR:HG22	2.17	0.45
1:AA:2575:U:O2	1:AA:2577:A:H8	2.00	0.45
3:AC:7:ARG:HH22	3:AC:219:MET:HB2	1.82	0.45
3:AC:16:ASP:OD2	3:AC:19:LYS:HB2	2.17	0.45
5:AE:110:GLY:O	65:AR:5101:HOH:O	2.21	0.45
7:AG:115:ARG:HH11	7:AG:137:GLU:CD	2.25	0.45
34:BA:949:A:H2'	34:BA:950:U:O4'	2.17	0.45
34:BA:1402:C:H2'	34:BA:1403:C:O4'	2.17	0.45
35:BB:172:ILE:H	35:BB:172:ILE:HG13	1.56	0.45
39:BF:33:TYR:HE2	39:BF:78:GLU:HG2	1.81	0.45
57:BX:19:G:C5	57:BX:57:A:C2	3.05	0.45
59:BZ:78:ARG:HE	59:BZ:357:ARG:CZ	2.29	0.45
59:BZ:82:ILE:HD13	59:BZ:100:VAL:HG12	1.98	0.45
1:CA:263:C:H2'	1:CA:264:C:O4'	2.17	0.45
1:CA:1019:U:O2'	1:CA:1021:A:H2	1.99	0.45
1:CA:1030:G:N2	33:C9:5:ALA:O	2.50	0.45
1:CA:1043:C:H2'	1:CA:1044:G:H8	1.82	0.45
2:CB:106:G:H5'	23:CZ:31:ARG:HG2	1.97	0.45
6:CF:196:LEU:HA	6:CF:196:LEU:HD23	1.54	0.45
8:CH:7:LEU:HD23	8:CH:69:ARG:NH1	2.31	0.45
22:CY:35:TYR:CD2	22:CY:69:ALA:HB3	2.51	0.45
34:DA:429:U:H5'	37:DD:9:CYS:SG	2.56	0.45
34:DA:1097:C:H2'	34:DA:1098:C:H6	1.81	0.45
38:DE:36:ASP:C	38:DE:38:GLN:H	2.24	0.45
44:DK:73:MET:HE1	44:DK:102:GLY:HA3	1.99	0.45
49:DP:14:ASN:N	49:DP:15:PRO:HD3	2.31	0.45
59:DZ:535:PRO:O	59:DZ:539:ILE:HG12	2.17	0.45
1:AA:733:G:OP1	31:A7:11:LYS:NZ	2.50	0.45
1:AA:1378:G:OP1	65:AA:3934:HOH:O	2.21	0.45
1:AA:1476:C:H2'	1:AA:1477:U:H6	1.81	0.45
1:AA:1478:C:H2'	1:AA:1479:U:O4'	2.16	0.45
1:AA:1671:C:H2'	1:AA:1672:G:O4'	2.17	0.45
3:AC:54:ARG:HH22	3:AC:56:ASP:HB3	1.76	0.45
23:AZ:45:ASP:CG	23:AZ:49:ARG:HH11	2.25	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:BA:443:C:O2	34:BA:491:G:N2	2.37	0.45
59:BZ:-32:LEU:HD23	59:BZ:-32:LEU:HA	1.82	0.45
59:BZ:14:ASN:HD22	59:BZ:329:ARG:HH21	1.64	0.45
59:BZ:87:HIS:CB	59:BZ:90:PHE:HB3	2.46	0.45
59:BZ:304:ASP:HA	59:BZ:305:PRO:HD2	1.81	0.45
1:CA:362:U:O2'	1:CA:363:G:H5'	2.17	0.45
1:CA:533:G:H5'	18:CU:24:TYR:CE1	2.52	0.45
1:CA:994:C:OP2	18:CU:54:LYS:NZ	2.50	0.45
1:CA:2751:G:H4'	8:CH:4:ILE:HD11	1.99	0.45
7:CG:115:ARG:HH11	7:CG:115:ARG:H	1.63	0.45
23:CZ:40:ASP:HB3	23:CZ:43:GLU:HG3	1.98	0.45
34:DA:644:G:H4'	41:DH:92:ARG:NH2	2.31	0.45
34:DA:926:G:C6	34:DA:1505:G:C5	3.05	0.45
36:DC:148:GLY:HA3	36:DC:172:ARG:O	2.16	0.45
1:AA:669:A:H4'	1:AA:670:C:C5	2.52	0.45
5:AE:47:VAL:HG22	5:AE:84:PHE:O	2.17	0.45
8:AH:13:LYS:HA	8:AH:14:GLY:HA2	1.71	0.45
8:AH:71:LEU:HD12	8:AH:71:LEU:HA	1.81	0.45
13:AP:125:VAL:O	13:AP:125:VAL:HG23	2.17	0.45
29:A5:35:GLU:HG3	29:A5:51:TYR:CG	2.52	0.45
51:BR:66:LEU:O	51:BR:70:ILE:HG13	2.17	0.45
53:BT:100:ILE:H	53:BT:100:ILE:HG12	1.43	0.45
59:BZ:98:MET:HG2	59:BZ:101:LEU:HD12	1.98	0.45
1:CA:271(A):A:N7	1:CA:271(W):G:N2	2.60	0.45
1:CA:2727:G:O2'	12:CO:70:LYS:NZ	2.48	0.45
23:CZ:120:ILE:HD11	23:CZ:171:ILE:C	2.42	0.45
25:C1:77:ALA:HB1	25:C1:82:LEU:HD11	1.99	0.45
34:DA:49:U:O4	34:DA:365:U:H5	2.00	0.45
34:DA:111:G:O6	34:DA:330:C:N4	2.44	0.45
34:DA:176:C:H2'	34:DA:177:C:H6	1.81	0.45
34:DA:297:G:N2	34:DA:300:A:OP2	2.45	0.45
34:DA:600:C:C2	34:DA:639:G:C2	3.05	0.45
34:DA:1058:G:H2'	34:DA:1059:C:C6	2.52	0.45
34:DA:1151:A:O2'	34:DA:1152:A:H8	2.00	0.45
34:DA:1157:A:H5'	34:DA:1158:C:C6	2.52	0.45
38:DE:71:LEU:HD21	38:DE:114:GLY:C	2.41	0.45
42:DI:9:ARG:O	42:DI:104:ARG:HG3	2.17	0.45
59:DZ:181:LEU:O	59:DZ:183:MET:N	2.50	0.45
59:DZ:517:LEU:HD13	59:DZ:564:LYS:HB2	1.99	0.45
1:AA:2228:G:O2'	1:AA:2229:A:OP1	2.31	0.45
2:AB:91:C:OP1	14:AQ:16:ARG:HG3	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:179:ALA:O	3:AC:180:SER:O	2.35	0.45
4:AD:93:ALA:HB3	4:AD:105:ILE:HG13	1.99	0.45
10:AL:103:GLN:HA	10:AL:106:GLU:HG2	1.98	0.45
15:AR:54:LEU:HD12	15:AR:54:LEU:HA	1.66	0.45
24:A0:24:LYS:O	24:A0:25:ARG:HD3	2.16	0.45
34:BA:453:A:C6	34:BA:454:C:C4	3.05	0.45
34:BA:620:C:H2'	34:BA:621:A:O4'	2.16	0.45
34:BA:838:G:N2	34:BA:849:C:C2	2.85	0.45
48:BO:14:GLU:O	48:BO:14:GLU:HG3	2.17	0.45
49:BP:74:LEU:HG	49:BP:79:VAL:HG21	1.99	0.45
59:BZ:-66:MET:N	59:BZ:-46:VAL:O	2.49	0.45
59:BZ:178:ILE:HA	59:BZ:185:ALA:HB2	1.99	0.45
1:CA:89:G:H3'	1:CA:90:U:H5"	1.98	0.45
1:CA:1059:G:O2'	10:CL:126:MET:O	2.28	0.45
1:CA:1494:A:H2'	1:CA:1495:A:C8	2.52	0.45
1:CA:2298:A:N6	1:CA:2318:G:C8	2.85	0.45
3:CC:30:VAL:CG2	3:CC:31:LYS:H	2.27	0.45
3:CC:179:ALA:O	3:CC:180:SER:O	2.35	0.45
5:CE:31:CYS:HA	5:CE:32:PRO:HD2	1.83	0.45
11:CN:58:ASP:OD1	11:CN:125:GLY:N	2.32	0.45
23:CZ:104:PHE:HA	23:CZ:139:VAL:HB	1.99	0.45
25:C1:3:LYS:HB2	25:C1:61:ARG:HH11	1.79	0.45
34:DA:10:A:OP2	38:DE:126:ARG:HD2	2.17	0.45
34:DA:1254:C:OP1	43:DJ:45:ARG:HA	2.16	0.45
36:DC:130:VAL:O	36:DC:134:ILE:HG12	2.17	0.45
38:DE:144:THR:OG1	38:DE:147:ASP:OD2	2.24	0.45
44:DK:48:ILE:C	44:DK:50:TYR:H	2.24	0.45
45:DL:70:ILE:HD13	45:DL:75:HIS:CD2	2.51	0.45
46:DM:59:TYR:CE1	46:DM:63:THR:HG21	2.52	0.45
50:DQ:40:LYS:HD3	50:DQ:42:TYR:CZ	2.52	0.45
56:DW:21:A:N6	56:DW:46:7MG:C4	2.85	0.45
59:DZ:246:ILE:HG23	59:DZ:255:ILE:HD11	1.99	0.45
59:DZ:257:PRO:HB2	59:DZ:259:PHE:HE1	1.82	0.45
59:DZ:462:ILE:O	59:DZ:466:LEU:HB2	2.17	0.45
1:AA:864:C:O2'	1:AA:886:U:H5"	2.17	0.44
1:AA:987:G:O2'	1:AA:988:U:H5'	2.17	0.44
1:AA:1002:A:N1	1:AA:2470:G:H4'	2.32	0.44
1:AA:1108:G:H1	1:AA:1122:C:H42	1.65	0.44
1:AA:2650:G:P	5:AE:82:ARG:NH2	2.90	0.44
5:AE:120:TRP:CE2	5:AE:155:LYS:HG2	2.52	0.44
11:AN:39:ARG:HA	11:AN:40:PRO:HD3	1.80	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:A4:15:ILE:HD13	28:A4:21:VAL:HG13	1.99	0.44
34:BA:43:C:H42	34:BA:399:G:H1	1.65	0.44
34:BA:506:G:C5	34:BA:507:C:C4	3.05	0.44
34:BA:551:U:H2'	34:BA:552:U:C6	2.52	0.44
34:BA:1005:A:H1'	34:BA:1036:G:H22	1.82	0.44
34:BA:1014:A:H4'	52:BS:14:HIS:CD2	2.52	0.44
34:BA:1152:A:OP1	43:BJ:68:HIS:ND1	2.49	0.44
35:BB:162:ILE:HD11	35:BB:184:VAL:HG22	1.99	0.44
43:BJ:78:ASN:O	43:BJ:80:LYS:N	2.50	0.44
52:BS:63:THR:HG23	52:BS:66:MET:HE3	1.98	0.44
59:BZ:-9:LEU:C	59:BZ:-7:GLU:H	2.25	0.44
1:CA:530:G:N3	1:CA:530:G:O4'	2.49	0.44
1:CA:1517:G:C6	1:CA:1518:U:N3	2.85	0.44
1:CA:2305:A:H2'	1:CA:2306:C:O4'	2.17	0.44
2:CB:3:C:H2'	2:CB:4:C:C6	2.52	0.44
3:CC:7:ARG:HH22	3:CC:219:MET:HB2	1.82	0.44
8:CH:3:ARG:HB3	8:CH:6:ARG:HG2	1.99	0.44
34:DA:15:G:H2'	34:DA:16:A:H8	1.81	0.44
34:DA:423:G:H3'	34:DA:423:G:N3	2.32	0.44
34:DA:838:G:H1	34:DA:848:C:N4	2.09	0.44
34:DA:1270:C:H2'	34:DA:1271:G:C8	2.51	0.44
34:DA:1320:C:OP1	52:DS:70:LYS:HE2	2.18	0.44
35:DB:54:THR:HG21	35:DB:201:ILE:HD11	1.98	0.44
37:DD:12:CYS:HB3	37:DD:17:VAL:O	2.17	0.44
47:DN:22:THR:HB	47:DN:33:VAL:CB	2.47	0.44
53:DT:56:MET:HE2	53:DT:56:MET:HB2	1.86	0.44
53:DT:92:LEU:HD23	53:DT:92:LEU:HA	1.81	0.44
58:DY:35:A:H2'	58:DY:36:A:O4'	2.17	0.44
58:DY:37:MIA:H2'	58:DY:38:A:O4'	2.17	0.44
59:DZ:552:SER:HB3	59:DZ:591:LYS:NZ	2.32	0.44
1:AA:116:A:H3'	1:AA:117:A:C5'	2.48	0.44
1:AA:320:C:H2'	1:AA:321:C:H6	1.81	0.44
1:AA:559:U:O2'	18:AU:49:HIS:ND1	2.46	0.44
1:AA:795:G:C8	20:AW:89:ALA:HB1	2.51	0.44
1:AA:866:A:H8	1:AA:866:A:H5'	1.82	0.44
1:AA:1099:C:H2'	1:AA:1100:A:H5"	1.99	0.44
1:AA:1177:G:H21	11:AN:73:THR:CG2	2.30	0.44
1:AA:1258:A:N3	1:AA:1284:G:O2'	2.49	0.44
1:AA:1355:G:P	31:A7:9:ARG:HD3	2.58	0.44
1:AA:1809:U:H2'	1:AA:1815:A:N6	2.33	0.44
34:BA:142:G:H2'	34:BA:143:A:C8	2.48	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:BA:841:U:H6	34:BA:841:U:OP2	2.00	0.44
34:BA:1036:G:H3'	34:BA:1037:C:C6	2.53	0.44
34:BA:1356:G:N2	34:BA:1367:C:O2	2.50	0.44
35:BB:223:ILE:HA	35:BB:226:ARG:HB2	2.00	0.44
42:BI:4:TYR:CE1	42:BI:88:TYR:HA	2.52	0.44
42:BI:26:VAL:HG22	42:BI:61:ALA:HB3	1.97	0.44
42:BI:49:PRO:HG3	42:BI:101:PHE:CD2	2.52	0.44
53:BT:45:GLN:HE21	53:BT:45:GLN:HB3	1.66	0.44
58:BY:48:C:OP1	58:BY:48:C:H2'	2.17	0.44
59:BZ:94:VAL:HA	59:BZ:97:SER:HB2	1.99	0.44
1:CA:118:A:O5'	1:CA:119:A:H5"	2.16	0.44
1:CA:300:A:H3'	22:CY:84:ARG:NH2	2.32	0.44
1:CA:601:C:OP1	6:CF:108:LYS:NZ	2.37	0.44
1:CA:647:G:H2'	1:CA:648:G:O4'	2.17	0.44
1:CA:851:U:H5'	27:C3:49:LYS:HD2	1.98	0.44
1:CA:1336:A:H2'	1:CA:1337:G:C8	2.53	0.44
1:CA:2139:C:N4	1:CA:2152:G:H1	2.15	0.44
1:CA:2303:G:O2'	7:CG:132:ASN:HB2	2.17	0.44
1:CA:2336:A:H61	24:C0:43:THR:CG2	2.30	0.44
4:CD:124:PRO:O	4:CD:126:GLN:N	2.51	0.44
7:CG:67:LYS:H	28:C4:6:HIS:CE1	2.35	0.44
10:CL:119:ASP:HB3	10:CL:120:LEU:H	1.66	0.44
28:C4:59:PHE:CE1	52:DS:64:GLU:HB2	2.52	0.44
34:DA:1252:A:H2'	34:DA:1253:G:O4'	2.17	0.44
35:DB:16:HIS:HB2	35:DB:204:ASN:ND2	2.32	0.44
36:DC:7:PRO:HG3	36:DC:201:TYR:CE2	2.51	0.44
38:DE:12:LEU:O	38:DE:30:ALA:HA	2.18	0.44
40:DG:73:MET:HE2	40:DG:73:MET:HB2	1.69	0.44
43:DJ:42:THR:CG2	43:DJ:68:HIS:HD2	2.30	0.44
50:DQ:7:THR:HA	50:DQ:57:VAL:O	2.17	0.44
59:DZ:632:LEU:HG	59:DZ:645:ALA:HA	1.99	0.44
1:AA:310:C:H2'	1:AA:311:C:C6	2.52	0.44
1:AA:395:C:H2'	1:AA:396:C:O4'	2.18	0.44
1:AA:886:U:H1'	1:AA:1236:G:H1'	1.99	0.44
1:AA:990:A:C4	1:AA:2460:A:C2	3.06	0.44
1:AA:2102:G:OP1	25:A1:35:THR:HG21	2.18	0.44
4:AD:246:PRO:O	4:AD:254:THR:HG22	2.17	0.44
13:AP:82:GLY:HA2	13:AP:113:LYS:O	2.17	0.44
34:BA:664:G:N2	34:BA:741:G:H1	2.03	0.44
34:BA:1075:C:H5"	35:BB:179:LYS:HE2	1.98	0.44
34:BA:1218:C:H2'	34:BA:1219:U:C6	2.51	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:BA:1323:G:H4'	34:BA:1363:C:N3	2.33	0.44
34:BA:1478:C:H2'	34:BA:1479:C:C6	2.52	0.44
38:BE:33:VAL:HG21	38:BE:109:ILE:HA	2.00	0.44
41:BH:86:ILE:HG21	41:BH:133:LEU:HD13	1.99	0.44
50:BQ:9:VAL:O	50:BQ:21:VAL:HA	2.17	0.44
58:BY:60:U:H5"	58:BY:61:C:C5	2.45	0.44
1:CA:661:C:H4'	13:CP:13:ASN:OD1	2.18	0.44
1:CA:1289:C:H2'	1:CA:1290:C:H6	1.80	0.44
1:CA:1434:A:H61	1:CA:1558:A:H62	1.64	0.44
1:CA:2607:G:H2'	1:CA:2608:G:O4'	2.17	0.44
34:DA:1082:G:H2'	34:DA:1083:U:O4'	2.17	0.44
34:DA:1119:C:OP1	42:DI:83:ARG:NH2	2.47	0.44
34:DA:1281:U:H5"	34:DA:1282:C:H5	1.81	0.44
35:DB:105:PHE:C	35:DB:107:THR:H	2.25	0.44
59:DZ:247:ARG:NH2	59:DZ:285:ASP:OD1	2.50	0.44
1:AA:1934:A:N1	34:BA:1407:C:O2'	2.48	0.44
5:AE:31:CYS:HA	5:AE:32:PRO:HD2	1.76	0.44
6:AF:64:ILE:HD11	6:AF:75:HIS:HB2	2.00	0.44
7:AG:121:ASN:HA	7:AG:122:PRO:HD3	1.81	0.44
13:AP:112:LEU:HD13	13:AP:127:ALA:HB2	1.99	0.44
14:AQ:62:GLY:HA2	23:AZ:116:VAL:HG21	2.00	0.44
26:A2:61:LEU:HD23	26:A2:61:LEU:HA	1.62	0.44
34:BA:102:G:O2'	34:BA:151:A:N3	2.44	0.44
34:BA:667:G:OP1	34:BA:732:C:O2'	2.21	0.44
34:BA:1129:C:H5"	42:BI:16:ARG:NH1	2.23	0.44
34:BA:1412:C:H2'	34:BA:1413:A:C8	2.53	0.44
35:BB:80:ILE:O	35:BB:80:ILE:HG13	2.17	0.44
35:BB:166:ASP:HB3	35:BB:169:LYS:HB2	1.99	0.44
38:BE:79:GLU:H	38:BE:79:GLU:HG3	1.61	0.44
41:BH:6:ILE:O	41:BH:10:LEU:HG	2.18	0.44
42:BI:11:LYS:C	42:BI:13:ALA:H	2.25	0.44
44:BK:30:VAL:HG21	44:BK:65:ALA:HA	1.98	0.44
59:BZ:418:LYS:HD3	59:BZ:418:LYS:HA	1.77	0.44
1:CA:858:U:O2	1:CA:2268:A:H2'	2.18	0.44
1:CA:1021:A:C8	1:CA:1021:A:C3'	3.00	0.44
1:CA:1434:A:O2'	1:CA:1435:G:H5'	2.17	0.44
1:CA:2466:C:H5'	33:C9:5:ALA:HB3	1.98	0.44
2:CB:8:U:O3'	16:CS:25:ARG:NH2	2.38	0.44
3:CC:16:ASP:OD2	3:CC:19:LYS:HB2	2.17	0.44
3:CC:174:ALA:HA	3:CC:175:PRO:HD3	1.82	0.44
4:CD:29:PRO:HA	4:CD:83:GLU:OE1	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:CD:94:LEU:O	4:CD:95:LEU:HD23	2.18	0.44
5:CE:96:PHE:O	5:CE:175:VAL:HG11	2.18	0.44
6:CF:36:VAL:HG11	6:CF:183:VAL:CG1	2.48	0.44
16:CS:25:ARG:NH1	16:CS:42:ASP:OD1	2.50	0.44
34:DA:235:C:H5'	50:DQ:70:ARG:HG2	1.98	0.44
34:DA:1013:G:N2	34:DA:1016:A:OP2	2.44	0.44
34:DA:1286:A:H8	34:DA:1287:A:H4'	1.81	0.44
34:DA:1323:G:H2'	34:DA:1324:A:C8	2.53	0.44
59:DZ:115:GLU:O	59:DZ:118:SER:HB2	2.17	0.44
59:DZ:127:LYS:HE2	59:DZ:128:TYR:HE2	1.81	0.44
1:AA:1495:G:H1'	1:AA:1574:A:N1	2.33	0.44
1:AA:2130:C:H2'	1:AA:2131:U:C6	2.51	0.44
1:AA:2417:G:OP1	13:AP:77:ARG:NH2	2.51	0.44
1:AA:2804:C:H2'	1:AA:2805:G:C8	2.53	0.44
27:A3:4:LEU:HD23	27:A3:4:LEU:HA	1.75	0.44
34:BA:410:G:H5"	34:BA:411:A:OP1	2.18	0.44
34:BA:1445:C:H2'	34:BA:1446:U:O4'	2.17	0.44
35:BB:71:VAL:HA	35:BB:93:VAL:HG23	2.00	0.44
1:CA:359:A:H2'	1:CA:360:G:O4'	2.18	0.44
1:CA:459:U:H5"	31:C7:40:TRP:CD2	2.53	0.44
1:CA:1074:G:H2'	1:CA:1075:C:C6	2.53	0.44
1:CA:1894:C:O2'	1:CA:1895:C:H5'	2.16	0.44
1:CA:2148:G:H2'	1:CA:2149:G:H8	1.81	0.44
1:CA:2638:G:P	5:CE:82:ARG:HH21	2.39	0.44
3:CC:68:GLY:N	3:CC:189:ASN:ND2	2.62	0.44
8:CH:73:ALA:O	8:CH:76:VAL:HB	2.18	0.44
13:CP:123:LEU:HD23	13:CP:123:LEU:HA	1.79	0.44
16:CS:105:ALA:O	16:CS:110:LEU:HB2	2.17	0.44
32:C8:31:HIS:O	32:C8:32:LEU:HB2	2.18	0.44
34:DA:235:C:H2'	34:DA:236:G:C8	2.52	0.44
34:DA:833:U:H2'	34:DA:834:C:H6	1.83	0.44
44:DK:43:SER:OG	44:DK:44:SER:N	2.51	0.44
59:DZ:168:ILE:N	59:DZ:176:GLY:O	2.50	0.44
59:DZ:604:PRO:HG2	59:DZ:649:LEU:HB3	1.98	0.44
1:AA:1941:A:H5"	1:AA:1942:C:OP2	2.17	0.44
3:AC:22:THR:HG23	3:AC:25:GLU:OE1	2.17	0.44
8:AH:29:PRO:HD2	8:AH:79:VAL:O	2.18	0.44
12:AO:69:ILE:O	12:AO:69:ILE:HG13	2.16	0.44
34:BA:418:C:H2'	34:BA:419:C:H6	1.83	0.44
34:BA:685:G:O2'	34:BA:686:U:H5'	2.18	0.44
34:BA:1326:C:H5"	54:BU:12:LYS:HE3	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:BA:1530:G:H4'	34:BA:1530:G:OP1	2.17	0.44
35:BB:28:PHE:CD1	35:BB:190:THR:HA	2.52	0.44
41:BH:112:LEU:HD13	41:BH:114:THR:HG23	1.98	0.44
54:BU:5:ASP:O	54:BU:11:GLY:HA3	2.17	0.44
59:BZ:553:GLY:H	59:BZ:557:GLY:HA2	1.82	0.44
1:CA:515:A:H1'	1:CA:581:C:H1'	1.99	0.44
1:CA:646:A:H2'	1:CA:647:G:O4'	2.17	0.44
1:CA:752:A:P	31:C7:3:ARG:HH22	2.41	0.44
1:CA:1847:A:H4'	1:CA:1848:A:OP2	2.17	0.44
1:CA:2238:G:H2'	1:CA:2238:G:N3	2.32	0.44
3:CC:22:THR:HG23	3:CC:25:GLU:OE1	2.17	0.44
3:CC:30:VAL:CG2	3:CC:31:LYS:N	2.78	0.44
3:CC:160:GLY:O	3:CC:161:ARG:C	2.61	0.44
10:CL:88:ALA:O	10:CL:90:LYS:N	2.50	0.44
34:DA:1014:A:OP1	52:DS:18:LYS:NZ	2.49	0.44
34:DA:1262:C:H2'	34:DA:1263:C:H6	1.83	0.44
34:DA:1272:G:C2	34:DA:1273:G:H1'	2.52	0.44
36:DC:7:PRO:O	36:DC:11:ARG:NH1	2.50	0.44
39:DF:49:ALA:HB2	51:DR:78:LEU:O	2.18	0.44
41:DH:97:VAL:HA	41:DH:100:ILE:HG13	1.98	0.44
46:DM:40:ASN:ND2	46:DM:41:PRO:HD2	2.32	0.44
52:DS:36:ARG:HD2	52:DS:52:TYR:O	2.18	0.44
59:DZ:681:LYS:HE2	59:DZ:681:LYS:HB3	1.72	0.44
1:AA:1188:A:C4	1:AA:1190:G:C8	3.06	0.44
1:AA:1889:G:N2	1:AA:1905:G:H2'	2.33	0.44
3:AC:5:GLY:O	3:AC:6:LYS:C	2.61	0.44
3:AC:39:ASP:O	3:AC:178:LYS:HE3	2.17	0.44
6:AF:53:THR:HG23	6:AF:55:GLY:H	1.81	0.44
7:AG:34:LEU:HD23	7:AG:34:LEU:HA	1.70	0.44
8:AH:111:HIS:CD2	8:AH:111:HIS:H	2.35	0.44
15:AR:55:ALA:HB2	15:AR:79:LEU:HD13	1.99	0.44
20:AW:18:ARG:HG2	20:AW:76:VAL:HB	2.00	0.44
21:AX:60:ARG:NH1	31:A7:47:ARG:HH21	2.15	0.44
28:A4:53:GLU:HB3	28:A4:54:GLY:HA2	2.00	0.44
34:BA:565:U:OP2	34:BA:566:G:O2'	2.32	0.44
34:BA:630:G:H2'	34:BA:631:G:H8	1.82	0.44
34:BA:977:A:O2'	34:BA:981:U:N3	2.47	0.44
34:BA:1159:U:OP1	35:BB:133:LYS:NZ	2.48	0.44
34:BA:1268:A:H2'	34:BA:1269:A:C8	2.52	0.44
35:BB:44:LEU:H	35:BB:44:LEU:HD22	1.82	0.44
39:BF:99:ALA:O	39:BF:100:ASN:HB2	2.16	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:BM:20:THR:C	46:BM:22:ILE:H	2.24	0.44
46:BM:49:THR:C	46:BM:51:ALA:H	2.24	0.44
59:BZ:-38:TYR:O	59:BZ:-34:ARG:HG2	2.18	0.44
59:BZ:-38:TYR:C	59:BZ:-35:PRO:HD2	2.42	0.44
59:BZ:177:ILE:O	59:BZ:185:ALA:HA	2.17	0.44
59:BZ:524:GLU:HB3	59:BZ:564:LYS:HG3	2.00	0.44
1:CA:271(X):G:C2	1:CA:271(Y):U:O4	2.70	0.44
1:CA:1076:C:H2'	1:CA:1077:A:C8	2.53	0.44
1:CA:1479:G:O2'	1:CA:1558:A:H5'	2.18	0.44
1:CA:1653:G:C6	15:CR:9:LYS:HG3	2.53	0.44
1:CA:2063:C:H1'	57:DX:76:31H:HCN	2.00	0.44
11:CN:103:VAL:O	11:CN:107:LEU:HG	2.17	0.44
17:CT:85:LYS:NZ	17:CT:87:ASP:OD2	2.46	0.44
21:CX:35:THR:HG22	21:CX:38:GLU:N	2.14	0.44
23:CZ:5:LEU:HD13	23:CZ:6:LYS:O	2.18	0.44
34:DA:839:U:H5"	34:DA:840:C:C5	2.51	0.44
34:DA:1165:C:H2'	34:DA:1166:G:O4'	2.18	0.44
37:DD:67:ILE:HG22	37:DD:68:TYR:CD2	2.52	0.44
53:DT:81:LYS:O	53:DT:85:MET:HG3	2.17	0.44
58:DY:55:PSU:HN1	58:DY:57:G:C5'	2.29	0.44
59:DZ:610:VAL:HG21	59:DZ:655:TYR:OH	2.18	0.44
1:AA:34:C:H5"	1:AA:35:G:OP2	2.18	0.44
1:AA:905:U:O2	1:AA:2280:A:H2'	2.17	0.44
1:AA:1576:G:H2'	1:AA:1577:C:O4'	2.18	0.44
1:AA:2034:G:OP1	20:AW:11:ARG:NH2	2.44	0.44
1:AA:2421:G:H2'	1:AA:2422:G:O4'	2.18	0.44
1:AA:2653:G:H5"	1:AA:2653:G:C8	2.52	0.44
1:AA:2693:C:OP2	5:AE:109:LYS:NZ	2.46	0.44
1:AA:2710:U:H2'	1:AA:2711:C:C6	2.53	0.44
4:AD:147:LEU:HD13	4:AD:155:LEU:HD11	1.99	0.44
10:AL:93:ARG:NH1	10:AL:94:GLU:HB2	2.33	0.44
18:AU:76:TYR:OH	18:AU:92:ARG:NH1	2.43	0.44
28:A4:59:PHE:HD2	52:BS:42:PRO:HG3	1.83	0.44
34:BA:96:U:O2'	34:BA:97:G:H5'	2.18	0.44
34:BA:200:G:N2	34:BA:218:C:C2	2.85	0.44
34:BA:1077:G:N2	34:BA:1080:A:OP2	2.46	0.44
34:BA:1226:C:H4'	52:BS:80:TYR:OH	2.18	0.44
43:BJ:6:ILE:O	43:BJ:71:LEU:HD12	2.18	0.44
46:BM:84:ILE:N	46:BM:85:GLY:HA2	2.33	0.44
59:BZ:94:VAL:HG12	59:BZ:97:SER:HB2	1.99	0.44
59:BZ:243:VAL:HG13	59:BZ:279:TYR:CE1	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:BZ:508:GLY:HA3	59:BZ:581:ALA:O	2.18	0.44
1:CA:251:A:C5	1:CA:252:G:H1'	2.53	0.44
1:CA:569:U:C4	1:CA:570:G:C6	3.06	0.44
1:CA:657:U:H2'	1:CA:658:C:H6	1.83	0.44
1:CA:771:G:OP1	31:C7:10:ARG:NH1	2.50	0.44
1:CA:1359:A:N1	1:CA:1372:U:O4	2.51	0.44
1:CA:1607:C:H4'	1:CA:1608:A:O5'	2.17	0.44
1:CA:2282:G:H4'	1:CA:2389:G:O2'	2.16	0.44
3:CC:39:ASP:O	3:CC:178:LYS:HE3	2.18	0.44
11:CN:39:ARG:HE	11:CN:39:ARG:HB3	1.48	0.44
13:CP:88:LEU:HD11	13:CP:114:ILE:HD12	1.99	0.44
14:CQ:16:ARG:HH11	14:CQ:16:ARG:CG	2.29	0.44
17:CT:53:ARG:O	17:CT:59:THR:HB	2.17	0.44
22:CY:38:ILE:HD13	22:CY:66:PRO:HA	2.00	0.44
23:CZ:53:ILE:HG22	23:CZ:71:VAL:HB	2.00	0.44
27:C3:5:LYS:NZ	27:C3:57:GLU:OE2	2.51	0.44
34:DA:25:C:O2'	34:DA:26:A:H5'	2.17	0.44
34:DA:309:G:H1'	34:DA:608:A:C2	2.52	0.44
34:DA:502:G:C2	34:DA:544:G:C2	3.06	0.44
34:DA:1239:A:H4'	34:DA:1240:U:C5'	2.44	0.44
34:DA:1328:C:OP1	54:DU:21:TYR:OH	2.28	0.44
35:DB:88:ALA:HB2	35:DB:219:VAL:HG13	1.99	0.44
41:DH:33:GLU:O	41:DH:36:LEU:N	2.46	0.44
41:DH:125:ARG:HE	41:DH:125:ARG:HB2	1.37	0.44
47:DN:15:LYS:HE2	47:DN:16:PHE:CZ	2.52	0.44
47:DN:45:ARG:O	47:DN:49:HIS:HD2	2.01	0.44
59:DZ:-53:ASP:H	59:DZ:-50:GLN:HE22	1.66	0.44
59:DZ:129:LYS:O	59:DZ:253:LEU:HD11	2.18	0.44
1:AA:104:C:H2'	1:AA:105:C:H6	1.83	0.44
1:AA:243:G:O6	32:A8:5:LYS:HG2	2.17	0.44
1:AA:324:A:P	22:AY:86:ARG:HH22	2.40	0.44
1:AA:504:A:C6	1:AA:506:A:C6	3.06	0.44
1:AA:553:A:C2	1:AA:2065:C:H5'	2.52	0.44
1:AA:808:A:OP1	65:AA:3935:HOH:O	2.21	0.44
1:AA:1249:A:N6	1:AA:1286:U:H2'	2.32	0.44
1:AA:1575:A:N6	1:AA:1588:G:O2'	2.45	0.44
1:AA:1900:G:H2'	1:AA:1901:C:C6	2.52	0.44
4:AD:40:THR:C	4:AD:42:GLY:H	2.26	0.44
4:AD:132:PRO:HD3	4:AD:190:TYR:CZ	2.53	0.44
9:AK:85:ASP:O	9:AK:87:VAL:N	2.51	0.44
13:AP:135:LEU:HD23	13:AP:135:LEU:HA	1.75	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:AW:61:ASN:HB2	20:AW:62:HIS:CD2	2.52	0.44
34:BA:1324:A:H2'	34:BA:1325:C:C6	2.52	0.44
47:BN:23:ARG:CZ	47:BN:30:ALA:HB2	2.48	0.44
59:BZ:107:VAL:HG13	59:BZ:135:PHE:HD2	1.83	0.44
59:BZ:606:MET:HE3	59:BZ:649:LEU:HD13	2.00	0.44
1:CA:493:G:H2'	1:CA:494:G:O4'	2.18	0.44
1:CA:651:G:OP2	32:C8:21:LYS:HE3	2.18	0.44
1:CA:848:G:O6	1:CA:928:G:H2'	2.17	0.44
1:CA:1235:G:C6	1:CA:1236:G:N1	2.85	0.44
1:CA:1495:A:H2'	1:CA:1496:A:H8	1.82	0.44
1:CA:1996:C:H4'	1:CA:1997:G:OP1	2.17	0.44
20:CW:59:VAL:HG12	20:CW:60:ASN:ND2	2.33	0.44
22:CY:35:TYR:CE2	22:CY:69:ALA:HB3	2.52	0.44
23:CZ:67:LEU:HD22	23:CZ:90:VAL:HG11	1.99	0.44
34:DA:513:C:H42	34:DA:538:G:H1	1.66	0.44
34:DA:537:G:H5"	45:DL:113:ARG:NH1	2.33	0.44
34:DA:1320:C:H5'	52:DS:70:LYS:HG3	2.00	0.44
35:DB:162:ILE:O	35:DB:185:ILE:HG12	2.18	0.44
41:DH:14:ARG:O	41:DH:18:ARG:HD3	2.18	0.44
46:DM:96:LEU:C	46:DM:110:ARG:HG2	2.42	0.44
52:DS:40:ILE:HB	52:DS:67:VAL:O	2.17	0.44
53:DT:79:ARG:HD2	53:DT:83:ARG:NH1	2.33	0.44
59:DZ:654:GLY:O	59:DZ:658:ASP:HB2	2.18	0.44
1:AA:386:U:H6	1:AA:386:U:H2'	1.60	0.43
1:AA:1014:U:H2'	1:AA:1015:C:C6	2.52	0.43
1:AA:1891:G:H5'	3:AC:206:LYS:CE	2.48	0.43
3:AC:60:ARG:HG3	3:AC:165:ARG:HB2	2.00	0.43
3:AC:194:ILE:HD11	3:AC:227:PRO:HB2	1.99	0.43
7:AG:43:LEU:HB3	7:AG:44:GLY:H	1.46	0.43
34:BA:757:U:O2'	34:BA:879:C:O2	2.28	0.43
34:BA:1066:C:O2'	34:BA:1067:A:H5'	2.18	0.43
34:BA:1251:A:H2'	34:BA:1252:A:H8	1.81	0.43
37:BD:13:ARG:HB3	37:BD:38:TYR:O	2.18	0.43
37:BD:121:VAL:O	37:BD:134:ASP:HA	2.18	0.43
38:BE:24:ARG:HH11	38:BE:24:ARG:HG2	1.83	0.43
48:BO:5:LYS:H	48:BO:5:LYS:HD2	1.83	0.43
51:BR:59:SER:OG	51:BR:62:GLU:HG2	2.18	0.43
58:BY:58:A:O2'	58:BY:60:U:H5	2.01	0.43
59:BZ:401:SER:O	59:BZ:402:ILE:HG12	2.18	0.43
1:CA:322:A:C5	1:CA:340:A:C2	3.06	0.43
1:CA:1158:C:H4'	27:C3:32:GLN:HB2	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:2892:A:C8	1:CA:2893:G:N7	2.86	0.43
4:CD:5:LYS:HE3	4:CD:5:LYS:HB3	1.63	0.43
7:CG:61:ALA:HA	7:CG:66:GLN:O	2.17	0.43
7:CG:96:ARG:O	7:CG:99:MET:HB3	2.18	0.43
11:CN:34:LEU:O	11:CN:49:GLY:HA3	2.17	0.43
23:CZ:10:ARG:NH2	23:CZ:26:GLY:O	2.49	0.43
23:CZ:39:VAL:HG21	23:CZ:44:PHE:HB2	2.00	0.43
27:C3:7:LYS:HB2	27:C3:34:GLU:HG3	1.99	0.43
34:DA:437:U:H5'	37:DD:155:LEU:HD21	2.00	0.43
34:DA:652:U:O4	34:DA:752:G:O2'	2.22	0.43
34:DA:685:G:N2	34:DA:686:U:C4	2.86	0.43
34:DA:881:G:P	45:DL:12:ARG:HH22	2.42	0.43
34:DA:1007:C:O2	34:DA:1023:G:N1	2.51	0.43
34:DA:1228:C:OP2	46:DM:111:LYS:HD3	2.18	0.43
34:DA:1324:A:O4'	34:DA:1362:C:H4'	2.18	0.43
34:DA:1410:G:H2'	34:DA:1411:C:H6	1.83	0.43
34:DA:1510:U:H2'	34:DA:1511:G:C8	2.52	0.43
35:DB:158:LEU:HA	35:DB:159:PRO:HD2	1.86	0.43
36:DC:77:ILE:HG13	36:DC:78:GLY:N	2.33	0.43
36:DC:113:ALA:HA	36:DC:116:VAL:HG23	2.00	0.43
38:DE:31:LEU:HD11	38:DE:132:ALA:HB2	1.99	0.43
43:DJ:78:ASN:C	43:DJ:80:LYS:H	2.26	0.43
44:DK:85:ARG:HG2	44:DK:111:ASP:O	2.18	0.43
49:DP:53:VAL:O	49:DP:54:GLU:C	2.61	0.43
56:DW:43:C:H2'	56:DW:44:G:C8	2.53	0.43
57:DX:67:C:H2'	57:DX:68:C:H5'	1.99	0.43
59:DZ:116:PRO:C	59:DZ:117:GLN:HG3	2.43	0.43
1:AA:1127:U:O3'	10:AL:117:THR:HB	2.18	0.43
1:AA:1485:A:H2'	1:AA:1486:G:O4'	2.18	0.43
1:AA:2867:G:N2	1:AA:2870:A:OP2	2.45	0.43
17:AT:80:SER:HA	17:AT:81:PRO:HD3	1.85	0.43
21:AX:88:LYS:NZ	21:AX:90:GLU:OE1	2.47	0.43
30:A6:18:ARG:HD2	30:A6:42:TRP:CG	2.53	0.43
34:BA:926:G:C6	34:BA:1505:G:C6	3.06	0.43
34:BA:1136:U:H5"	34:BA:1137:C:N3	2.33	0.43
35:BB:45:GLN:O	35:BB:49:GLU:HG3	2.18	0.43
48:BO:54:ARG:HG2	48:BO:58:MET:HE2	2.00	0.43
55:BV:14:A:N6	55:BV:15:A:C6	2.87	0.43
59:BZ:-7:GLU:HA	59:BZ:-4:ALA:HB3	1.98	0.43
1:CA:300:A:H1'	1:CA:319:C:H1'	1.99	0.43
1:CA:2175:C:H1'	3:CC:218:THR:O	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:2461:C:H2'	1:CA:2462:U:C6	2.54	0.43
7:CG:116:ASP:N	7:CG:116:ASP:OD1	2.51	0.43
14:CQ:7:MET:HE2	14:CQ:7:MET:HB3	1.87	0.43
16:CS:15:ARG:C	16:CS:19:LYS:HE2	2.43	0.43
21:CX:32:PRO:HA	21:CX:77:LYS:HD2	2.00	0.43
28:C4:46:GLN:HG2	28:C4:48:ARG:HH21	1.83	0.43
34:DA:1029:C:H2'	34:DA:1030:C:H5"	2.00	0.43
34:DA:1434:A:H2'	34:DA:1435:G:O4'	2.18	0.43
35:DB:48:MET:C	35:DB:50:GLU:H	2.26	0.43
35:DB:187:LEU:HA	35:DB:201:ILE:HB	1.99	0.43
40:DG:149:ARG:HG2	44:DK:59:TYR:CE1	2.54	0.43
41:DH:34:GLU:O	41:DH:38:ILE:HG12	2.18	0.43
41:DH:121:ASP:OD1	41:DH:121:ASP:N	2.49	0.43
43:DJ:52:GLY:HA2	43:DJ:53:PRO:HD3	1.82	0.43
46:DM:57:ARG:O	46:DM:61:GLU:HB2	2.18	0.43
49:DP:5:ARG:HB3	49:DP:67:THR:CG2	2.48	0.43
52:DS:27:GLU:HB2	52:DS:28:LYS:NZ	2.33	0.43
59:DZ:-53:ASP:O	59:DZ:-50:GLN:HB3	2.17	0.43
59:DZ:493:VAL:HG21	59:DZ:593:ALA:HB2	2.00	0.43
1:AA:2219:U:C5	1:AA:2236:G:C6	3.06	0.43
3:AC:160:GLY:O	3:AC:161:ARG:C	2.61	0.43
4:AD:275:LYS:HB3	4:AD:276:LYS:H	1.52	0.43
5:AE:12:THR:HG22	5:AE:13:ARG:N	2.32	0.43
9:AK:118:THR:O	9:AK:120:LYS:N	2.47	0.43
12:AO:122:LEU:HD13	17:AT:72:VAL:HG11	1.98	0.43
25:A1:86:SER:OG	25:A1:89:GLU:HG2	2.18	0.43
34:BA:299:G:H2'	34:BA:300:A:C8	2.54	0.43
34:BA:406:G:N2	34:BA:437:U:O2	2.51	0.43
34:BA:688:G:H2'	34:BA:689:C:C6	2.54	0.43
34:BA:925:G:H1'	34:BA:1502:A:C4	2.53	0.43
34:BA:1020:U:H2'	34:BA:1021:G:H8	1.83	0.43
34:BA:1058:G:N2	43:BJ:53:PRO:HG3	2.33	0.43
35:BB:16:HIS:C	35:BB:17:PHE:HD1	2.26	0.43
35:BB:121:LEU:HD13	35:BB:121:LEU:HA	1.85	0.43
37:BD:120:LEU:HA	37:BD:120:LEU:HD23	1.70	0.43
38:BE:76:ILE:HB	38:BE:77:PRO:HD2	2.01	0.43
46:BM:14:ARG:HB2	46:BM:17:VAL:HG23	2.00	0.43
46:BM:73:GLU:O	46:BM:77:ASN:ND2	2.48	0.43
59:BZ:289:ILE:H	59:BZ:289:ILE:HG13	1.50	0.43
1:CA:724:U:H2'	1:CA:725:G:O4'	2.18	0.43
1:CA:945:A:C4	1:CA:2448:A:C2	3.06	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:1557:C:H5"	1:CA:1558:A:OP2	2.17	0.43
1:CA:2086:U:H2'	1:CA:2087:G:C8	2.52	0.43
1:CA:2110:G:H4'	1:CA:2111:C:OP2	2.17	0.43
1:CA:2132:U:C2	3:CC:6:LYS:CE	3.01	0.43
8:CH:154:PRO:HB3	8:CH:163:TYR:CZ	2.53	0.43
34:DA:60:A:H4'	34:DA:61:G:O5'	2.19	0.43
34:DA:620:C:C2	37:DD:135:LEU:HG	2.53	0.43
34:DA:815:A:N7	34:DA:1509:C:O2'	2.48	0.43
34:DA:1051:C:H2'	34:DA:1052:U:C6	2.53	0.43
34:DA:1342:C:O2'	42:DI:124:GLN:HG2	2.17	0.43
36:DC:178:LEU:HD13	36:DC:178:LEU:HA	1.85	0.43
45:DL:31:PRO:HB2	45:DL:32:PHE:CD2	2.53	0.43
46:DM:25:ILE:HD11	46:DM:66:LEU:HD23	1.99	0.43
58:DY:39:PSU:C2	58:DY:40:C:C4	3.07	0.43
58:DY:65:G:H2'	58:DY:66:U:C6	2.53	0.43
1:AA:85:C:O2'	1:AA:86:C:H5'	2.18	0.43
1:AA:278:G:OP1	25:A1:76:ARG:HD2	2.18	0.43
1:AA:1617:A:H2'	1:AA:1618:A:C8	2.53	0.43
1:AA:1922:A:N1	1:AA:1992:A:C6	2.87	0.43
1:AA:2453:C:OP2	1:AA:2598:C:O2'	2.36	0.43
2:AB:28:C:H2'	2:AB:29:A:O4'	2.18	0.43
7:AG:137:GLU:HB3	7:AG:139:LEU:HD12	2.01	0.43
8:AH:38:SER:C	8:AH:40:GLU:H	2.24	0.43
16:AS:36:TYR:N	16:AS:36:TYR:CD1	2.86	0.43
17:AT:24:PRO:HA	17:AT:49:VAL:HG22	2.01	0.43
22:AY:20:TYR:CE1	22:AY:43:ASN:HA	2.53	0.43
28:A4:6:HIS:HA	28:A4:7:PRO:HD3	1.79	0.43
29:A5:38:ALA:CB	29:A5:48:GLU:HG3	2.49	0.43
34:BA:235:C:H5'	50:BQ:70:ARG:HG2	2.00	0.43
34:BA:761:G:C6	34:BA:762:C:C4	3.06	0.43
34:BA:1116:C:O2'	42:BI:108:VAL:HG21	2.18	0.43
34:BA:1434:A:H2'	34:BA:1435:G:O4'	2.18	0.43
35:BB:68:ILE:HG12	35:BB:161:ALA:HB3	2.00	0.43
36:BC:58:GLU:HB2	36:BC:65:ALA:CB	2.48	0.43
36:BC:100:ALA:O	36:BC:101:LEU:HB2	2.19	0.43
39:BF:55:ASP:HA	39:BF:56:PRO:HD3	1.85	0.43
44:BK:43:SER:HB3	44:BK:68:ALA:HB2	2.00	0.43
46:BM:70:LEU:O	46:BM:74:VAL:HG23	2.19	0.43
52:BS:50:ALA:HB1	52:BS:57:HIS:HB3	1.99	0.43
56:BW:7:A:H5'	56:BW:8:4SU:H5	1.99	0.43
56:BW:39:PSU:H2'	56:BW:40:C:C6	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:BY:53:G:H1	58:BY:61:C:H42	1.64	0.43
1:CA:652(C):G:H5"	1:CA:652(D):C:OP2	2.19	0.43
1:CA:1144:G:H2'	1:CA:1145:C:H6	1.81	0.43
1:CA:1719:G:C6	1:CA:1720:U:C4	3.07	0.43
1:CA:1960:A:HO2'	34:DA:1484:C:HO2'	1.63	0.43
2:CB:8:U:H6	2:CB:8:U:H5"	1.83	0.43
3:CC:5:GLY:O	3:CC:6:LYS:C	2.61	0.43
7:CG:145:THR:HG22	7:CG:148:MET:CG	2.47	0.43
12:CO:120:GLU:HG2	12:CO:122:LEU:HG	1.99	0.43
17:CT:120:ARG:HA	17:CT:123:GLN:HG3	2.00	0.43
34:DA:35:G:H2'	34:DA:36:C:C6	2.53	0.43
34:DA:961:U:H2'	34:DA:962:C:O4'	2.19	0.43
34:DA:1187:G:H4'	42:DI:111:ARG:HH11	1.84	0.43
34:DA:1321:C:H5"	34:DA:1322:C:H2'	2.00	0.43
35:DB:25:ASN:HA	35:DB:26:PRO:HD3	1.82	0.43
43:DJ:39:PRO:HA	43:DJ:70:ARG:HD3	2.00	0.43
59:DZ:74:TRP:HE1	59:DZ:274:ASP:N	2.17	0.43
59:DZ:169:GLY:HA3	59:DZ:173:THR:O	2.18	0.43
1:AA:438:G:C5	13:AP:72:PRO:HB3	2.53	0.43
1:AA:1604:C:H5"	1:AA:1605:A:OP2	2.19	0.43
1:AA:2784:C:H2'	1:AA:2785:C:C6	2.53	0.43
5:AE:131:ALA:HB1	5:AE:134:ILE:HD11	2.00	0.43
22:AY:90:LEU:HB2	22:AY:94:LYS:O	2.18	0.43
23:AZ:146:ILE:HA	23:AZ:147:GLY:HA2	1.65	0.43
23:AZ:151:HIS:C	23:AZ:153:SER:H	2.22	0.43
31:A7:5:TRP:CD1	31:A7:7:PRO:HD3	2.53	0.43
32:A8:36:LYS:HB2	32:A8:41:ILE:HD11	1.99	0.43
34:BA:950:U:H2'	34:BA:951:G:C8	2.53	0.43
34:BA:1131:G:O5'	34:BA:1131:G:H8	2.01	0.43
34:BA:1189:C:OP1	43:BJ:51:ARG:NH2	2.51	0.43
35:BB:192:SER:O	35:BB:194:PRO:HD3	2.18	0.43
1:CA:141:A:C8	1:CA:1408:C:O2'	2.69	0.43
1:CA:1071:G:H1'	1:CA:1089:G:H2'	2.00	0.43
2:CB:24:G:N7	2:CB:56:G:H2'	2.33	0.43
3:CC:54:ARG:HE	3:CC:57:GLN:HG2	1.83	0.43
4:CD:3:VAL:HG13	4:CD:17:THR:HB	2.00	0.43
4:CD:146:GLU:HB2	4:CD:189:CYS:CB	2.49	0.43
8:CH:126:PRO:HB2	8:CH:127:GLU:H	1.64	0.43
13:CP:100:LEU:HD23	13:CP:100:LEU:HA	1.77	0.43
19:CV:1:MET:HG3	19:CV:43:GLU:OE2	2.18	0.43
23:CZ:75:ASN:O	23:CZ:84:GLU:HG2	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:C4:34:GLU:HG2	46:DM:3:ARG:CB	2.48	0.43
34:DA:189:G:H2'	34:DA:189(A):C:C6	2.54	0.43
34:DA:394:G:H2'	34:DA:395:C:C6	2.54	0.43
34:DA:1074:G:C6	34:DA:1075:C:C4	3.07	0.43
34:DA:1316:G:H22	34:DA:1319:A:C5'	2.31	0.43
34:DA:1399:C:C2	34:DA:1502:A:N6	2.87	0.43
34:DA:1465:C:H2'	34:DA:1466:C:O4'	2.19	0.43
38:DE:42:GLY:HA2	38:DE:65:ASN:O	2.19	0.43
43:DJ:50:ILE:HD11	43:DJ:57:LYS:HE2	1.99	0.43
50:DQ:6:LEU:O	50:DQ:58:GLU:HA	2.19	0.43
59:DZ:428:LEU:HD13	59:DZ:440:VAL:HG11	2.01	0.43
59:DZ:438:PHE:CE2	59:DZ:440:VAL:HG23	2.50	0.43
1:AA:861:C:H4'	1:AA:1270:C:O2	2.19	0.43
1:AA:1549:U:H2'	1:AA:1550:C:C6	2.53	0.43
1:AA:2316:G:H22	1:AA:2324:U:H3	1.66	0.43
1:AA:2649:U:H5"	5:AE:82:ARG:HH21	1.83	0.43
1:AA:2724:U:O2'	1:AA:2726:A:H5'	2.19	0.43
1:AA:2724:U:OP1	1:AA:2727:G:H4'	2.18	0.43
6:AF:124:LEU:O	6:AF:193:VAL:HA	2.19	0.43
23:AZ:150:LEU:HB3	23:AZ:171:ILE:HD11	2.01	0.43
23:AZ:155:LEU:HD12	23:AZ:155:LEU:HA	1.76	0.43
32:A8:37:SER:OG	32:A8:39:LYS:N	2.52	0.43
34:BA:486:U:H2'	34:BA:487:A:H8	1.84	0.43
34:BA:1324:A:O4'	34:BA:1362:C:H4'	2.18	0.43
36:BC:44:GLU:HA	36:BC:52:LEU:HD13	1.99	0.43
43:BJ:70:ARG:HA	43:BJ:70:ARG:HD3	1.88	0.43
50:BQ:92:ARG:HA	50:BQ:92:ARG:HD3	1.83	0.43
59:BZ:7:ASN:HB3	59:BZ:10:LYS:HE2	1.99	0.43
59:BZ:131:PRO:HG2	59:BZ:281:PRO:HG2	2.00	0.43
59:BZ:411:VAL:HB	59:BZ:459:LEU:HD13	2.01	0.43
1:CA:671:C:H2'	1:CA:672:C:C6	2.54	0.43
1:CA:729:G:C6	4:CD:208:LYS:HB2	2.52	0.43
1:CA:1056:G:H5"	1:CA:1057:A:O4'	2.17	0.43
1:CA:1754:C:H5"	17:CT:113:LYS:HE3	1.99	0.43
1:CA:2218:U:O4'	25:C1:52:ARG:NH2	2.51	0.43
2:CB:22:U:H3	2:CB:61:G:H1	1.66	0.43
7:CG:52:ILE:O	7:CG:53:LEU:HD23	2.18	0.43
13:CP:55:ARG:HA	65:CP:303:HOH:O	2.19	0.43
14:CQ:3:MET:HE2	14:CQ:3:MET:HB3	1.86	0.43
23:CZ:18:LEU:HD13	23:CZ:18:LEU:HA	1.78	0.43
24:C0:53:MET:HG3	24:C0:59:LEU:CD2	2.46	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:DA:89:C:H2'	34:DA:90:U:O4'	2.18	0.43
34:DA:1291:G:OP1	40:DG:37:ASN:ND2	2.51	0.43
36:DC:16:ARG:HD2	36:DC:16:ARG:HA	1.66	0.43
39:DF:79:LEU:HD23	39:DF:79:LEU:HA	1.83	0.43
43:DJ:46:ARG:NH2	43:DJ:64:GLU:OE1	2.52	0.43
47:DN:23:ARG:HD2	47:DN:28:GLY:O	2.19	0.43
59:DZ:319:ASP:HA	59:DZ:320:PRO:HD3	1.84	0.43
59:DZ:459:LEU:HD23	59:DZ:459:LEU:HA	1.83	0.43
1:AA:310:C:H2'	1:AA:311:C:H6	1.83	0.43
1:AA:2478:C:OP1	33:A9:4:ARG:HB3	2.19	0.43
6:AF:199:TRP:O	6:AF:203:GLN:HG2	2.18	0.43
8:AH:98:LEU:HD12	8:AH:98:LEU:HA	1.84	0.43
11:AN:15:LEU:HD22	11:AN:16:ILE:N	2.33	0.43
22:AY:28:LYS:HB3	22:AY:28:LYS:HE3	1.79	0.43
27:A3:23:LEU:HD12	27:A3:23:LEU:HA	1.81	0.43
34:BA:194:C:H2'	34:BA:195:A:H5"	2.01	0.43
34:BA:448:A:C4	34:BA:487:A:C2	3.07	0.43
34:BA:548:G:C6	34:BA:549:C:C4	3.06	0.43
34:BA:1284:C:H3'	34:BA:1285:A:C8	2.53	0.43
34:BA:1437:C:H2'	34:BA:1438:G:C8	2.54	0.43
36:BC:59:ARG:O	43:BJ:92:THR:HG22	2.18	0.43
38:BE:143:ARG:NH1	41:BH:77:GLU:OE2	2.52	0.43
38:BE:152:ARG:HA	41:BH:64:LYS:HZ2	1.83	0.43
53:BT:97:ALA:N	53:BT:98:PRO:HD3	2.33	0.43
58:BY:25:C:C2	58:BY:26:A:C8	3.07	0.43
59:BZ:114:VAL:HG12	59:BZ:115:GLU:N	2.32	0.43
59:BZ:330:VAL:HB	59:BZ:371:ALA:HA	2.01	0.43
59:BZ:519:ARG:NH2	59:BZ:678:GLU:H	2.16	0.43
1:CA:41:C:H2'	1:CA:42:G:O4'	2.19	0.43
1:CA:57:C:H2'	1:CA:58:G:O4'	2.19	0.43
1:CA:597:U:H2'	1:CA:598:G:C8	2.54	0.43
1:CA:1110:G:N3	1:CA:1110:G:C2'	2.82	0.43
1:CA:1266:G:O2'	1:CA:2012:G:O6	2.36	0.43
1:CA:1452:A:O2'	1:CA:1453:U:H2'	2.19	0.43
1:CA:1628:G:H2'	1:CA:1629:U:H6	1.84	0.43
1:CA:1857:G:C6	1:CA:1858:G:N1	2.87	0.43
1:CA:2692:C:O2'	1:CA:2693:A:H5'	2.19	0.43
8:CH:148:ILE:O	8:CH:151:ILE:HB	2.19	0.43
23:CZ:70:LEU:HD23	23:CZ:70:LEU:HA	1.79	0.43
23:CZ:130:PRO:C	23:CZ:132:ASN:H	2.25	0.43
34:DA:539:A:OP2	45:DL:115:LYS:NZ	2.48	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:DA:632:A:OP2	34:DA:632:A:H8	2.02	0.43
34:DA:735:C:O2'	34:DA:736:C:H5'	2.18	0.43
36:DC:110:ASN:HB3	36:DC:141:VAL:HA	2.01	0.43
36:DC:173:VAL:O	36:DC:175:LEU:HD12	2.18	0.43
45:DL:7:ILE:O	45:DL:11:VAL:HG23	2.18	0.43
46:DM:14:ARG:HB3	46:DM:16:ASP:OD1	2.18	0.43
56:DW:76:F3N:H5"	56:DW:76:F3N:O	2.17	0.43
59:DZ:123:ARG:HD2	59:DZ:675:HIS:ND1	2.34	0.43
59:DZ:160:ARG:HH21	59:DZ:253:LEU:HA	1.84	0.43
59:DZ:309:LEU:HA	59:DZ:333:GLY:HA3	2.01	0.43
1:AA:142:G:H1'	21:AX:37:THR:CG2	2.49	0.43
1:AA:313:A:H2'	1:AA:314:G:O4'	2.18	0.43
1:AA:733:G:N2	1:AA:835:A:H61	2.17	0.43
4:AD:8:PRO:HB3	4:AD:14:ARG:HB2	1.99	0.43
5:AE:49:LEU:HD12	5:AE:49:LEU:HA	1.78	0.43
8:AH:86:GLU:OE2	8:AH:132:ARG:NH2	2.52	0.43
22:AY:49:VAL:HG11	22:AY:61:ILE:HD13	1.99	0.43
28:A4:10:VAL:N	28:A4:26:SER:O	2.37	0.43
34:BA:377:G:OP1	49:BP:5:ARG:HD2	2.19	0.43
34:BA:872:A:C5	34:BA:874:G:C8	3.06	0.43
34:BA:1279:A:N1	36:BC:26:LYS:NZ	2.67	0.43
41:BH:114:THR:HG22	41:BH:130:GLY:C	2.44	0.43
59:BZ:69:VAL:HG11	59:BZ:374:LEU:HD22	2.01	0.43
59:BZ:486:THR:O	59:BZ:599:PRO:HA	2.18	0.43
1:CA:443:A:H5"	1:CA:444:C:OP1	2.19	0.43
1:CA:2328:A:H2'	1:CA:2329:G:H8	1.83	0.43
3:CC:195:ARG:HH11	3:CC:195:ARG:HG3	1.83	0.43
6:CF:140:LEU:HD13	6:CF:170:LEU:HD21	2.00	0.43
11:CN:43:THR:HB	11:CN:46:VAL:CG2	2.49	0.43
16:CS:15:ARG:HB3	16:CS:19:LYS:HZ1	1.83	0.43
16:CS:67:ARG:O	16:CS:71:ARG:HG3	2.18	0.43
16:CS:69:VAL:O	16:CS:72:ALA:HB3	2.19	0.43
18:CU:104:GLN:NE2	18:CU:105:VAL:HG23	2.34	0.43
25:C1:50:ARG:HG2	25:C1:59:THR:HB	2.01	0.43
34:DA:152:A:N6	34:DA:170:U:C2	2.86	0.43
34:DA:707:C:H2'	34:DA:708:C:C6	2.52	0.43
34:DA:1097:C:H2'	34:DA:1098:C:C6	2.54	0.43
35:DB:71:VAL:O	35:DB:165:VAL:HG23	2.19	0.43
39:DF:82:ARG:HD2	39:DF:82:ARG:HA	1.70	0.43
40:DG:29:LYS:HB3	40:DG:105:VAL:HG21	2.00	0.43
46:DM:50:GLU:O	46:DM:54:VAL:HG22	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:DN:24:CYS:HA	47:DN:38:GLY:O	2.18	0.43
59:DZ:87:HIS:O	59:DZ:89:ASP:N	2.47	0.43
59:DZ:228:MET:O	59:DZ:232:LEU:HD22	2.18	0.43
59:DZ:292:THR:C	59:DZ:397:VAL:HG23	2.44	0.43
1:AA:275:C:H2'	1:AA:276:C:C6	2.53	0.43
1:AA:313:A:N6	1:AA:375:G:H1'	2.33	0.43
1:AA:694:G:N2	1:AA:696:C:O2	2.31	0.43
1:AA:2163:G:N7	1:AA:2173:G:N2	2.67	0.43
5:AE:28:ALA:HB3	5:AE:93:VAL:HG13	2.00	0.43
5:AE:79:ARG:HD3	5:AE:79:ARG:HA	1.84	0.43
12:AO:69:ILE:HD11	12:AO:105:GLU:OE1	2.18	0.43
14:AQ:56:ARG:HA	14:AQ:56:ARG:HD2	1.45	0.43
34:BA:872:A:C4	34:BA:874:G:N7	2.87	0.43
37:BD:166:LYS:N	37:BD:168:ARG:HH12	2.17	0.43
39:BF:19:LEU:HD11	39:BF:59:TYR:CZ	2.54	0.43
59:BZ:536:LYS:H	59:BZ:536:LYS:HD2	1.83	0.43
1:CA:982:C:O5'	1:CA:982:C:H6	2.02	0.43
1:CA:1095:A:H2'	1:CA:1096:A:C8	2.54	0.43
1:CA:1668:A:H4'	1:CA:1669:A:O5'	2.18	0.43
1:CA:2468:G:C6	1:CA:2481:G:C4	3.07	0.43
1:CA:2850:A:N7	1:CA:2868:A:O2'	2.50	0.43
3:CC:60:ARG:HG3	3:CC:165:ARG:HB2	2.01	0.43
6:CF:57:VAL:HG13	6:CF:59:TYR:CD2	2.53	0.43
7:CG:50:ALA:O	7:CG:51:ARG:C	2.62	0.43
34:DA:735:C:H2'	34:DA:736:C:H6	1.84	0.43
34:DA:1206:G:C6	34:DA:1207:G:C5	3.07	0.43
34:DA:1356:G:N2	34:DA:1367:C:O2	2.51	0.43
35:DB:94:ASN:HA	35:DB:94:ASN:HD22	1.56	0.43
35:DB:102:LEU:HD23	35:DB:182:ILE:HD12	2.00	0.43
39:DF:96:PRO:HB3	51:DR:30:ASP:OD2	2.19	0.43
59:DZ:-58:LEU:HB3	59:DZ:-55:LEU:HB2	2.01	0.43
59:DZ:38:ARG:HH12	59:DZ:270:GLN:HE22	1.66	0.43
59:DZ:324:ARG:HD3	59:DZ:380:LEU:O	2.19	0.43
1:AA:613:A:H2'	1:AA:614:C:O4'	2.19	0.43
1:AA:933:C:OP1	1:AA:933:C:H4'	2.18	0.43
1:AA:1384:G:N7	21:AX:62:LYS:NZ	2.59	0.43
1:AA:1975:A:H2	1:AA:2561:G:N3	2.17	0.43
1:AA:2569:G:H2'	1:AA:2570:C:C6	2.54	0.43
3:AC:6:LYS:N	3:AC:9:ARG:HH12	2.17	0.43
7:AG:77:ILE:O	7:AG:82:LEU:N	2.49	0.43
12:AO:10:VAL:HG21	12:AO:16:ALA:HB3	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:AQ:2:LEU:HB2	14:AQ:70:PRO:HG3	2.01	0.43
14:AQ:39:PRO:HA	14:AQ:97:VAL:O	2.19	0.43
30:A6:50:ARG:HE	30:A6:50:ARG:HB2	1.65	0.43
34:BA:1437:C:H2'	34:BA:1438:G:H8	1.84	0.43
36:BC:78:GLY:HA3	36:BC:83:ARG:H	1.83	0.43
37:BD:173:TRP:HB2	37:BD:187:ARG:O	2.19	0.43
38:BE:64:ARG:HE	38:BE:64:ARG:HB3	1.70	0.43
42:BI:81:ILE:HA	42:BI:84:ALA:HB3	2.00	0.43
48:BO:32:LEU:O	48:BO:35:ARG:N	2.51	0.43
52:BS:20:LEU:HD21	52:BS:43:GLU:HG2	2.00	0.43
59:BZ:146:LEU:HD22	59:BZ:150:ILE:HD11	2.00	0.43
1:CA:25:U:H2'	1:CA:26:G:O4'	2.19	0.43
1:CA:171:G:H2'	1:CA:172:C:C6	2.54	0.43
1:CA:289:A:N6	1:CA:351:G:O2'	2.49	0.43
1:CA:571:A:O2'	19:CV:78:LYS:HE2	2.18	0.43
1:CA:699:A:C2	1:CA:1633:G:N3	2.86	0.43
1:CA:699:A:H2'	1:CA:700:G:O4'	2.19	0.43
1:CA:760:G:H2'	1:CA:761:A:O4'	2.19	0.43
1:CA:867:C:N4	1:CA:868:U:O4	2.52	0.43
1:CA:1064:C:H4'	10:CL:89:HIS:HB3	2.00	0.43
1:CA:2290:G:C2	1:CA:2343:C:O2	2.72	0.43
1:CA:2489:G:C6	1:CA:2490:G:N1	2.87	0.43
3:CC:31:LYS:H	3:CC:31:LYS:HG2	1.57	0.43
4:CD:94:LEU:HD22	4:CD:95:LEU:N	2.33	0.43
5:CE:103:ASP:OD2	5:CE:168:MET:HE2	2.19	0.43
5:CE:195:LEU:HD21	65:CE:412:HOH:O	2.19	0.43
13:CP:39:LYS:HB2	13:CP:45:LEU:CG	2.40	0.43
34:DA:73:G:C6	34:DA:76:C:C4	3.07	0.43
34:DA:612:C:O2	34:DA:629:G:N2	2.52	0.43
34:DA:833:U:H2'	34:DA:834:C:C6	2.54	0.43
34:DA:1004:A:N6	34:DA:1037:C:C2	2.87	0.43
46:DM:80:ARG:O	46:DM:84:ILE:HG12	2.19	0.43
53:DT:44:ALA:HB1	53:DT:91:LEU:HB2	2.00	0.43
57:DX:23:C:H2'	57:DX:24:U:H6	1.83	0.43
59:DZ:-62:LEU:N	59:DZ:-62:LEU:HD12	2.34	0.43
59:DZ:420:ASP:OD1	59:DZ:423:LYS:HB2	2.19	0.43
1:AA:553:A:N1	1:AA:2064:A:H2'	2.33	0.42
1:AA:589:U:H2'	1:AA:590:A:O4'	2.19	0.42
1:AA:866:A:H8	1:AA:866:A:C5'	2.31	0.42
1:AA:1003:U:OP2	14:AQ:14:ARG:HD3	2.19	0.42
1:AA:1692:G:H5"	1:AA:1693:C:H5'	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:2203:G:O2'	1:AA:2204:G:OP1	2.30	0.42
1:AA:2589:A:H5'	29:A5:3:LYS:HD2	2.00	0.42
3:AC:11:LEU:HD11	3:AC:35:THR:HG23	2.01	0.42
3:AC:195:ARG:HG3	3:AC:195:ARG:NH1	2.34	0.42
12:AO:104:ARG:HH12	17:AT:43:GLN:NE2	2.17	0.42
23:AZ:89:PHE:HE2	23:AZ:96:VAL:HG23	1.84	0.42
34:BA:15:G:H1'	38:BE:19:MET:HE2	2.01	0.42
34:BA:445:G:C6	34:BA:490:G:C6	3.07	0.42
34:BA:908:A:H2'	34:BA:909:A:C8	2.54	0.42
34:BA:1513:A:H2'	34:BA:1514:C:C6	2.53	0.42
35:BB:24:TRP:CE3	35:BB:26:PRO:HA	2.54	0.42
35:BB:173:ALA:O	35:BB:176:GLU:N	2.52	0.42
38:BE:112:LEU:C	38:BE:114:GLY:H	2.28	0.42
44:BK:86:GLY:H	44:BK:112:THR:HG1	1.65	0.42
50:BQ:41:LYS:HZ3	50:BQ:92:ARG:HH21	1.66	0.42
57:BX:2:G:H2'	57:BX:3:C:C6	2.54	0.42
59:BZ:88:VAL:HG22	59:BZ:120:THR:HG21	2.01	0.42
59:BZ:201:ILE:H	59:BZ:201:ILE:HG13	1.67	0.42
59:BZ:309:LEU:HD13	59:BZ:334:THR:C	2.45	0.42
1:CA:528:A:OP2	11:CN:114:ARG:NH1	2.51	0.42
1:CA:639:U:H2'	1:CA:640:C:H6	1.81	0.42
1:CA:830:G:H4'	1:CA:831:G:OP2	2.17	0.42
1:CA:1027:A:C2	1:CA:2488:A:H5'	2.54	0.42
1:CA:1570:A:H2'	1:CA:1571:A:C8	2.54	0.42
3:CC:11:LEU:HD11	3:CC:35:THR:HG23	2.01	0.42
4:CD:106:ILE:HD13	4:CD:106:ILE:HG21	1.80	0.42
7:CG:109:VAL:C	7:CG:112:PRO:HD2	2.44	0.42
32:C8:57:ARG:O	32:C8:60:LEU:N	2.49	0.42
34:DA:7:G:H5'	34:DA:298:A:O4'	2.19	0.42
34:DA:253:U:H2'	34:DA:254:G:C8	2.54	0.42
34:DA:1438:G:H2'	34:DA:1439:C:C6	2.53	0.42
35:DB:70:PHE:CE1	35:DB:163:PHE:HD2	2.37	0.42
35:DB:112:VAL:C	35:DB:114:ARG:H	2.27	0.42
37:DD:153:ARG:HD3	37:DD:181:MET:HE1	2.01	0.42
50:DQ:31:LEU:HD23	50:DQ:32:TYR:CZ	2.54	0.42
59:DZ:295:GLU:H	59:DZ:295:GLU:HG3	1.48	0.42
1:AA:180:A:H2'	1:AA:181:C:C6	2.54	0.42
1:AA:1240:G:O2'	1:AA:1272:A:N1	2.46	0.42
2:AB:28:C:OP1	16:AS:36:TYR:OH	2.34	0.42
7:AG:101:ILE:HG22	7:AG:105:LYS:HE2	2.01	0.42
16:AS:78:LEU:HD21	16:AS:83:LYS:HG3	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:BA:991:U:C4	34:BA:1212:U:H1'	2.54	0.42
34:BA:1123:A:H61	34:BA:1149:C:N4	2.14	0.42
34:BA:1149:C:H2'	34:BA:1150:U:H6	1.84	0.42
34:BA:1492:A:H4'	45:BL:47:LYS:HE3	2.01	0.42
34:BA:1504:G:OP1	34:BA:1507:A:H4'	2.19	0.42
35:BB:215:LEU:HA	35:BB:215:LEU:HD23	1.79	0.42
41:BH:88:LYS:O	41:BH:92:ARG:HD3	2.19	0.42
52:BS:27:GLU:HA	52:BS:28:LYS:HA	1.91	0.42
59:BZ:98:MET:C	59:BZ:100:VAL:H	2.27	0.42
59:BZ:639:ASN:N	59:BZ:640:ALA:HB3	2.33	0.42
1:CA:746:A:H2'	1:CA:2612:C:H5"	2.00	0.42
1:CA:1154:G:H8	1:CA:1154:G:O5'	2.02	0.42
1:CA:1805:U:O2	4:CD:50:THR:HB	2.18	0.42
1:CA:2529:G:O6	33:C9:31:LYS:NZ	2.52	0.42
13:CP:55:ARG:HG2	13:CP:56:SER:N	2.34	0.42
16:CS:3:ARG:O	16:CS:4:LEU:HD23	2.19	0.42
17:CT:99:LEU:HD22	17:CT:101:PHE:HE1	1.84	0.42
22:CY:76:CYS:SG	22:CY:78:ALA:HB3	2.59	0.42
23:CZ:97:GLU:H	23:CZ:97:GLU:HG2	1.55	0.42
25:C1:25:LYS:C	25:C1:27:GLU:H	2.27	0.42
34:DA:67:C:H4'	34:DA:172:A:O4'	2.18	0.42
34:DA:814:A:N7	34:DA:816:A:C4	2.87	0.42
34:DA:872:A:C4	34:DA:874:G:N7	2.87	0.42
34:DA:1048:G:OP1	47:DN:3:ARG:NH2	2.52	0.42
34:DA:1221:G:H4'	52:DS:53:ASN:O	2.19	0.42
35:DB:47:THR:HG23	35:DB:202:PRO:HG2	2.01	0.42
36:DC:47:LEU:HB3	36:DC:52:LEU:HB3	2.00	0.42
40:DG:52:GLU:H	40:DG:52:GLU:HG2	1.60	0.42
41:DH:21:LYS:O	41:DH:65:TYR:OH	2.30	0.42
43:DJ:23:ILE:HD13	43:DJ:23:ILE:HA	1.84	0.42
46:DM:17:VAL:O	46:DM:20:THR:OG1	2.35	0.42
56:DW:54:5MU:C4	56:DW:55:PSU:C2	3.07	0.42
59:DZ:638:GLY:C	59:DZ:640:ALA:HB3	2.44	0.42
1:AA:2284:U:H5"	1:AA:2285:A:OP1	2.19	0.42
1:AA:2566:U:H2'	1:AA:2567:U:C6	2.54	0.42
3:AC:195:ARG:HG3	3:AC:195:ARG:HH11	1.83	0.42
19:AV:49:THR:O	19:AV:49:THR:CG2	2.67	0.42
30:A6:12:GLU:HA	30:A6:19:ARG:HA	2.00	0.42
34:BA:1002:G:H2'	34:BA:1003:G:O4'	2.20	0.42
34:BA:1072:G:C6	34:BA:1073:U:C4	3.08	0.42
34:BA:1148:U:H2'	34:BA:1149:C:O4'	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:BD:194:LEU:HD12	37:BD:195:ALA:N	2.34	0.42
39:BF:10:LEU:HD23	39:BF:61:LEU:HD23	2.01	0.42
41:BH:8:ASP:O	41:BH:11:THR:N	2.46	0.42
50:BQ:89:LEU:HA	50:BQ:89:LEU:HD23	1.61	0.42
59:BZ:13:ARG:NH1	59:BZ:247:ARG:NH2	2.55	0.42
59:BZ:438:PHE:HB3	59:BZ:458:HIS:CE1	2.54	0.42
59:BZ:509:HIS:NE2	59:BZ:511:LYS:HE2	2.35	0.42
1:CA:637:A:H5"	13:CP:117:GLU:HG2	2.01	0.42
1:CA:1141:U:H4'	1:CA:1142(A):A:O4'	2.19	0.42
1:CA:1239:G:H2'	1:CA:1240:U:O4'	2.19	0.42
1:CA:2439:A:C8	1:CA:2439:A:H5'	2.55	0.42
6:CF:33:LEU:HA	6:CF:33:LEU:HD12	1.61	0.42
7:CG:31:VAL:HG22	7:CG:32:PRO:HD2	2.01	0.42
7:CG:33:ARG:NH1	7:CG:33:ARG:HB2	2.34	0.42
8:CH:15:VAL:HG23	8:CH:28:GLY:HA3	2.00	0.42
11:CN:91:LEU:HA	11:CN:91:LEU:HD23	1.74	0.42
17:CT:30:VAL:HG13	17:CT:86:ILE:HG12	2.02	0.42
27:C3:8:LEU:HD23	27:C3:8:LEU:HA	1.79	0.42
34:DA:1326:C:H2'	34:DA:1327:C:H6	1.84	0.42
36:DC:142:MET:HE3	36:DC:142:MET:HB3	1.93	0.42
37:DD:11:LEU:O	37:DD:15:GLU:HG2	2.18	0.42
39:DF:89:MET:HE3	39:DF:91:VAL:HG21	2.02	0.42
39:DF:94:GLN:HE22	51:DR:72:ARG:HH12	1.67	0.42
53:DT:90:GLN:O	53:DT:93:GLU:HG3	2.19	0.42
57:DX:47:U:H3'	57:DX:48:C:C5'	2.50	0.42
59:DZ:114:VAL:HG23	59:DZ:152:THR:HB	2.01	0.42
59:DZ:160:ARG:HD3	59:DZ:256:THR:OG1	2.20	0.42
59:DZ:193:GLY:O	59:DZ:196:ILE:HG22	2.18	0.42
1:AA:734:C:H5"	31:A7:2:LYS:HE2	2.02	0.42
1:AA:1137:G:C6	1:AA:1147:U:C2	3.07	0.42
1:AA:1346:U:H4'	1:AA:1347:A:H5"	2.01	0.42
1:AA:2402:U:O2'	1:AA:2403:G:H5'	2.19	0.42
1:AA:2407:C:H2'	1:AA:2408:G:O4'	2.19	0.42
7:AG:60:LEU:HA	7:AG:60:LEU:HD13	1.67	0.42
8:AH:7:LEU:HD12	8:AH:7:LEU:HA	1.89	0.42
8:AH:69:ARG:HG3	8:AH:70:THR:N	2.28	0.42
17:AT:39:ARG:HH22	34:BA:345:C:H5	1.66	0.42
34:BA:254:G:OP1	50:BQ:67:LYS:O	2.37	0.42
34:BA:690:G:C6	34:BA:691:G:C6	3.07	0.42
34:BA:1100:C:O2'	34:BA:1102:A:OP1	2.38	0.42
34:BA:1272:G:H2'	34:BA:1273:G:O4'	2.18	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:BA:1292:U:H2'	34:BA:1293:G:C8	2.55	0.42
34:BA:1521:G:H2'	34:BA:1522:U:C6	2.54	0.42
35:BB:50:GLU:O	35:BB:54:THR:N	2.50	0.42
35:BB:200:ILE:H	35:BB:200:ILE:HG12	1.47	0.42
37:BD:52:SER:O	37:BD:56:VAL:HG23	2.20	0.42
37:BD:147:ALA:HA	37:BD:182:LYS:HA	2.01	0.42
37:BD:196:LEU:C	37:BD:198:VAL:H	2.27	0.42
42:BI:127:LYS:O	42:BI:128:ARG:HG2	2.19	0.42
59:BZ:-29:LEU:H	59:BZ:-29:LEU:HD23	1.84	0.42
59:BZ:417:THR:HA	59:BZ:418:LYS:CB	2.49	0.42
1:CA:271(A):A:N1	1:CA:272(D):G:O2'	2.43	0.42
1:CA:1022:G:H22	1:CA:1142(A):A:H2	1.62	0.42
1:CA:1354:A:H2'	1:CA:1355:G:O4'	2.19	0.42
1:CA:1514:U:H2'	1:CA:1515:G:H8	1.84	0.42
1:CA:2130:U:OP1	3:CC:6:LYS:HG2	2.20	0.42
1:CA:2243:U:H2'	1:CA:2244:U:H6	1.83	0.42
65:CA:3745:HOH:O	5:CE:135:HIS:NE2	2.30	0.42
3:CC:27:ALA:O	3:CC:30:VAL:CG2	2.64	0.42
10:CL:90:LYS:HD3	10:CL:93:ARG:NH2	2.33	0.42
26:C2:21:LEU:HA	26:C2:21:LEU:HD23	1.81	0.42
31:C7:19:ARG:HG2	31:C7:19:ARG:HH11	1.83	0.42
34:DA:189(L):G:H2'	34:DA:190:U:C6	2.54	0.42
34:DA:229:U:H2'	34:DA:230:G:O4'	2.19	0.42
34:DA:575:G:C6	34:DA:821:G:N7	2.87	0.42
34:DA:991:U:H3'	34:DA:1212:U:C4	2.54	0.42
34:DA:1303:C:N4	34:DA:1304:G:C6	2.87	0.42
35:DB:105:PHE:O	35:DB:107:THR:N	2.52	0.42
37:DD:64:LEU:HB2	37:DD:198:VAL:HG11	2.01	0.42
37:DD:191:ARG:HD2	37:DD:191:ARG:HA	1.73	0.42
42:DI:17:VAL:HA	42:DI:63:ILE:HG12	2.02	0.42
46:DM:29:ARG:HG3	46:DM:64:TRP:CH2	2.54	0.42
1:AA:485:U:H5"	31:A7:40:TRP:CD2	2.54	0.42
1:AA:579:G:H2'	1:AA:580:U:C6	2.55	0.42
1:AA:1271:G:O3'	19:AV:84:LYS:HE2	2.19	0.42
1:AA:2267:G:H21	24:A0:9:SER:HB3	1.84	0.42
1:AA:2595:G:N3	56:BW:76:F3N:C2	2.82	0.42
2:AB:66:A:N6	2:AB:108:U:H2'	2.35	0.42
11:AN:85:ILE:HA	11:AN:86:PRO:HD3	1.81	0.42
19:AV:28:GLU:HG3	19:AV:29:PRO:HD2	2.01	0.42
21:AX:24:GLY:O	21:AX:83:VAL:HG22	2.19	0.42
34:BA:342:C:O2'	34:BA:343:U:H5'	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:BA:924:C:H2'	34:BA:925:G:H8	1.85	0.42
34:BA:1055:A:C5	34:BA:1206:G:C2	3.07	0.42
43:BJ:61:GLU:OE1	47:BN:49:HIS:HE1	2.03	0.42
50:BQ:87:LYS:HA	50:BQ:87:LYS:HD3	1.84	0.42
58:BY:38:A:H2'	58:BY:39:PSU:O4'	2.20	0.42
59:BZ:73:PHE:CZ	59:BZ:78:ARG:NH1	2.79	0.42
59:BZ:247:ARG:HG3	59:BZ:247:ARG:NH1	2.34	0.42
59:BZ:422:GLU:H	59:BZ:422:GLU:HG3	1.61	0.42
1:CA:924:C:H2'	1:CA:925:C:C6	2.54	0.42
1:CA:1404:C:H2'	1:CA:1405:U:H6	1.85	0.42
1:CA:2126:A:N6	1:CA:2163:C:H5'	2.34	0.42
2:CB:78:A:C2	2:CB:100:A:C4	3.07	0.42
4:CD:16:MET:CE	4:CD:208:LYS:HD3	2.50	0.42
4:CD:102:LYS:C	4:CD:103:ARG:HG2	2.44	0.42
5:CE:11:MET:HE3	5:CE:186:GLY:O	2.20	0.42
6:CF:31:HIS:O	6:CF:34:TRP:HB3	2.20	0.42
11:CN:34:LEU:HD12	11:CN:34:LEU:HA	1.61	0.42
11:CN:43:THR:HA	11:CN:44:PRO:HD3	1.82	0.42
15:CR:18:LEU:HD23	15:CR:18:LEU:HA	1.64	0.42
23:CZ:100:VAL:HA	23:CZ:101:PRO:HD3	1.90	0.42
24:C0:72:ARG:HE	24:C0:75:LEU:HD12	1.85	0.42
26:C2:22:GLU:OE2	26:C2:68:ARG:NH2	2.52	0.42
30:C6:8:LYS:HD3	32:C8:34:TRP:CG	2.54	0.42
33:C9:14:CYS:HA	33:C9:27:CYS:HB2	2.02	0.42
34:DA:1074:G:O2'	34:DA:1101:A:N1	2.44	0.42
42:DI:8:GLY:O	42:DI:14:VAL:HA	2.19	0.42
1:AA:726:C:H2'	1:AA:727:G:H8	1.85	0.42
1:AA:2150:C:H2'	1:AA:2151:C:H6	1.84	0.42
1:AA:2595:G:N3	56:BW:76:F3N:H2	2.35	0.42
10:AL:101:TRP:O	10:AL:105:LEU:HD12	2.19	0.42
34:BA:155:C:N4	34:BA:167:G:O6	2.53	0.42
34:BA:162:A:C8	34:BA:163:C:H1'	2.55	0.42
34:BA:836:G:OP2	51:BR:61:LYS:HE3	2.19	0.42
34:BA:1002:G:C2	34:BA:1003:G:H1'	2.55	0.42
36:BC:23:TYR:CD2	36:BC:23:TYR:C	2.97	0.42
37:BD:158:ILE:H	37:BD:158:ILE:HG12	1.61	0.42
41:BH:49:GLU:HG2	41:BH:62:TYR:HE1	1.85	0.42
45:BL:24:VAL:HB	45:BL:27:LEU:HD22	2.01	0.42
45:BL:27:LEU:HD12	45:BL:27:LEU:HA	1.84	0.42
47:BN:33:VAL:HA	47:BN:40:CYS:HA	2.02	0.42
51:BR:45:SER:OG	51:BR:47:THR:HG22	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:BZ:-34:ARG:O	59:BZ:-32:LEU:N	2.52	0.42
59:BZ:100:VAL:HG12	59:BZ:100:VAL:O	2.19	0.42
1:CA:18:C:H2'	1:CA:19:C:H6	1.83	0.42
1:CA:315:G:H2'	1:CA:316:C:C6	2.55	0.42
1:CA:330:A:H2	1:CA:1210:A:HO2'	1.65	0.42
1:CA:686:G:N2	1:CA:788:A:H61	2.17	0.42
1:CA:794:G:H2'	1:CA:795:C:C6	2.55	0.42
1:CA:814:C:H2'	1:CA:815:C:H6	1.85	0.42
1:CA:862:G:O2'	2:CB:78:A:N3	2.53	0.42
1:CA:956:G:N2	1:CA:959:A:H3'	2.34	0.42
1:CA:1104:C:H2'	1:CA:1105:U:C6	2.55	0.42
1:CA:1473:G:H2'	1:CA:1474:C:O4'	2.19	0.42
1:CA:2756:U:H1'	1:CA:2757:A:H5"	2.01	0.42
3:CC:195:ARG:HG3	3:CC:195:ARG:NH1	2.35	0.42
7:CG:86:MET:HA	7:CG:87:PRO:HD2	1.93	0.42
7:CG:136:ARG:HD2	7:CG:137:GLU:HG3	2.01	0.42
12:CO:98:VAL:CG1	12:CO:117:LEU:HB3	2.48	0.42
13:CP:84:ASN:OD1	13:CP:117:GLU:HB2	2.19	0.42
13:CP:85:LEU:HD23	13:CP:88:LEU:HD12	2.01	0.42
25:C1:80:LEU:HD23	25:C1:82:LEU:HD21	2.01	0.42
34:DA:26:A:O2'	37:DD:209:ARG:NH2	2.53	0.42
34:DA:165:C:H2'	34:DA:166:G:H8	1.84	0.42
34:DA:923:A:N6	34:DA:1392:G:O6	2.52	0.42
36:DC:22:TRP:HB2	36:DC:23:TYR:H	1.69	0.42
40:DG:26:PHE:CD1	40:DG:62:PHE:CE1	3.07	0.42
40:DG:28:ASN:HD21	40:DG:36:LYS:NZ	2.16	0.42
40:DG:79:ARG:HB3	40:DG:80:VAL:H	1.42	0.42
56:DW:37:MIA:H2'	56:DW:38:A:O4'	2.19	0.42
59:DZ:31:ARG:HA	59:DZ:31:ARG:HE	1.83	0.42
59:DZ:285:ASP:OD2	59:DZ:285:ASP:N	2.53	0.42
59:DZ:443:HIS:HA	59:DZ:444:PRO:HD2	1.79	0.42
59:DZ:480:GLN:C	59:DZ:482:ALA:H	2.27	0.42
1:AA:1634:C:H2'	1:AA:1635:C:C6	2.53	0.42
1:AA:1911:A:N1	1:AA:2246:G:H1'	2.34	0.42
1:AA:2289:G:OP2	24:A0:10:THR:HG21	2.20	0.42
3:AC:225:ILE:O	3:AC:227:PRO:HD3	2.19	0.42
6:AF:181:LEU:HA	6:AF:181:LEU:HD12	1.81	0.42
14:AQ:31:ASP:OD2	14:AQ:107:ALA:HA	2.20	0.42
17:AT:18:ASP:OD2	17:AT:18:ASP:N	2.53	0.42
17:AT:53:ARG:CZ	17:AT:53:ARG:HB3	2.49	0.42
24:A0:56:ASP:O	24:A0:57:PHE:HB2	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:BA:134:A:N6	49:BP:25:ARG:NH1	2.68	0.42
34:BA:1092:A:N3	34:BA:1183:A:N6	2.67	0.42
34:BA:1486:G:H2'	34:BA:1487:G:O4'	2.20	0.42
51:BR:46:GLU:H	51:BR:46:GLU:HG3	1.52	0.42
56:BW:19:G:H4'	56:BW:20:U:OP1	2.19	0.42
59:BZ:21:ILE:HD12	59:BZ:87:HIS:NE2	2.35	0.42
1:CA:86:C:P	22:CY:32:PRO:HG2	2.60	0.42
1:CA:590:A:H2'	1:CA:591:C:O4'	2.19	0.42
1:CA:610:G:N2	1:CA:619:G:H1'	2.34	0.42
1:CA:910:A:H2'	1:CA:2264:C:O2'	2.20	0.42
1:CA:1070:A:H5'	1:CA:1072:C:OP2	2.19	0.42
1:CA:1615:C:C5	1:CA:1617:C:C4	3.07	0.42
1:CA:1889:A:N1	1:CA:2234:G:H1'	2.34	0.42
2:CB:11:C:OP2	2:CB:12:C:N4	2.33	0.42
3:CC:6:LYS:N	3:CC:9:ARG:HH12	2.17	0.42
7:CG:33:ARG:HB2	7:CG:33:ARG:CZ	2.50	0.42
9:CK:56:ASN:HA	9:CK:83:TYR:HA	2.02	0.42
13:CP:2:LYS:HE2	13:CP:2:LYS:HB2	1.84	0.42
34:DA:784:C:H2'	34:DA:785:G:C8	2.54	0.42
34:DA:1041:A:H5'	34:DA:1042:G:OP2	2.20	0.42
34:DA:1418:A:H5"	34:DA:1419:G:OP2	2.19	0.42
35:DB:55:PHE:HD1	35:DB:58:ILE:HD12	1.83	0.42
36:DC:32:LEU:O	36:DC:36:ASP:HB2	2.19	0.42
38:DE:100:VAL:HG12	38:DE:107:ARG:HH21	1.85	0.42
59:DZ:630:GLN:CG	59:DZ:646:PHE:HB2	2.50	0.42
1:AA:645:G:H2'	1:AA:645:G:N3	2.33	0.42
1:AA:1117:G:O2'	1:AA:1135:G:OP2	2.30	0.42
1:AA:2200:C:H2'	1:AA:2201:C:C6	2.55	0.42
1:AA:2703:C:O3'	1:AA:2881:C:H4'	2.20	0.42
3:AC:54:ARG:HE	3:AC:57:GLN:HG2	1.83	0.42
8:AH:33:LEU:HD21	8:AH:136:ILE:HG13	2.01	0.42
11:AN:4:TYR:CE2	18:AU:100:VAL:HG11	2.54	0.42
13:AP:65:ARG:HG3	13:AP:66:GLY:N	2.34	0.42
16:AS:110:LEU:HD12	16:AS:110:LEU:HA	1.75	0.42
23:AZ:98:MET:O	23:AZ:125:LEU:HD12	2.18	0.42
23:AZ:107:THR:HA	23:AZ:108:PRO:HD3	1.71	0.42
34:BA:1028:C:H2'	34:BA:1029:C:H4'	2.02	0.42
34:BA:1054:C:C4	56:BW:34:G:H1'	2.55	0.42
34:BA:1250:A:H4'	42:BI:68:GLY:N	2.35	0.42
36:BC:8:ILE:HG22	47:BN:49:HIS:O	2.19	0.42
37:BD:116:GLN:NE2	37:BD:157:LEU:HD11	2.35	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:BE:31:LEU:HD23	38:BE:45:PHE:CD1	2.55	0.42
40:BG:103:TRP:CH2	40:BG:141:VAL:HG21	2.55	0.42
53:BT:99:LEU:HA	53:BT:100:ILE:O	2.19	0.42
57:BX:39:C:O2'	58:BY:35:A:O2'	2.38	0.42
59:BZ:2:LYS:HA	59:BZ:5:LEU:HB2	2.00	0.42
59:BZ:111:SER:O	59:BZ:148:LEU:HD21	2.20	0.42
59:BZ:268:GLY:HA2	59:BZ:271:LEU:HD13	2.02	0.42
1:CA:373:U:H1'	1:CA:423:A:N3	2.34	0.42
1:CA:572:A:H5"	1:CA:573:G:OP2	2.19	0.42
1:CA:1155:A:H5"	18:CU:55:ARG:NH1	2.26	0.42
1:CA:1810:A:H2'	1:CA:1811:G:O4'	2.18	0.42
1:CA:2112:G:C5	1:CA:2113:U:H1'	2.55	0.42
1:CA:2712:U:H2'	1:CA:2714:G:H5"	2.01	0.42
3:CC:20:VAL:O	3:CC:21:TYR:CB	2.59	0.42
3:CC:225:ILE:O	3:CC:227:PRO:HD3	2.19	0.42
15:CR:12:ARG:HG3	15:CR:12:ARG:HH11	1.84	0.42
17:CT:41:ARG:NH1	34:DA:346:G:OP1	2.49	0.42
22:CY:68:HIS:CE1	22:CY:70:SER:HB3	2.55	0.42
23:CZ:40:ASP:OD2	23:CZ:42:VAL:HG12	2.20	0.42
34:DA:685:G:C2	34:DA:686:U:C4	3.08	0.42
34:DA:1144:G:N2	34:DA:1146:A:H62	2.18	0.42
44:DK:84:VAL:HG11	44:DK:91:ARG:HD2	2.00	0.42
49:DP:36:ILE:HD12	49:DP:56:ALA:HB2	2.02	0.42
50:DQ:52:LYS:HB2	50:DQ:52:LYS:HE3	1.83	0.42
53:DT:57:ARG:HH12	53:DT:100:ILE:CD1	2.33	0.42
59:DZ:280:LEU:HA	59:DZ:281:PRO:HD3	1.92	0.42
59:DZ:286:ILE:O	59:DZ:286:ILE:HG12	2.19	0.42
1:AA:233:A:C2	1:AA:244:A:C4	3.07	0.42
1:AA:330:U:H2'	1:AA:331:G:O4'	2.20	0.42
1:AA:540:A:H2	1:AA:1306:G:N3	2.17	0.42
1:AA:800:C:H2'	1:AA:801:C:H6	1.85	0.42
1:AA:1764:G:C6	1:AA:1765:U:C4	3.08	0.42
1:AA:1831:C:OP2	4:AD:183:ARG:NH2	2.53	0.42
1:AA:2022:G:OP1	15:AR:5:LYS:NZ	2.49	0.42
1:AA:2340:A:H2'	1:AA:2341:G:C8	2.54	0.42
1:AA:2408:G:H5'	25:A1:25:LYS:HE2	2.02	0.42
5:AE:40:GLU:CD	5:AE:40:GLU:H	2.26	0.42
5:AE:49:LEU:HD22	5:AE:81:ILE:HG13	2.01	0.42
33:A9:17:ILE:HD12	33:A9:17:ILE:HA	1.72	0.42
34:BA:106:C:O2	34:BA:379:C:H4'	2.20	0.42
34:BA:342:C:N3	34:BA:348:G:N2	2.68	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:BA:1368:G:OP2	42:BI:112:LYS:HG3	2.20	0.42
35:BB:24:TRP:CD1	35:BB:24:TRP:H	2.38	0.42
36:BC:143:GLU:C	36:BC:145:GLY:H	2.28	0.42
37:BD:52:SER:HG	37:BD:55:ALA:H	1.63	0.42
40:BG:45:ASP:O	40:BG:49:ILE:HG13	2.20	0.42
40:BG:78:ARG:HG2	40:BG:79:ARG:N	2.35	0.42
51:BR:40:LEU:C	51:BR:42:ARG:N	2.78	0.42
53:BT:81:LYS:O	53:BT:85:MET:HG3	2.19	0.42
59:BZ:25:LYS:NZ	64:BZ:702:GDP:O3B	2.42	0.42
59:BZ:147:TRP:CD1	59:BZ:147:TRP:H	2.37	0.42
1:CA:86:C:H4'	1:CA:104:U:H1'	2.02	0.42
1:CA:814:C:O2'	1:CA:815:C:H5'	2.20	0.42
1:CA:2285:C:OP2	30:C6:6:ARG:NH1	2.52	0.42
1:CA:2628:C:H1'	1:CA:2781:A:H2'	2.01	0.42
1:CA:2689:U:P	1:CA:2719:G:H22	2.43	0.42
3:CC:48:LEU:CD2	3:CC:59:VAL:HG21	2.50	0.42
4:CD:132:PRO:HD3	4:CD:190:TYR:CZ	2.55	0.42
5:CE:24:THR:HG23	5:CE:184:VAL:HG13	2.00	0.42
5:CE:36:ARG:HG2	5:CE:47:VAL:HG12	2.01	0.42
6:CF:60:SER:OG	6:CF:61:GLY:N	2.51	0.42
8:CH:42:ARG:HH12	8:CH:53:GLU:HB2	1.84	0.42
8:CH:88:LEU:HD22	8:CH:165:ALA:HA	2.00	0.42
11:CN:120:LEU:HD22	11:CN:122:VAL:HG23	2.01	0.42
13:CP:47:ASP:HA	13:CP:48:PRO:HD3	1.87	0.42
15:CR:51:LEU:HD23	15:CR:51:LEU:HA	1.74	0.42
17:CT:118:ARG:HG2	34:DA:1442(A):G:C8	2.55	0.42
26:C2:2:LYS:HE3	26:C2:2:LYS:HB3	1.92	0.42
34:DA:232:G:H1'	34:DA:262:A:N1	2.35	0.42
34:DA:688:G:H2'	34:DA:689:C:C6	2.55	0.42
34:DA:992:U:H3	34:DA:1044:A:N6	2.12	0.42
34:DA:1004:A:H62	34:DA:1037:C:C2'	2.30	0.42
35:DB:184:VAL:N	35:DB:198:ASP:OD2	2.50	0.42
57:DX:47:U:N3	57:DX:50:U:OP1	2.52	0.42
57:DX:58:A:H4'	57:DX:59:A:OP1	2.18	0.42
59:DZ:463:VAL:HA	59:DZ:466:LEU:HB2	2.02	0.42
1:AA:1091:A:C8	1:AA:1093:G:C2	3.08	0.42
1:AA:1500:A:O2'	1:AA:1501:U:H2'	2.20	0.42
1:AA:1938:A:H2'	1:AA:1939:U:O4'	2.20	0.42
1:AA:1944:G:H2'	1:AA:1945:U:C6	2.54	0.42
1:AA:2554:A:H4'	1:AA:2555:G:C8	2.55	0.42
5:AE:51:PHE:CE2	5:AE:52:LEU:HG	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AG:143:GLU:CD	7:AG:143:GLU:H	2.28	0.42
17:AT:45:PHE:CE1	17:AT:65:LYS:HD3	2.55	0.42
22:AY:55:TYR:H	22:AY:55:TYR:HD1	1.68	0.42
22:AY:90:LEU:HD12	22:AY:90:LEU:HA	1.75	0.42
23:AZ:104:PHE:HB3	23:AZ:141:VAL:HG21	2.01	0.42
25:A1:23:LYS:HB2	25:A1:23:LYS:HE3	1.90	0.42
25:A1:85:LEU:HA	25:A1:85:LEU:HD23	1.75	0.42
32:A8:52:LYS:N	32:A8:53:PRO:HD2	2.35	0.42
34:BA:864:A:H2'	34:BA:865:A:C8	2.55	0.42
39:BF:4:TYR:HD1	39:BF:92:LYS:HA	1.85	0.42
41:BH:64:LYS:HB3	41:BH:79:VAL:HG21	2.01	0.42
53:BT:14:LYS:O	53:BT:18:GLN:HG3	2.20	0.42
59:BZ:21:ILE:HD11	59:BZ:117:GLN:CD	2.45	0.42
59:BZ:94:VAL:HB	59:BZ:98:MET:HB2	2.02	0.42
59:BZ:246:ILE:C	59:BZ:250:THR:HG1	2.27	0.42
1:CA:503:A:H4'	1:CA:504:U:H5"	2.02	0.42
1:CA:748:G:O6	20:CW:90:ARG:NH1	2.52	0.42
1:CA:857:C:OP2	24:C0:77:ARG:NH2	2.52	0.42
1:CA:1268:A:H2'	1:CA:1269:A:O4'	2.20	0.42
1:CA:1651:G:H2'	1:CA:1652:A:O4'	2.20	0.42
1:CA:1713:U:H2'	1:CA:1714:G:C8	2.55	0.42
1:CA:2335:A:C8	1:CA:2337:G:C5	3.07	0.42
1:CA:2583:G:N3	56:DW:76:F3N:H2	2.35	0.42
9:CK:4:LYS:HA	9:CK:5:ARG:HA	1.86	0.42
12:CO:15:GLY:O	12:CO:47:ILE:HG13	2.20	0.42
16:CS:63:THR:HG23	16:CS:64:GLU:N	2.35	0.42
21:CX:5:TYR:CE2	26:C2:30:ARG:HB3	2.54	0.42
21:CX:5:TYR:HB3	26:C2:33:MET:HB2	2.02	0.42
23:CZ:145:GLU:HG2	23:CZ:146:ILE:HD12	2.01	0.42
23:CZ:150:LEU:HB3	23:CZ:171:ILE:HD11	2.02	0.42
34:DA:834:C:C4	34:DA:835:U:C4	3.08	0.42
34:DA:1218:C:P	47:DN:9:LYS:HZ3	2.42	0.42
34:DA:1263:C:H2'	34:DA:1264:C:C6	2.55	0.42
36:DC:18:TRP:HE3	36:DC:18:TRP:H	1.68	0.42
38:DE:24:ARG:NH1	55:DV:24:A:OP2	2.52	0.42
44:DK:72:ALA:HB1	44:DK:77:MET:HB2	2.01	0.42
45:DL:32:PHE:CB	45:DL:84:LEU:HD11	2.46	0.42
45:DL:84:LEU:HD13	45:DL:85:ILE:N	2.35	0.42
53:DT:55:ILE:HA	53:DT:55:ILE:HD13	1.82	0.42
57:DX:72:A:H2'	57:DX:73:A:C8	2.55	0.42
1:AA:1185:C:O3'	11:AN:25:ARG:NH1	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1715:A:H4'	1:AA:1716:A:O5'	2.20	0.41
1:AA:1961:U:OP1	1:AA:2616:U:O2'	2.34	0.41
1:AA:2132:G:C6	1:AA:2142:G:C8	3.08	0.41
1:AA:2348:A:N6	24:A0:43:THR:HG21	2.33	0.41
1:AA:2429:C:OP1	13:AP:65:ARG:NH2	2.53	0.41
2:AB:88:C:H2'	2:AB:89:G:O4'	2.19	0.41
3:AC:48:LEU:CD2	3:AC:59:VAL:HG21	2.50	0.41
11:AN:115:ARG:HA	11:AN:118:LYS:HE3	2.02	0.41
16:AS:74:ALA:HA	16:AS:110:LEU:HD22	2.02	0.41
17:AT:32:TYR:HD2	17:AT:34:VAL:HG23	1.85	0.41
19:AV:97:LYS:HA	19:AV:97:LYS:HD2	1.46	0.41
22:AY:76:CYS:HA	22:AY:77:PRO:HD3	1.89	0.41
31:A7:31:LEU:HD22	31:A7:42:LEU:HD13	2.00	0.41
34:BA:99:U:H2'	34:BA:100:C:C6	2.55	0.41
34:BA:107:G:H2'	34:BA:108:G:O4'	2.20	0.41
34:BA:109:A:H2'	34:BA:326:G:H21	1.83	0.41
34:BA:392:G:H2'	34:BA:393:A:C8	2.55	0.41
34:BA:567:G:H2'	34:BA:568:G:O4'	2.19	0.41
34:BA:955:U:O2'	52:BS:83:HIS:CD2	2.73	0.41
37:BD:202:LEU:HD23	37:BD:202:LEU:HA	1.74	0.41
38:BE:83:GLU:HG2	38:BE:88:LYS:HB2	2.02	0.41
39:BF:2:ARG:CZ	39:BF:69:GLU:HG2	2.50	0.41
52:BS:31:ILE:HD12	52:BS:49:ILE:HG12	2.01	0.41
53:BT:63:ILE:HG22	53:BT:77:ALA:HB1	2.02	0.41
1:CA:403:U:H4'	1:CA:404:C:H5'	2.01	0.41
1:CA:623:G:H2'	1:CA:624:C:C6	2.55	0.41
1:CA:687:C:H1'	31:C7:4:THR:HG22	2.02	0.41
1:CA:1816:G:C8	4:CD:62:TYR:CE2	3.09	0.41
1:CA:2378:A:H4'	16:CS:23:ARG:NH1	2.35	0.41
3:CC:60:ARG:NH2	3:CC:165:ARG:HH21	2.18	0.41
5:CE:51:PHE:CE2	5:CE:52:LEU:HD13	2.55	0.41
11:CN:58:ASP:OD2	11:CN:59:LYS:HE3	2.20	0.41
13:CP:3:LEU:HD12	13:CP:3:LEU:HA	1.88	0.41
13:CP:46:LYS:HE3	13:CP:46:LYS:HB3	1.87	0.41
34:DA:114:U:O2'	34:DA:115:G:H5'	2.20	0.41
34:DA:519:C:H2'	34:DA:520:A:O4'	2.20	0.41
34:DA:519:C:H2'	34:DA:520:A:C8	2.55	0.41
34:DA:918:A:H2'	34:DA:919:A:O4'	2.20	0.41
34:DA:1018:C:H2'	34:DA:1019:C:O4'	2.20	0.41
34:DA:1328:C:H2'	34:DA:1329:A:O4'	2.20	0.41
34:DA:1429:C:H2'	34:DA:1430:C:C6	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:DB:214:ILE:H	35:DB:214:ILE:HG12	1.64	0.41
37:DD:28:SER:HB2	37:DD:29:PRO:HD2	2.01	0.41
40:DG:104:LEU:HD13	40:DG:104:LEU:HA	1.73	0.41
41:DH:97:VAL:HG21	41:DH:128:GLY:HA2	2.02	0.41
56:DW:13:C:HO2'	56:DW:14:A:P	2.43	0.41
57:DX:49:G:N2	57:DX:66:C:O2	2.53	0.41
59:DZ:494:GLU:CD	59:DZ:511:LYS:HE2	2.44	0.41
1:AA:696:C:P	1:AA:696:C:H6	2.43	0.41
1:AA:1042:A:H4'	18:AU:91:ASP:OD2	2.20	0.41
1:AA:1403:U:H2'	1:AA:1404:G:O4'	2.20	0.41
1:AA:2431:U:H2'	1:AA:2432:C:C6	2.56	0.41
1:AA:2481:A:H5'	1:AA:2482:G:OP2	2.20	0.41
5:AE:144:ARG:HB3	5:AE:145:LYS:H	1.45	0.41
7:AG:145:THR:H	7:AG:148:MET:HE2	1.85	0.41
7:AG:155:MET:HE2	7:AG:155:MET:HB3	2.00	0.41
12:AO:19:ILE:HB	12:AO:41:ALA:HB1	2.01	0.41
13:AP:3:LEU:HD12	13:AP:3:LEU:HA	1.75	0.41
15:AR:100:LEU:HD11	15:AR:113:LEU:HD23	2.02	0.41
21:AX:41:ASN:O	21:AX:45:THR:HG23	2.20	0.41
30:A6:19:ARG:HD2	30:A6:19:ARG:N	2.35	0.41
34:BA:62:U:H5"	34:BA:385:C:H1'	2.02	0.41
34:BA:143:A:H2	34:BA:220:G:H1	1.66	0.41
34:BA:382:A:H2'	34:BA:383:A:C8	2.55	0.41
34:BA:1152:A:H5'	43:BJ:13:HIS:ND1	2.35	0.41
34:BA:1352:C:OP1	54:BU:3:LYS:NZ	2.46	0.41
34:BA:1516:G:H2'	34:BA:1518:A:OP2	2.20	0.41
35:BB:145:LEU:HD12	35:BB:149:LEU:HD12	2.01	0.41
38:BE:127:ASN:HA	38:BE:128:PRO:HD3	1.79	0.41
45:BL:39:VAL:HG11	45:BL:41:ARG:NH1	2.35	0.41
51:BR:40:LEU:O	51:BR:43:PHE:N	2.38	0.41
59:BZ:6:GLU:O	59:BZ:10:LYS:N	2.53	0.41
59:BZ:264:LEU:HB2	64:BZ:702:GDP:C6	2.55	0.41
1:CA:443:A:H1'	1:CA:1201:C:O4'	2.19	0.41
1:CA:590:A:OP1	6:CF:95:ARG:NH1	2.49	0.41
1:CA:815:C:H2'	1:CA:816:C:H6	1.84	0.41
1:CA:888:C:P	46:DM:93:ARG:HD3	2.59	0.41
1:CA:1469:A:H2'	1:CA:1470:G:O4'	2.20	0.41
1:CA:2127:G:OP1	1:CA:2127:G:H4'	2.20	0.41
1:CA:2137:C:H2'	1:CA:2138:C:C6	2.55	0.41
1:CA:2183:C:H2'	1:CA:2184:G:C8	2.52	0.41
1:CA:2206:G:H3'	1:CA:2207:G:H8	1.75	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:CE:48:GLN:OE1	5:CE:78:LEU:HG	2.21	0.41
6:CF:64:ILE:HD12	6:CF:65:TRP:CZ3	2.55	0.41
16:CS:87:PHE:CE1	16:CS:102:ALA:HB2	2.55	0.41
18:CU:79:PHE:O	18:CU:83:LEU:HD22	2.20	0.41
18:CU:86:ALA:O	19:CV:49:THR:HG23	2.20	0.41
19:CV:82:ARG:O	19:CV:83:ARG:HD3	2.20	0.41
23:CZ:8:TYR:HB2	23:CZ:38:TYR:CZ	2.55	0.41
23:CZ:102:LEU:HD11	23:CZ:121:HIS:O	2.20	0.41
23:CZ:157:LEU:HB3	23:CZ:161:VAL:HG13	2.02	0.41
30:C6:40:CYS:SG	30:C6:42:TRP:HB2	2.59	0.41
34:DA:396:G:O2'	34:DA:398:C:OP1	2.24	0.41
34:DA:730:G:O2'	34:DA:766:A:H5'	2.20	0.41
34:DA:1049:U:C6	34:DA:1201:A:H5'	2.55	0.41
34:DA:1090:U:H2'	34:DA:1091:U:H6	1.86	0.41
34:DA:1119:C:H2'	34:DA:1120:G:C8	2.54	0.41
36:DC:184:TYR:HD1	36:DC:201:TYR:CE2	2.38	0.41
43:DJ:38:ILE:HG12	43:DJ:71:LEU:O	2.20	0.41
46:DM:88:ARG:HG2	46:DM:98:VAL:HG12	2.03	0.41
56:DW:9:A:H8	56:DW:11:C:H41	1.67	0.41
1:AA:50:G:H4'	1:AA:51:A:H5'	2.01	0.41
1:AA:469:A:C6	6:AF:45:ARG:HD2	2.55	0.41
1:AA:1067:A:C8	1:AA:1067:A:C3'	3.03	0.41
1:AA:1098:C:H2'	1:AA:1099:C:H6	1.84	0.41
1:AA:2124:U:H2'	1:AA:2125:C:C6	2.54	0.41
1:AA:2164:C:H2'	1:AA:2165:C:C6	2.55	0.41
4:AD:260:ARG:NH2	4:AD:264:LYS:HD3	2.35	0.41
5:AE:108:SER:O	5:AE:162:ALA:HA	2.20	0.41
7:AG:11:TYR:HA	7:AG:15:VAL:HB	2.01	0.41
8:AH:84:SER:HA	8:AH:133:VAL:O	2.20	0.41
15:AR:21:TYR:OH	15:AR:43:GLU:HG2	2.20	0.41
16:AS:97:ARG:O	16:AS:100:ALA:HB3	2.20	0.41
23:AZ:129:SER:HA	23:AZ:130:PRO:HD3	1.74	0.41
28:A4:64:GLY:C	28:A4:66:SER:H	2.27	0.41
34:BA:78:G:H22	34:BA:92:C:H42	1.67	0.41
34:BA:243:A:C2	34:BA:246:A:C8	3.09	0.41
34:BA:715:A:H2'	34:BA:716:A:C8	2.55	0.41
34:BA:1118:C:H1'	34:BA:1179:A:C4	2.56	0.41
34:BA:1250:A:H2'	34:BA:1251:A:C8	2.56	0.41
38:BE:74:GLY:HA3	38:BE:116:THR:HG22	2.01	0.41
44:BK:33:THR:HA	44:BK:39:PRO:HA	2.02	0.41
48:BO:32:LEU:O	48:BO:33:THR:C	2.60	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:BS:48:THR:HA	52:BS:60:VAL:O	2.19	0.41
59:BZ:257:PRO:HB2	59:BZ:259:PHE:CE1	2.55	0.41
1:CA:271(F):C:H2'	1:CA:271(G):C:O4'	2.20	0.41
1:CA:583:G:OP2	18:CU:10:ARG:HD2	2.20	0.41
1:CA:863:A:H2'	1:CA:864:G:H8	1.84	0.41
1:CA:1082:U:H5"	10:CL:122:ALA:HB1	2.02	0.41
1:CA:1107:G:C2	1:CA:1108:U:C4	3.08	0.41
1:CA:1401:G:H2'	1:CA:1402:C:O4'	2.21	0.41
1:CA:1638:C:H5"	1:CA:2710:C:O2'	2.20	0.41
1:CA:1647:G:H3'	1:CA:1647:G:OP2	2.20	0.41
1:CA:1656:C:H2'	1:CA:1657:C:C6	2.56	0.41
1:CA:2536:G:C6	1:CA:2537:U:C4	3.09	0.41
3:CC:189:ASN:O	3:CC:190:ILE:C	2.63	0.41
9:CK:118:THR:O	9:CK:120:LYS:N	2.51	0.41
13:CP:36:LYS:O	13:CP:40:SER:HB3	2.20	0.41
13:CP:87:ASP:HB3	13:CP:105:LEU:HD22	2.02	0.41
20:CW:53:SER:O	20:CW:56:ALA:HB3	2.20	0.41
22:CY:98:VAL:HG23	22:CY:99:CYS:O	2.20	0.41
23:CZ:67:LEU:HA	23:CZ:68:PRO:HD3	1.73	0.41
26:C2:49:LYS:HE2	26:C2:49:LYS:HB3	1.89	0.41
32:C8:57:ARG:O	32:C8:58:ILE:C	2.64	0.41
34:DA:64:G:H4'	34:DA:65:U:C3'	2.49	0.41
34:DA:137:C:H2'	34:DA:138:G:H8	1.84	0.41
34:DA:391:G:C6	34:DA:392:G:C5	3.08	0.41
34:DA:1106:G:H4'	36:DC:171:GLY:O	2.20	0.41
34:DA:1130:A:H5'	42:DI:18:PHE:CE2	2.55	0.41
34:DA:1314:C:OP2	52:DS:4:SER:OG	2.12	0.41
37:DD:60:GLU:OE1	37:DD:199:ASN:N	2.52	0.41
40:DG:26:PHE:HB2	40:DG:101:LEU:HD22	2.01	0.41
1:AA:170:A:H2'	1:AA:171:A:C8	2.55	0.41
1:AA:659:C:H2'	1:AA:660:C:C6	2.55	0.41
1:AA:2147:G:OP1	3:AC:71:LYS:NZ	2.52	0.41
1:AA:2173:G:H2'	1:AA:2174:G:C8	2.56	0.41
7:AG:43:LEU:HD12	7:AG:43:LEU:HA	1.81	0.41
7:AG:97:ASP:O	7:AG:101:ILE:HG13	2.20	0.41
8:AH:56:SER:OG	8:AH:61:HIS:ND1	2.40	0.41
15:AR:36:THR:HG22	15:AR:37:THR:H	1.84	0.41
17:AT:109:GLU:HG2	17:AT:112:ARG:HH21	1.85	0.41
23:AZ:150:LEU:O	23:AZ:171:ILE:HG13	2.20	0.41
23:AZ:152:ALA:HA	23:AZ:155:LEU:HD22	2.02	0.41
34:BA:565:U:H3'	34:BA:566:G:H2'	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:BA:1220:G:N2	52:BS:54:GLY:O	2.50	0.41
34:BA:1261:A:H3'	34:BA:1262:C:H6	1.84	0.41
36:BC:131:ARG:HH11	38:BE:50:GLU:HG3	1.86	0.41
40:BG:125:MET:HB3	40:BG:125:MET:HE2	1.76	0.41
47:BN:8:GLU:OE2	47:BN:11:LYS:HD2	2.21	0.41
52:BS:65:ASN:HD22	52:BS:65:ASN:H	1.67	0.41
53:BT:53:LEU:O	53:BT:57:ARG:HG3	2.20	0.41
59:BZ:-9:LEU:C	59:BZ:-7:GLU:N	2.78	0.41
59:BZ:427:ALA:O	59:BZ:431:LEU:HD22	2.20	0.41
59:BZ:471:LYS:HE2	59:BZ:471:LYS:HB3	1.97	0.41
59:BZ:606:MET:HE3	59:BZ:649:LEU:HB2	2.02	0.41
1:CA:888:C:H5"	1:CA:889:C:OP2	2.20	0.41
1:CA:1652:A:O2'	1:CA:1653:G:H5'	2.20	0.41
1:CA:1804:C:O5'	1:CA:1804:C:H6	2.02	0.41
1:CA:1860:G:H4'	3:CC:206:LYS:HG3	1.76	0.41
34:DA:520:A:N1	34:DA:536:C:H1'	2.35	0.41
34:DA:546:G:P	37:DD:72:GLU:HB3	2.60	0.41
34:DA:719:C:O2'	51:DR:49:LYS:HB3	2.21	0.41
34:DA:1343:G:H2'	34:DA:1344:C:C6	2.55	0.41
35:DB:212:GLN:O	35:DB:216:SER:OG	2.35	0.41
37:DD:100:ARG:HH11	37:DD:100:ARG:HG2	1.84	0.41
39:DF:61:LEU:HD23	39:DF:63:TYR:OH	2.20	0.41
48:DO:32:LEU:HA	48:DO:32:LEU:HD23	1.75	0.41
56:DW:4:C:N4	56:DW:5:G:O6	2.53	0.41
59:DZ:165:GLN:O	59:DZ:166:LEU:HD12	2.20	0.41
59:DZ:201:ILE:HG22	59:DZ:202:PRO:O	2.20	0.41
1:AA:1400:A:C8	1:AA:1401:G:C8	3.09	0.41
1:AA:1704:C:H2'	1:AA:1705:C:C6	2.55	0.41
1:AA:1841:A:H2'	1:AA:1842:G:O4'	2.20	0.41
2:AB:41:U:C5	7:AG:70:VAL:HB	2.56	0.41
3:AC:31:LYS:H	3:AC:31:LYS:HG2	1.57	0.41
5:AE:27:LEU:HD22	17:AT:1:MET:HE3	2.03	0.41
7:AG:44:GLY:C	7:AG:46:ALA:N	2.78	0.41
11:AN:138:LEU:HD22	11:AN:138:LEU:HA	1.74	0.41
14:AQ:31:ASP:HB2	14:AQ:32:TYR:HD2	1.85	0.41
16:AS:67:ARG:HD2	16:AS:71:ARG:NH2	2.35	0.41
23:AZ:111:VAL:HG12	23:AZ:112:ARG:N	2.35	0.41
25:A1:23:LYS:HB3	25:A1:29:GLY:HA3	2.02	0.41
28:A4:69:LYS:HE2	52:BS:20:LEU:HD13	2.02	0.41
31:A7:33:ARG:NH2	65:A7:202:HOH:O	2.54	0.41
34:BA:7:G:H5'	34:BA:298:A:O4'	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:BA:368:U:P	59:BZ:351:ARG:HH11	2.43	0.41
34:BA:1053:G:O2'	34:BA:1199:U:OP2	2.21	0.41
34:BA:1130:A:C4	34:BA:1146:A:C2	3.08	0.41
34:BA:1183:A:H3'	34:BA:1184:G:C5'	2.51	0.41
34:BA:1318:A:H2'	34:BA:1319:A:H5"	2.03	0.41
35:BB:167:PRO:HG3	35:BB:186:ALA:HB1	2.02	0.41
46:BM:4:ILE:HA	46:BM:5:ALA:HA	1.90	0.41
57:BX:19:G:H4'	57:BX:20:U:OP2	2.21	0.41
59:BZ:-20:LEU:HD22	59:BZ:-20:LEU:HA	1.70	0.41
59:BZ:78:ARG:HH11	59:BZ:78:ARG:CB	2.32	0.41
59:BZ:414:GLU:O	59:BZ:416:LYS:N	2.54	0.41
1:CA:297:C:H2'	1:CA:298:G:O4'	2.20	0.41
1:CA:620:G:N3	1:CA:620:G:H2'	2.35	0.41
1:CA:643:A:N1	1:CA:2369:A:O2'	2.52	0.41
4:CD:68:LYS:O	4:CD:69:ARG:HB2	2.21	0.41
13:CP:3:LEU:HD12	13:CP:6:LEU:HD12	2.02	0.41
30:C6:34:LEU:HB2	30:C6:51:GLU:HB2	2.03	0.41
34:DA:344:A:H4'	34:DA:345:C:OP2	2.21	0.41
34:DA:511:C:C2	34:DA:512:U:C5	3.08	0.41
34:DA:869:G:H8	34:DA:869:G:O5'	2.03	0.41
34:DA:921:U:O2'	38:DE:19:MET:O	2.26	0.41
36:DC:33:LEU:O	36:DC:37:GLN:N	2.52	0.41
36:DC:112:SER:O	36:DC:115:LEU:HB2	2.21	0.41
37:DD:78:LEU:HB3	37:DD:93:PHE:HE1	1.86	0.41
38:DE:129:ILE:O	38:DE:132:ALA:HB3	2.20	0.41
39:DF:5:GLU:N	39:DF:91:VAL:O	2.47	0.41
40:DG:26:PHE:CZ	40:DG:30:ILE:HD11	2.56	0.41
40:DG:155:ARG:CZ	40:DG:155:ARG:HB3	2.49	0.41
41:DH:9:MET:SD	41:DH:26:VAL:HG21	2.61	0.41
45:DL:124:LYS:HA	45:DL:125:PRO:HD3	1.79	0.41
59:DZ:38:ARG:HE	59:DZ:38:ARG:HB2	1.60	0.41
1:AA:52:A:H2'	1:AA:53:G:O4'	2.20	0.41
1:AA:268:G:O2'	1:AA:269:G:H8	2.02	0.41
1:AA:277:G:H2'	1:AA:278:G:C8	2.55	0.41
1:AA:2140:U:OP1	1:AA:2170:G:H4'	2.20	0.41
1:AA:2202:U:C4	1:AA:2203:G:N7	2.88	0.41
1:AA:2595:G:H2'	1:AA:2596:U:O4'	2.21	0.41
4:AD:34:VAL:HA	4:AD:62:TYR:O	2.21	0.41
7:AG:140:ILE:HG22	7:AG:141:PHE:CD1	2.56	0.41
16:AS:89:ARG:HD2	16:AS:92:TYR:O	2.21	0.41
24:A0:70:GLN:HG2	24:A0:72:ARG:HG3	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:A6:26:ASN:OD1	30:A6:26:ASN:C	2.63	0.41
34:BA:5:U:H5"	34:BA:6:G:C5	2.55	0.41
34:BA:149:A:H2'	34:BA:150:C:H6	1.84	0.41
34:BA:303:A:H2'	34:BA:304:U:O4'	2.20	0.41
34:BA:321:A:C2	34:BA:333:G:C2	3.08	0.41
34:BA:911:U:OP2	45:BL:97:ARG:NH1	2.54	0.41
34:BA:982:U:H4'	34:BA:983:A:O5'	2.21	0.41
37:BD:110:PHE:CE2	37:BD:148:VAL:HG23	2.55	0.41
41:BH:113:SER:O	41:BH:131:GLY:HA3	2.21	0.41
42:BI:23:ASN:HB2	42:BI:25:LYS:NZ	2.35	0.41
46:BM:19:LEU:HD12	46:BM:19:LEU:HA	1.85	0.41
59:BZ:88:VAL:HG23	59:BZ:117:GLN:HA	2.02	0.41
59:BZ:309:LEU:HD21	59:BZ:335:LEU:HD13	2.03	0.41
59:BZ:443:HIS:HA	59:BZ:444:PRO:HD2	1.91	0.41
1:CA:184:C:H2'	1:CA:185:U:H6	1.86	0.41
1:CA:777:A:O2'	1:CA:778:G:H5'	2.20	0.41
1:CA:1081:U:O5'	10:CL:125:ARG:HD3	2.20	0.41
1:CA:1645:G:H5"	1:CA:1646:C:O4'	2.21	0.41
1:CA:2557:G:H2'	1:CA:2558:C:C6	2.55	0.41
2:CB:19:G:H2'	2:CB:20:C:O4'	2.21	0.41
16:CS:39:ILE:HD13	16:CS:85:VAL:HG21	2.01	0.41
16:CS:65:VAL:O	16:CS:68:GLN:HB2	2.21	0.41
22:CY:49:VAL:HG11	22:CY:55:TYR:HD2	1.85	0.41
23:CZ:153:SER:HB3	23:CZ:167:PRO:HB3	2.03	0.41
26:C2:2:LYS:HG2	26:C2:5:GLU:OE1	2.20	0.41
34:DA:67:C:H2'	34:DA:68:G:C8	2.55	0.41
34:DA:841:U:H6	34:DA:841:U:P	2.43	0.41
34:DA:1319:A:N6	34:DA:1361:G:H21	2.18	0.41
35:DB:155:LEU:HD11	35:DB:159:PRO:HD3	2.02	0.41
38:DE:60:TYR:CE1	38:DE:64:ARG:HD3	2.54	0.41
40:DG:26:PHE:CD1	40:DG:62:PHE:HE1	2.39	0.41
41:DH:132:GLU:O	41:DH:134:ILE:N	2.54	0.41
1:AA:381:A:H2'	1:AA:382:U:O4'	2.21	0.41
1:AA:667:G:H21	1:AA:671:A:H2	1.69	0.41
1:AA:1020:C:OP1	65:AA:3936:HOH:O	2.22	0.41
1:AA:2044:U:HO2'	1:AA:2629:C:H5'	1.83	0.41
1:AA:2170:G:H2'	1:AA:2171:G:H8	1.86	0.41
7:AG:111:LEU:HD23	7:AG:111:LEU:HA	1.89	0.41
13:AP:63:PRO:HD3	32:A8:27:THR:HG22	2.02	0.41
18:AU:112:ARG:HH11	18:AU:112:ARG:HG2	1.84	0.41
19:AV:25:LEU:HD12	19:AV:92:THR:HG21	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:AZ:104:PHE:O	23:AZ:106:GLY:N	2.54	0.41
34:BA:452:A:OP1	49:BP:43:LYS:NZ	2.30	0.41
34:BA:741:G:H2'	34:BA:742:G:O4'	2.21	0.41
34:BA:786:G:C2	34:BA:797:C:C2	3.09	0.41
38:BE:96:PRO:HA	38:BE:117:ASP:OD2	2.21	0.41
41:BH:36:LEU:HD23	41:BH:36:LEU:HA	1.80	0.41
43:BJ:38:ILE:HG13	43:BJ:71:LEU:HB3	2.02	0.41
46:BM:121:LYS:NZ	56:BW:40:C:H4'	2.36	0.41
49:BP:5:ARG:O	49:BP:20:VAL:N	2.46	0.41
53:BT:29:LYS:O	53:BT:33:ILE:HG13	2.21	0.41
59:BZ:160:ARG:HD3	59:BZ:254:LYS:C	2.46	0.41
1:CA:335:C:H4'	22:CY:73:ARG:NE	2.35	0.41
1:CA:623:G:C6	1:CA:624:C:C4	3.09	0.41
1:CA:652:C:C2'	1:CA:652(A):A:H5'	2.50	0.41
1:CA:1291:C:H2'	1:CA:1292:U:C6	2.56	0.41
1:CA:1890:A:O5'	1:CA:1890:A:H8	2.04	0.41
1:CA:2380:C:O5'	1:CA:2380:C:H6	2.02	0.41
1:CA:2732:G:H3'	1:CA:2733:A:O4'	2.21	0.41
6:CF:20:LEU:HD23	6:CF:20:LEU:HA	1.75	0.41
8:CH:106:THR:O	8:CH:106:THR:OG1	2.35	0.41
16:CS:93:LYS:HG2	16:CS:95:HIS:HB3	2.02	0.41
18:CU:76:TYR:O	18:CU:79:PHE:HB3	2.20	0.41
23:CZ:14:LYS:HA	23:CZ:15:PRO:HD3	1.79	0.41
25:C1:83:GLU:HA	25:C1:84:GLY:HA2	1.60	0.41
34:DA:255:G:H1'	50:DQ:16:GLN:NE2	2.36	0.41
34:DA:407:G:H5"	37:DD:115:ARG:HB3	2.02	0.41
34:DA:662:G:H2'	34:DA:663:A:C8	2.56	0.41
34:DA:1151:A:O2'	34:DA:1152:A:O5'	2.36	0.41
34:DA:1373:G:H8	34:DA:1373:G:O5'	2.02	0.41
34:DA:1410:G:H2'	34:DA:1411:C:C6	2.56	0.41
34:DA:1429:C:H2'	34:DA:1430:C:H6	1.85	0.41
37:DD:15:GLU:HB3	37:DD:63:LYS:HD2	2.03	0.41
39:DF:96:PRO:HB3	51:DR:30:ASP:CG	2.45	0.41
42:DI:17:VAL:HG23	42:DI:63:ILE:HG12	2.03	0.41
45:DL:52:LEU:HD12	45:DL:52:LEU:HA	1.78	0.41
47:DN:14:PRO:HB2	47:DN:16:PHE:O	2.21	0.41
57:DX:14:A:C5	57:DX:22:G:C6	3.08	0.41
59:DZ:88:VAL:HG23	59:DZ:117:GLN:HE21	1.86	0.41
1:AA:552:C:C4	1:AA:2792:U:H2'	2.55	0.41
1:AA:599:U:H2'	1:AA:600:G:C8	2.56	0.41
1:AA:2227:G:H3'	1:AA:2228:G:N7	2.36	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:2287:C:O2	14:AQ:85:LYS:HE2	2.20	0.41
1:AA:2325:C:H4'	7:AG:91:ARG:HG3	2.02	0.41
3:AC:60:ARG:NH2	3:AC:165:ARG:HH21	2.18	0.41
6:AF:64:ILE:H	6:AF:64:ILE:HG13	1.59	0.41
8:AH:83:TYR:CE2	8:AH:138:LYS:HB2	2.55	0.41
17:AT:61:PHE:CE1	17:AT:76:PHE:HB2	2.56	0.41
17:AT:117:ASP:O	17:AT:121:ILE:HG13	2.21	0.41
32:A8:31:HIS:O	32:A8:32:LEU:HB2	2.20	0.41
34:BA:418:C:H2'	34:BA:419:C:C6	2.56	0.41
34:BA:1072:G:C5	34:BA:1073:U:C4	3.09	0.41
34:BA:1187:G:H2'	34:BA:1188:A:C8	2.56	0.41
36:BC:85:ARG:O	36:BC:89:GLU:HG2	2.21	0.41
38:BE:40:ARG:HB3	38:BE:66:MET:CE	2.51	0.41
46:BM:49:THR:O	46:BM:53:VAL:HG23	2.20	0.41
48:BO:66:LEU:HD12	48:BO:66:LEU:HA	1.76	0.41
51:BR:39:VAL:O	51:BR:42:ARG:HB2	2.20	0.41
59:BZ:538:TYR:OH	59:BZ:577:SER:O	2.30	0.41
1:CA:443:A:C6	6:CF:45:ARG:HD2	2.56	0.41
1:CA:479:A:H4'	1:CA:480:A:OP1	2.20	0.41
1:CA:1125:G:H5'	33:C9:37:GLY:HA2	2.03	0.41
1:CA:1445(A):C:H2'	1:CA:1446:C:H6	1.86	0.41
1:CA:1657:C:H2'	1:CA:1658:C:H6	1.85	0.41
1:CA:1823:G:OP1	4:CD:54:ARG:NH1	2.54	0.41
3:CC:44:VAL:HG23	3:CC:176:VAL:CG2	2.51	0.41
5:CE:33:VAL:HG13	5:CE:89:ASP:C	2.46	0.41
7:CG:15:VAL:HG22	7:CG:175:LEU:HB3	2.02	0.41
12:CO:68:GLU:OE2	12:CO:78:ARG:NH1	2.51	0.41
17:CT:109:GLU:O	17:CT:113:LYS:HB2	2.21	0.41
23:CZ:30:ASN:ND2	23:CZ:90:VAL:HB	2.35	0.41
25:C1:53:VAL:O	25:C1:56:GLN:HB2	2.21	0.41
25:C1:95:LEU:O	25:C1:98:LEU:HB2	2.20	0.41
30:C6:9:LEU:HD11	30:C6:23:THR:HG23	2.02	0.41
32:C8:23:VAL:HA	32:C8:48:PHE:O	2.20	0.41
34:DA:336:C:O2'	34:DA:337:C:H5'	2.21	0.41
34:DA:694:A:H2'	34:DA:695:A:O4'	2.21	0.41
34:DA:1057:G:H2'	34:DA:1058:G:O4'	2.21	0.41
34:DA:1273:G:H5'	34:DA:1274:G:OP2	2.21	0.41
34:DA:1319:A:H61	34:DA:1361:G:H21	1.68	0.41
35:DB:91:PRO:HB3	35:DB:154:LEU:HB3	2.03	0.41
38:DE:41:VAL:HG22	38:DE:113:ALA:HA	2.02	0.41
46:DM:24:GLY:C	46:DM:25:ILE:HD12	2.46	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:DP:58:TYR:O	49:DP:61:SER:N	2.52	0.41
53:DT:63:ILE:HG21	53:DT:81:LYS:HG3	2.02	0.41
58:DY:36:A:H2'	58:DY:37:MIA:O4'	2.20	0.41
59:DZ:590:ILE:HD13	59:DZ:590:ILE:HA	1.83	0.41
59:DZ:641:GLN:HE21	59:DZ:641:GLN:HB2	1.63	0.41
59:DZ:655:TYR:CZ	59:DZ:659:LEU:HG	2.56	0.41
1:AA:139:A:C8	1:AA:1454:C:O2'	2.67	0.41
1:AA:354:A:O2'	1:AA:355:A:C8	2.72	0.41
1:AA:505:A:N3	1:AA:507:G:H5"	2.35	0.41
1:AA:841:G:H2'	1:AA:842:C:H6	1.85	0.41
1:AA:926:G:H8	1:AA:926:G:O5'	2.02	0.41
1:AA:1401:G:P	4:AD:38:LYS:HE2	2.61	0.41
1:AA:1572:G:C6	1:AA:1573:G:C2	3.08	0.41
1:AA:1756:U:H2'	1:AA:1757:C:C6	2.56	0.41
1:AA:1815:A:H4'	1:AA:1816:A:C5'	2.51	0.41
1:AA:1957:G:H1'	1:AA:1986:G:N2	2.36	0.41
1:AA:2356:U:O2'	30:A6:36:LEU:HD22	2.21	0.41
3:AC:11:LEU:HD22	3:AC:11:LEU:H	1.86	0.41
3:AC:206:LYS:HB3	3:AC:206:LYS:HZ3	1.85	0.41
4:AD:33:LEU:HD23	4:AD:33:LEU:HA	1.94	0.41
12:AO:17:ARG:N	12:AO:45:GLU:O	2.40	0.41
17:AT:1:MET:HE2	17:AT:3:ARG:HG2	2.03	0.41
18:AU:47:TYR:HA	18:AU:50:ARG:NH2	2.35	0.41
19:AV:71:LEU:HD23	19:AV:71:LEU:HA	1.94	0.41
34:BA:443:C:H2'	34:BA:444:C:H6	1.86	0.41
34:BA:501:C:H1'	34:BA:549:C:H1'	2.03	0.41
34:BA:509:A:H3'	34:BA:509:A:C8	2.55	0.41
34:BA:973:G:OP1	43:BJ:57:LYS:HE3	2.20	0.41
34:BA:981:U:OP1	47:BN:6:LEU:HD11	2.21	0.41
34:BA:1142:G:H2'	34:BA:1143:G:O4'	2.21	0.41
34:BA:1169:A:N6	34:BA:1170:A:N1	2.69	0.41
34:BA:1304:G:C6	34:BA:1305:G:N1	2.89	0.41
35:BB:21:ARG:HB3	35:BB:39:ILE:HA	2.02	0.41
35:BB:204:ASN:OD1	35:BB:205:ASP:N	2.54	0.41
36:BC:108:ASN:HA	36:BC:109:PRO:HD2	1.91	0.41
37:BD:167:GLY:H	37:BD:168:ARG:NH2	2.19	0.41
38:BE:85:GLY:O	38:BE:86:ALA:HB3	2.21	0.41
44:BK:56:GLY:O	44:BK:89:ALA:HB3	2.21	0.41
46:BM:49:THR:C	46:BM:51:ALA:N	2.78	0.41
46:BM:78:ILE:O	46:BM:82:MET:HG3	2.21	0.41
49:BP:7:ALA:O	49:BP:9:PHE:CD1	2.73	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:BT:18:GLN:O	53:BT:22:ARG:HG3	2.21	0.41
59:BZ:125:ALA:CB	59:BZ:132:ARG:NH1	2.84	0.41
59:BZ:291:GLY:HA3	59:BZ:301:ILE:HD11	2.01	0.41
59:BZ:603:GLU:HG2	59:BZ:679:VAL:HG12	2.03	0.41
1:CA:1002:G:H2'	1:CA:1003:G:O4'	2.21	0.41
1:CA:1485:G:H2'	1:CA:1486:A:O4'	2.20	0.41
1:CA:2404:C:O3'	13:CP:77:ARG:NH2	2.54	0.41
1:CA:2544:G:H1'	1:CA:2646:C:H4'	2.03	0.41
1:CA:2630:G:H2'	1:CA:2631:G:H8	1.86	0.41
1:CA:2801(A):A:H1'	1:CA:2895:U:H1'	2.03	0.41
1:CA:2876:G:OP1	17:CT:3:ARG:HB2	2.21	0.41
3:CC:11:LEU:HD22	3:CC:11:LEU:H	1.86	0.41
3:CC:16:ASP:HA	3:CC:17:PRO:HD2	1.90	0.41
6:CF:103:LYS:HA	6:CF:106:ARG:HG3	2.01	0.41
6:CF:197:ASP:O	6:CF:200:GLU:HB2	2.21	0.41
11:CN:91:LEU:O	11:CN:95:PRO:HB3	2.20	0.41
13:CP:93:GLY:H	13:CP:123:LEU:HD21	1.86	0.41
14:CQ:83:MET:HE2	14:CQ:83:MET:HA	2.02	0.41
14:CQ:114:ALA:O	14:CQ:115:MET:C	2.62	0.41
18:CU:76:TYR:CZ	18:CU:80:ILE:HG13	2.55	0.41
19:CV:1:MET:HG2	19:CV:41:GLY:O	2.20	0.41
20:CW:10:VAL:HG21	20:CW:103:ILE:HD12	2.01	0.41
21:CX:4:ALA:HB1	21:CX:42:ALA:HA	2.01	0.41
32:C8:26:LYS:HG2	32:C8:48:PHE:CD1	2.56	0.41
34:DA:401:C:H1'	34:DA:622:A:H1'	2.02	0.41
34:DA:790:A:OP1	57:DX:38:A:O2'	2.37	0.41
34:DA:796:C:H6	34:DA:796:C:O5'	2.04	0.41
34:DA:1122:U:H2'	34:DA:1123:A:O4'	2.20	0.41
34:DA:1277:C:O2'	34:DA:1279:A:H1'	2.20	0.41
34:DA:1281:U:H5"	34:DA:1282:C:C5	2.56	0.41
37:DD:26:CYS:HA	63:DD:501:SF4:S3	2.61	0.41
40:DG:110:GLN:HE21	40:DG:110:GLN:HB3	1.71	0.41
40:DG:120:ILE:HG22	40:DG:124:LEU:CD1	2.50	0.41
41:DH:9:MET:HE1	41:DH:32:LYS:O	2.21	0.41
41:DH:39:LEU:HD13	41:DH:39:LEU:HA	1.96	0.41
41:DH:134:ILE:HG22	41:DH:135:CYS:SG	2.61	0.41
46:DM:60:VAL:HG23	46:DM:64:TRP:CE3	2.56	0.41
50:DQ:89:LEU:HD23	50:DQ:89:LEU:HA	1.64	0.41
53:DT:36:LEU:HD13	53:DT:36:LEU:HA	1.57	0.41
56:DW:13:C:O2'	56:DW:14:A:P	2.79	0.41
59:DZ:164:MET:HG3	59:DZ:257:PRO:HB3	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:DZ:168:ILE:HG12	59:DZ:205:TYR:CD2	2.55	0.41
1:AA:438:G:OP2	1:AA:2418:U:O2'	2.36	0.41
1:AA:789:G:H4'	1:AA:1723:A:H5'	2.03	0.41
1:AA:1002:A:H5'	14:AQ:76:LYS:HG2	2.03	0.41
1:AA:1712:A:H2'	1:AA:1713:G:O4'	2.20	0.41
1:AA:1772:C:H6	1:AA:1772:C:O5'	2.04	0.41
1:AA:2555:G:H2'	1:AA:2556:G:C8	2.56	0.41
3:AC:224:ARG:HE	3:AC:224:ARG:HB3	1.73	0.41
6:AF:62:ARG:HB3	6:AF:62:ARG:NH1	2.36	0.41
12:AO:66:LYS:HA	12:AO:79:PHE:O	2.21	0.41
13:AP:85:LEU:HD12	13:AP:116:GLY:O	2.20	0.41
23:AZ:138:GLU:H	23:AZ:156:LYS:HD3	1.86	0.41
34:BA:1118:C:OP1	42:BI:9:ARG:NH1	2.54	0.41
34:BA:1254:C:H2'	34:BA:1255:G:O4'	2.21	0.41
35:BB:215:LEU:O	35:BB:219:VAL:HG23	2.21	0.41
37:BD:188:LEU:HD23	37:BD:188:LEU:H	1.86	0.41
59:BZ:-27:THR:O	59:BZ:-23:LEU:HB2	2.21	0.41
59:BZ:350:GLU:OE1	59:BZ:382:GLU:N	2.53	0.41
59:BZ:499:ARG:HB2	59:BZ:506:GLN:HB2	2.04	0.41
1:CA:224:G:N7	1:CA:420:C:H4'	2.36	0.41
1:CA:1405:U:H2'	1:CA:1406:U:C6	2.55	0.41
1:CA:2330:G:H2'	1:CA:2331:G:O4'	2.20	0.41
1:CA:2733:A:H2	5:CE:204:ALA:H	1.68	0.41
1:CA:2745:C:H4'	8:CH:142:GLY:O	2.20	0.41
3:CC:54:ARG:CZ	3:CC:55:SER:O	2.69	0.41
7:CG:53:LEU:HD23	7:CG:53:LEU:HA	1.83	0.41
12:CO:113:LYS:O	12:CO:117:LEU:HD12	2.21	0.41
14:CQ:85:LYS:HD3	24:C0:7:LEU:HG	2.02	0.41
20:CW:70:TYR:O	20:CW:107:LEU:HD12	2.21	0.41
22:CY:5:MET:HG2	22:CY:30:VAL:HG11	2.03	0.41
22:CY:99:CYS:SG	22:CY:102:CYS:N	2.93	0.41
34:DA:253:U:H2'	34:DA:254:G:H8	1.85	0.41
34:DA:1030(A):G:N2	34:DA:1030(C):G:H3'	2.36	0.41
34:DA:1310:G:H5'	46:DM:77:ASN:OD1	2.21	0.41
39:DF:6:VAL:C	39:DF:7:ASN:HD22	2.28	0.41
59:DZ:327:PHE:CE1	59:DZ:376:ALA:HB2	2.56	0.41
59:DZ:382:GLU:H	59:DZ:382:GLU:HG2	1.76	0.41
59:DZ:628:ARG:HD2	59:DZ:680:PRO:HG2	2.03	0.41
1:AA:100:G:H5"	26:A2:3:LEU:CD1	2.51	0.40
1:AA:253:C:O2'	1:AA:254:A:H2'	2.22	0.40
1:AA:254:A:N6	1:AA:454:U:O2'	2.46	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:325:G:C4	1:AA:326:C:C5	3.09	0.40
1:AA:347:G:C8	6:AF:171:PRO:HG3	2.56	0.40
1:AA:895:G:H2'	1:AA:896:A:C8	2.56	0.40
1:AA:1855:G:OP1	4:AD:52:ARG:NH1	2.46	0.40
1:AA:1985:U:H4'	1:AA:1986:G:OP1	2.20	0.40
1:AA:2146:G:H5"	3:AC:175:PRO:HG3	2.03	0.40
1:AA:2819:A:C6	1:AA:2901:A:C8	3.09	0.40
3:AC:194:ILE:CD1	3:AC:227:PRO:CB	2.99	0.40
7:AG:132:ASN:HA	7:AG:157:ILE:O	2.22	0.40
8:AH:98:LEU:HD13	8:AH:125:VAL:CG2	2.51	0.40
11:AN:10:GLU:OE1	11:AN:11:PRO:HD2	2.21	0.40
12:AO:47:ILE:HB	12:AO:48:PRO:HD2	2.03	0.40
14:AQ:81:VAL:HB	24:A0:7:LEU:HD11	2.01	0.40
17:AT:118:ARG:HH11	17:AT:118:ARG:HG3	1.86	0.40
28:A4:44:THR:O	28:A4:44:THR:OG1	2.33	0.40
34:BA:435:C:H2'	34:BA:436:C:H6	1.85	0.40
34:BA:622:A:C8	34:BA:623:C:C5	3.09	0.40
34:BA:1015:A:N3	34:BA:1218:C:O2'	2.45	0.40
35:BB:84:GLU:O	35:BB:219:VAL:HG21	2.20	0.40
35:BB:87:ARG:NH2	35:BB:220:ASP:OD1	2.42	0.40
38:BE:100:VAL:O	38:BE:101:ILE:HD13	2.21	0.40
42:BI:26:VAL:HG13	42:BI:61:ALA:HB3	2.03	0.40
47:BN:13:THR:HA	47:BN:14:PRO:HD3	1.78	0.40
48:BO:27:VAL:O	48:BO:31:LEU:HG	2.21	0.40
49:BP:48:TRP:CD1	49:BP:48:TRP:H	2.39	0.40
50:BQ:27:PHE:CE2	50:BQ:36:ILE:HD11	2.55	0.40
50:BQ:29:HIS:HA	50:BQ:30:PRO:HD2	1.79	0.40
1:CA:190:A:OP2	25:C1:39:LYS:HE3	2.22	0.40
1:CA:811:U:P	13:CP:29:LYS:H	2.45	0.40
1:CA:856:C:H3'	1:CA:856:C:C6	2.56	0.40
1:CA:1283:G:N2	1:CA:1285:G:H3'	2.36	0.40
1:CA:1297:C:H2'	1:CA:1298:C:H6	1.86	0.40
1:CA:1652:A:OP1	15:CR:8:ARG:HD3	2.21	0.40
1:CA:1654:A:OP1	15:CR:1:MET:HA	2.20	0.40
1:CA:2164:C:H3'	1:CA:2165:G:O4'	2.21	0.40
1:CA:2309:A:C6	1:CA:2310:A:C6	3.09	0.40
1:CA:2494:G:O2'	14:CQ:80:GLU:HA	2.22	0.40
1:CA:2683:C:O2	12:CO:70:LYS:NZ	2.42	0.40
1:CA:2689:U:O2	1:CA:2689:U:H2'	2.21	0.40
3:CC:165:ARG:C	3:CC:172:ILE:HD12	2.47	0.40
5:CE:67:PHE:CE2	5:CE:74:PRO:HA	2.56	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:CE:179:GLU:O	5:CE:180:ASN:HB2	2.22	0.40
11:CN:128:HIS:HA	11:CN:129:PRO:HD3	1.75	0.40
22:CY:5:MET:HE3	22:CY:32:PRO:HA	2.03	0.40
32:C8:26:LYS:HG2	32:C8:48:PHE:HD1	1.86	0.40
33:C9:9:ARG:HG2	33:C9:14:CYS:HB2	2.03	0.40
34:DA:939:G:C6	34:DA:940:C:N4	2.90	0.40
34:DA:1207:G:H2'	34:DA:1208:C:C6	2.55	0.40
37:DD:173:TRP:CD1	37:DD:174:LEU:HG	2.56	0.40
43:DJ:47:PHE:CZ	47:DN:37:PHE:HE1	2.40	0.40
46:DM:20:THR:HG22	46:DM:26:GLY:O	2.21	0.40
49:DP:21:VAL:CG1	49:DP:34:GLU:HB3	2.51	0.40
51:DR:76:LEU:HA	51:DR:76:LEU:HD12	1.56	0.40
59:DZ:221:ALA:HB1	59:DZ:228:MET:HB2	2.02	0.40
1:AA:1445:C:N4	65:AA:4104:HOH:O	2.53	0.40
1:AA:1686:U:H4'	1:AA:2711:C:H4'	2.03	0.40
1:AA:2108:U:H2'	1:AA:2109:G:C8	2.56	0.40
1:AA:2650:G:P	5:AE:82:ARG:HH22	2.44	0.40
5:AE:120:TRP:CE3	5:AE:155:LYS:HE2	2.56	0.40
6:AF:200:GLU:O	6:AF:203:GLN:HB2	2.22	0.40
12:AO:98:VAL:HG22	12:AO:118:ALA:HA	2.04	0.40
13:AP:106:LEU:HA	13:AP:106:LEU:HD23	1.80	0.40
13:AP:144:GLU:HA	13:AP:145:PRO:HD3	1.84	0.40
16:AS:74:ALA:HB2	16:AS:105:ALA:HA	2.03	0.40
17:AT:23:ARG:HG3	17:AT:120:ARG:NH1	2.35	0.40
23:AZ:102:LEU:HD12	23:AZ:102:LEU:HA	1.79	0.40
34:BA:375:U:C2	34:BA:376:G:C8	3.10	0.40
38:BE:143:ARG:NH1	41:BH:77:GLU:OE1	2.54	0.40
46:BM:60:VAL:HG13	46:BM:64:TRP:CZ3	2.55	0.40
47:BN:27:CYS:SG	47:BN:29:ARG:HB2	2.61	0.40
50:BQ:48:GLU:O	50:BQ:49:GLU:C	2.64	0.40
56:BW:52:G:H2'	56:BW:53:G:O4'	2.21	0.40
59:BZ:188:TYR:CE1	59:BZ:196:ILE:HD12	2.56	0.40
1:CA:248:G:H2'	65:CA:3872:HOH:O	2.20	0.40
1:CA:947:G:H2'	1:CA:948:G:C8	2.57	0.40
1:CA:1627:G:OP2	65:CA:3735:HOH:O	2.22	0.40
1:CA:1721:G:H5'	1:CA:1722:A:OP2	2.22	0.40
1:CA:2203:U:H2'	1:CA:2205:C:C6	2.56	0.40
1:CA:2626:C:H2'	1:CA:2627:G:O4'	2.21	0.40
4:CD:218:ARG:HB3	4:CD:219:PRO:HD2	2.03	0.40
5:CE:75:VAL:HG13	5:CE:77:ILE:H	1.86	0.40
14:CQ:65:PHE:HB2	14:CQ:105:GLU:HB2	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:CY:30:VAL:O	22:CY:32:PRO:HD3	2.22	0.40
34:DA:338:A:H2'	34:DA:339:C:O4'	2.21	0.40
34:DA:555:C:H2'	34:DA:556:C:C6	2.56	0.40
34:DA:1014:A:H2'	34:DA:1015:A:N9	2.36	0.40
35:DB:149:LEU:O	35:DB:153:ARG:N	2.47	0.40
40:DG:139:GLU:O	40:DG:143:ARG:N	2.53	0.40
57:DX:8:4SU:O2	57:DX:21:A:H2	2.05	0.40
1:AA:96:C:OP1	26:A2:2:LYS:HE2	2.22	0.40
1:AA:174:U:H4'	1:AA:207:A:H4'	2.03	0.40
1:AA:1824:C:H2'	1:AA:1825:U:C6	2.57	0.40
1:AA:2221:A:H3'	1:AA:2222:C:H6	1.86	0.40
1:AA:2603:C:P	4:AD:239:ARG:HG3	2.62	0.40
3:AC:54:ARG:CZ	3:AC:55:SER:O	2.69	0.40
3:AC:165:ARG:C	3:AC:172:ILE:HD12	2.47	0.40
4:AD:223:GLY:HA3	4:AD:231:HIS:CE1	2.56	0.40
10:AL:84:LEU:HD21	10:AL:96:VAL:HB	2.03	0.40
14:AQ:37:LEU:HA	14:AQ:37:LEU:HD23	1.65	0.40
14:AQ:109:VAL:HG13	14:AQ:113:GLN:HB2	2.03	0.40
21:AX:65:ARG:HB2	21:AX:70:LEU:HD22	2.04	0.40
25:A1:20:ARG:HD3	25:A1:20:ARG:HH11	1.71	0.40
34:BA:708:C:H2'	34:BA:709:G:C8	2.56	0.40
34:BA:986:A:H2'	34:BA:987:G:O4'	2.21	0.40
34:BA:1316:G:O2'	47:BN:18:VAL:HG11	2.20	0.40
34:BA:1510:U:H2'	34:BA:1511:G:C8	2.57	0.40
36:BC:18:TRP:H	36:BC:18:TRP:HE3	1.68	0.40
38:BE:8:GLU:HG3	38:BE:34:VAL:HG23	2.03	0.40
41:BH:6:ILE:H	41:BH:6:ILE:HG12	1.53	0.40
46:BM:56:LEU:O	46:BM:60:VAL:HG23	2.22	0.40
56:BW:24:G:C5	56:BW:25:C:C4	3.10	0.40
58:BY:20:U:H4'	58:BY:21:A:OP1	2.20	0.40
1:CA:527:C:C5	1:CA:2779:U:H2'	2.57	0.40
1:CA:1093:G:H1'	1:CA:1099:G:N2	2.37	0.40
1:CA:1301:A:C8	1:CA:1303:G:C8	3.09	0.40
1:CA:1826:G:H4'	4:CD:242:ARG:CZ	2.51	0.40
1:CA:2178:C:HO2'	3:CC:169:THR:HB	1.80	0.40
1:CA:2306:C:C4	1:CA:2307:G:C6	3.10	0.40
1:CA:2667:C:N3	8:CH:110:SER:OG	2.54	0.40
1:CA:2787:C:O2'	1:CA:2810:A:O2'	2.29	0.40
2:CB:79:C:H2'	2:CB:80:U:O4'	2.21	0.40
4:CD:26:LYS:HE2	4:CD:28:GLU:O	2.21	0.40
6:CF:155:LEU:CD2	6:CF:186:ILE:HG13	2.50	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:CQ:18:LYS:HB2	14:CQ:18:LYS:HE3	1.75	0.40
15:CR:84:ALA:HB3	15:CR:85:PRO:HD3	2.03	0.40
22:CY:49:VAL:HG21	22:CY:61:ILE:HG23	2.03	0.40
25:C1:25:LYS:C	25:C1:27:GLU:N	2.80	0.40
26:C2:53:LEU:O	26:C2:57:ILE:HG13	2.21	0.40
33:C9:17:ILE:HD12	33:C9:18:ARG:H	1.86	0.40
34:DA:684:A:H1'	44:DK:38:ASN:HB3	2.04	0.40
34:DA:1073:U:O2'	35:DB:104:ASN:OD1	2.35	0.40
34:DA:1090:U:H2'	34:DA:1091:U:C6	2.56	0.40
34:DA:1104:G:O5'	35:DB:111:ARG:HD2	2.21	0.40
34:DA:1229:A:H2'	34:DA:1230:C:H6	1.85	0.40
34:DA:1237:C:OP1	34:DA:1238:A:H1'	2.21	0.40
35:DB:193:ASP:HA	35:DB:194:PRO:HD2	1.84	0.40
37:DD:196:LEU:O	37:DD:198:VAL:N	2.48	0.40
39:DF:100:ASN:HD21	51:DR:23:LYS:HG2	1.86	0.40
40:DG:36:LYS:O	40:DG:39:ALA:HB3	2.22	0.40
49:DP:68:ASP:C	49:DP:70:ALA:H	2.29	0.40
51:DR:21:LYS:HE2	51:DR:21:LYS:HB2	1.85	0.40
56:DW:32:PSU:C2	56:DW:33:U:C4	3.09	0.40
59:DZ:84:THR:O	59:DZ:84:THR:OG1	2.39	0.40
1:AA:461:U:H1'	1:AA:462:C:H5	1.86	0.40
1:AA:632:A:H2'	1:AA:633:G:O4'	2.22	0.40
1:AA:704:U:H2'	1:AA:705:C:H6	1.86	0.40
1:AA:1249:A:H61	1:AA:1286:U:H2'	1.86	0.40
1:AA:2203:G:HO2'	1:AA:2204:G:P	2.44	0.40
1:AA:2225:U:O4'	4:AD:151:LYS:HE2	2.21	0.40
1:AA:2247:G:H2'	1:AA:2248:C:C6	2.56	0.40
1:AA:2367:C:O3'	24:A0:24:LYS:HE3	2.21	0.40
2:AB:43:C:O2'	7:AG:95:ARG:HD2	2.22	0.40
5:AE:21:VAL:HG23	5:AE:185:LYS:HD2	2.04	0.40
5:AE:52:LEU:O	5:AE:76:ARG:N	2.54	0.40
6:AF:139:PHE:HB2	6:AF:166:ALA:HB1	2.03	0.40
6:AF:140:LEU:HD12	6:AF:140:LEU:HA	1.75	0.40
7:AG:161:THR:HG22	7:AG:163:ALA:N	2.33	0.40
9:AK:23:SER:HA	9:AK:117:LEU:O	2.21	0.40
11:AN:121:LYS:HG2	11:AN:130:HIS:CE1	2.57	0.40
34:BA:619:U:N3	37:BD:134:ASP:OD2	2.42	0.40
34:BA:954:G:H2'	34:BA:955:U:O4'	2.21	0.40
34:BA:1330:U:C2'	34:BA:1331:G:H5'	2.51	0.40
34:BA:1350:A:N7	42:BI:118:LYS:NZ	2.70	0.40
35:BB:71:VAL:HG22	35:BB:93:VAL:CG2	2.52	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:BC:56:ASP:HB2	36:BC:67:THR:HB	2.03	0.40
38:BE:48:ALA:HB3	38:BE:54:ALA:HB2	2.03	0.40
38:BE:51:VAL:HB	38:BE:52:PRO:HD3	2.04	0.40
41:BH:112:LEU:HB3	41:BH:133:LEU:HA	2.03	0.40
46:BM:80:ARG:NH2	52:BS:69:HIS:CE1	2.90	0.40
48:BO:43:LEU:HA	48:BO:43:LEU:HD23	1.78	0.40
50:BQ:9:VAL:H	50:BQ:9:VAL:HG23	1.57	0.40
50:BQ:81:ARG:HA	50:BQ:81:ARG:HD2	1.90	0.40
59:BZ:404:VAL:HA	59:BZ:405:PRO:HD3	1.80	0.40
59:BZ:462:ILE:O	59:BZ:466:LEU:HB2	2.21	0.40
1:CA:1913:A:H4'	1:CA:1914:C:O5'	2.20	0.40
1:CA:1913:A:C8	34:DA:1494:G:H4'	2.57	0.40
1:CA:2280:G:N3	1:CA:2388:A:H2	2.19	0.40
1:CA:2830:G:O2'	1:CA:2883:A:N1	2.47	0.40
2:CB:13:A:N1	2:CB:69:G:O2'	2.40	0.40
13:CP:39:LYS:CB	13:CP:45:LEU:HG	2.41	0.40
14:CQ:32:TYR:CZ	14:CQ:133:ARG:HD3	2.56	0.40
16:CS:110:LEU:HA	16:CS:110:LEU:HD12	1.74	0.40
19:CV:35:LEU:HA	19:CV:36:PRO:HD3	1.94	0.40
22:CY:79:CYS:O	22:CY:81:LYS:HG3	2.21	0.40
34:DA:186:C:H2'	34:DA:187:C:C6	2.56	0.40
34:DA:499:A:H4'	34:DA:500:G:OP1	2.20	0.40
35:DB:16:HIS:CD2	35:DB:17:PHE:N	2.90	0.40
35:DB:223:ILE:H	35:DB:223:ILE:HG13	1.74	0.40
36:DC:181:ASN:OD1	36:DC:204:LEU:HD12	2.21	0.40
37:DD:97:LEU:HD23	37:DD:97:LEU:HA	1.93	0.40
39:DF:100:ASN:ND2	51:DR:23:LYS:HE3	2.37	0.40
40:DG:59:LEU:O	40:DG:63:LYS:HE2	2.21	0.40
41:DH:51:VAL:HG12	41:DH:52:ASP:H	1.86	0.40
41:DH:84:ARG:HD2	41:DH:86:ILE:HD13	2.03	0.40
42:DI:4:TYR:CG	42:DI:88:TYR:HB2	2.57	0.40
43:DJ:29:ARG:HA	43:DJ:29:ARG:HD3	1.83	0.40
59:DZ:105:ILE:HG22	59:DZ:280:LEU:HD11	2.03	0.40
59:DZ:116:PRO:O	59:DZ:117:GLN:HG3	2.22	0.40
59:DZ:355:LEU:HD12	59:DZ:355:LEU:HA	1.93	0.40
1:AA:863:C:H2'	1:AA:864:C:H6	1.86	0.40
1:AA:955:A:H2'	1:AA:958:C:H5	1.86	0.40
1:AA:2371:C:H2'	1:AA:2372:A:O4'	2.22	0.40
3:AC:189:ASN:O	3:AC:190:ILE:C	2.64	0.40
5:AE:21:VAL:HA	5:AE:22:PRO:HD3	1.89	0.40
6:AF:129:PHE:HB3	6:AF:132:VAL:CG1	2.52	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AF:150:GLY:HA2	6:AF:172:TRP:CE3	2.56	0.40
22:AY:54:LYS:HA	22:AY:55:TYR:HA	1.95	0.40
34:BA:45:U:O5'	34:BA:45:U:H6	2.04	0.40
34:BA:456:C:H42	34:BA:475:G:H1	1.68	0.40
34:BA:1082:G:H2'	34:BA:1083:U:O4'	2.22	0.40
34:BA:1106:G:H5"	36:BC:172:ARG:HG2	2.04	0.40
34:BA:1250:A:C2	34:BA:1370:G:H1'	2.56	0.40
34:BA:1417:G:H22	34:BA:1482:G:H2'	1.86	0.40
36:BC:20:SER:HB3	36:BC:22:TRP:NE1	2.37	0.40
36:BC:33:LEU:HD11	47:BN:53:LEU:HD23	2.03	0.40
36:BC:113:ALA:HB3	36:BC:114:PRO:HD3	2.04	0.40
37:BD:61:LYS:HA	37:BD:203:VAL:HG22	2.03	0.40
37:BD:110:PHE:H	37:BD:110:PHE:HD1	1.70	0.40
1:CA:277:C:H1'	1:CA:278:A:P	2.62	0.40
1:CA:307:G:H2'	1:CA:309:G:OP2	2.21	0.40
1:CA:1171:G:N2	1:CA:1179:C:C2	2.89	0.40
1:CA:1341:U:O2	21:CX:80:ILE:HD12	2.22	0.40
1:CA:1740:G:H2'	1:CA:1741:A:C8	2.57	0.40
1:CA:2576:G:H1'	65:CA:3954:HOH:O	2.21	0.40
2:CB:101:G:H2'	2:CB:102:A:O4'	2.21	0.40
4:CD:242:ARG:N	4:CD:242:ARG:HD3	2.36	0.40
5:CE:51:PHE:C	5:CE:75:VAL:HG22	2.46	0.40
6:CF:36:VAL:HG12	6:CF:40:GLN:OE1	2.21	0.40
6:CF:148:LEU:HD11	6:CF:193:VAL:HG21	2.03	0.40
14:CQ:118:LEU:HD23	14:CQ:118:LEU:HA	1.93	0.40
18:CU:61:TRP:CD2	18:CU:93:LYS:HA	2.56	0.40
22:CY:13:VAL:O	22:CY:24:VAL:HA	2.21	0.40
34:DA:188:C:H2'	34:DA:189:G:C8	2.53	0.40
34:DA:643:C:H5'	41:DH:31:PHE:CD1	2.57	0.40
34:DA:719:C:N4	51:DR:71:LYS:HE2	2.37	0.40
34:DA:865:A:H5'	34:DA:1078:U:O4	2.21	0.40
34:DA:976:G:N2	34:DA:1362:C:H2'	2.37	0.40
34:DA:1125:U:O2'	34:DA:1126:U:H2'	2.21	0.40
34:DA:1132:C:H2'	34:DA:1133:G:H8	1.86	0.40
34:DA:1222:G:C2	34:DA:1223:C:C2	3.09	0.40
34:DA:1409:C:H2'	34:DA:1410:G:H8	1.86	0.40
35:DB:97:TRP:CH2	35:DB:102:LEU:HD13	2.57	0.40
36:DC:8:ILE:HG13	36:DC:16:ARG:HG2	2.02	0.40
36:DC:140:ARG:NH1	36:DC:141:VAL:HG23	2.36	0.40
37:DD:38:TYR:CE1	37:DD:45:GLN:HG3	2.57	0.40
37:DD:203:VAL:O	37:DD:206:PHE:HB3	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:DF:50:TYR:CE2	51:DR:77:GLY:HA2	2.56	0.40
41:DH:40:ALA:O	41:DH:43:GLY:N	2.46	0.40
42:DI:111:ARG:O	42:DI:113:LYS:HD2	2.20	0.40
49:DP:55:ARG:O	49:DP:58:TYR:HB3	2.21	0.40
58:DY:8:4SU:H1'	58:DY:48:C:O2	2.21	0.40
59:DZ:71:THR:HG22	59:DZ:80:ASN:OD1	2.22	0.40
59:DZ:160:ARG:HB3	59:DZ:256:THR:H	1.87	0.40
59:DZ:659:LEU:HD23	59:DZ:659:LEU:HA	1.87	0.40
59:DZ:682:GLN:O	59:DZ:686:LYS:HB3	2.21	0.40

All (19) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:9:ARG:NH2	59:DZ:504:ARG:NH1[3_654]	0.73	1.47
59:BZ:504:ARG:NH2	3:CC:9:ARG:NE[2_655]	1.08	1.12
59:BZ:504:ARG:NH1	3:CC:9:ARG:NH1[2_655]	1.09	1.11
59:BZ:504:ARG:NH1	3:CC:9:ARG:CZ[2_655]	1.43	0.77
59:BZ:504:ARG:CZ	3:CC:9:ARG:NE[2_655]	1.49	0.71
3:AC:6:LYS:O	59:DZ:501:THR:O[3_654]	1.74	0.46
59:BZ:504:ARG:NH1	3:CC:9:ARG:NE[2_655]	1.80	0.40
59:BZ:504:ARG:CZ	3:CC:9:ARG:CZ[2_655]	1.83	0.37
3:AC:9:ARG:CZ	59:DZ:504:ARG:NH1[3_654]	1.85	0.35
59:BZ:502:GLY:CA	3:CC:9:ARG:CB[2_655]	1.85	0.35
59:BZ:504:ARG:CZ	3:CC:9:ARG:CD[2_655]	1.85	0.35
3:AC:9:ARG:NH2	59:DZ:504:ARG:CZ[3_654]	1.86	0.34
59:BZ:504:ARG:NH2	3:CC:9:ARG:CZ[2_655]	1.91	0.29
59:BZ:504:ARG:NH1	3:CC:9:ARG:CD[2_655]	2.04	0.16
59:BZ:504:ARG:NH2	3:CC:9:ARG:CD[2_655]	2.07	0.13
1:AA:2154:U:O4	59:DZ:501:THR:OG1[3_654]	2.08	0.12
1:AA:2158:C:O2'	34:DA:1000:U:O2'[3_654]	2.08	0.12
3:AC:9:ARG:CB	59:DZ:502:GLY:CA[3_654]	2.10	0.10
59:BZ:502:GLY:N	3:CC:9:ARG:CB[2_655]	2.17	0.03

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	AC	133/228 (58%)	90 (68%)	25 (19%)	18 (14%)	0	0
3	CC	133/228 (58%)	90 (68%)	25 (19%)	18 (14%)	0	0
4	AD	273/276 (99%)	248 (91%)	22 (8%)	3 (1%)	11	36
4	CD	273/276 (99%)	245 (90%)	25 (9%)	3 (1%)	11	36
5	AE	202/206 (98%)	189 (94%)	12 (6%)	1 (0%)	24	55
5	CE	202/206 (98%)	189 (94%)	10 (5%)	3 (2%)	8	28
6	AF	201/210 (96%)	185 (92%)	16 (8%)	0	100	100
6	CF	201/210 (96%)	189 (94%)	8 (4%)	4 (2%)	6	21
7	AG	179/182 (98%)	159 (89%)	14 (8%)	6 (3%)	3	11
7	CG	179/182 (98%)	154 (86%)	19 (11%)	6 (3%)	3	11
8	AH	172/180 (96%)	160 (93%)	11 (6%)	1 (1%)	21	51
8	CH	172/180 (96%)	153 (89%)	13 (8%)	6 (4%)	3	10
9	AK	128/173 (74%)	74 (58%)	26 (20%)	28 (22%)	0	0
9	CK	128/173 (74%)	80 (62%)	28 (22%)	20 (16%)	0	0
10	AL	64/147 (44%)	47 (73%)	13 (20%)	4 (6%)	1	3
10	CL	64/147 (44%)	44 (69%)	17 (27%)	3 (5%)	2	6
11	AN	138/140 (99%)	130 (94%)	8 (6%)	0	100	100
11	CN	138/140 (99%)	126 (91%)	10 (7%)	2 (1%)	9	30
12	AO	120/122 (98%)	110 (92%)	9 (8%)	1 (1%)	16	44
12	CO	120/122 (98%)	110 (92%)	9 (8%)	1 (1%)	16	44
13	AP	147/150 (98%)	133 (90%)	12 (8%)	2 (1%)	9	30
13	CP	147/150 (98%)	129 (88%)	15 (10%)	3 (2%)	6	21
14	AQ	139/141 (99%)	128 (92%)	11 (8%)	0	100	100
14	CQ	139/141 (99%)	123 (88%)	13 (9%)	3 (2%)	5	19
15	AR	116/118 (98%)	109 (94%)	6 (5%)	1 (1%)	14	41
15	CR	116/118 (98%)	104 (90%)	11 (10%)	1 (1%)	14	41
16	AS	108/112 (96%)	99 (92%)	8 (7%)	1 (1%)	14	41
16	CS	108/112 (96%)	89 (82%)	17 (16%)	2 (2%)	6	22
17	AT	129/146 (88%)	119 (92%)	10 (8%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
17	CT	129/146 (88%)	120 (93%)	9 (7%)	0	100 100
18	AU	114/118 (97%)	112 (98%)	2 (2%)	0	100 100
18	CU	114/118 (97%)	108 (95%)	6 (5%)	0	100 100
19	AV	99/101 (98%)	93 (94%)	5 (5%)	1 (1%)	12 38
19	CV	99/101 (98%)	90 (91%)	7 (7%)	2 (2%)	6 21
20	AW	110/113 (97%)	108 (98%)	2 (2%)	0	100 100
20	CW	110/113 (97%)	108 (98%)	2 (2%)	0	100 100
21	AX	93/96 (97%)	89 (96%)	3 (3%)	1 (1%)	11 36
21	CX	93/96 (97%)	88 (95%)	4 (4%)	1 (1%)	11 36
22	AY	105/110 (96%)	95 (90%)	9 (9%)	1 (1%)	12 38
22	CY	105/110 (96%)	90 (86%)	11 (10%)	4 (4%)	2 9
23	AZ	169/206 (82%)	136 (80%)	28 (17%)	5 (3%)	3 12
23	CZ	172/206 (84%)	144 (84%)	25 (14%)	3 (2%)	7 25
24	A0	81/85 (95%)	74 (91%)	6 (7%)	1 (1%)	10 34
24	C0	81/85 (95%)	76 (94%)	5 (6%)	0	100 100
25	A1	95/98 (97%)	86 (90%)	9 (10%)	0	100 100
25	C1	95/98 (97%)	91 (96%)	3 (3%)	1 (1%)	11 36
26	A2	68/72 (94%)	66 (97%)	2 (3%)	0	100 100
26	C2	68/72 (94%)	64 (94%)	4 (6%)	0	100 100
27	A3	57/60 (95%)	55 (96%)	2 (4%)	0	100 100
27	C3	57/60 (95%)	52 (91%)	4 (7%)	1 (2%)	6 23
28	A4	67/71 (94%)	44 (66%)	16 (24%)	7 (10%)	0 1
28	C4	67/71 (94%)	49 (73%)	13 (19%)	5 (8%)	1 2
29	A5	57/60 (95%)	55 (96%)	2 (4%)	0	100 100
29	C5	57/60 (95%)	57 (100%)	0	0	100 100
30	A6	51/54 (94%)	48 (94%)	3 (6%)	0	100 100
30	C6	51/54 (94%)	45 (88%)	6 (12%)	0	100 100
31	A7	46/49 (94%)	46 (100%)	0	0	100 100
31	C7	46/49 (94%)	44 (96%)	0	2 (4%)	2 7
32	A8	62/65 (95%)	59 (95%)	3 (5%)	0	100 100
32	C8	62/65 (95%)	58 (94%)	2 (3%)	2 (3%)	3 11

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
33	A9	35/37 (95%)	35 (100%)	0	0	100 100
33	C9	35/37 (95%)	35 (100%)	0	0	100 100
35	BB	229/256 (90%)	187 (82%)	29 (13%)	13 (6%)	1 4
35	DB	229/256 (90%)	177 (77%)	37 (16%)	15 (7%)	1 3
36	BC	204/239 (85%)	171 (84%)	25 (12%)	8 (4%)	2 8
36	DC	204/239 (85%)	171 (84%)	30 (15%)	3 (2%)	8 28
37	BD	206/209 (99%)	186 (90%)	16 (8%)	4 (2%)	6 22
37	DD	206/209 (99%)	180 (87%)	20 (10%)	6 (3%)	3 13
38	BE	146/162 (90%)	128 (88%)	13 (9%)	5 (3%)	3 11
38	DE	146/162 (90%)	128 (88%)	12 (8%)	6 (4%)	2 8
39	BF	98/101 (97%)	89 (91%)	7 (7%)	2 (2%)	6 21
39	DF	98/101 (97%)	91 (93%)	6 (6%)	1 (1%)	12 38
40	BG	153/156 (98%)	142 (93%)	9 (6%)	2 (1%)	9 31
40	DG	153/156 (98%)	132 (86%)	19 (12%)	2 (1%)	9 31
41	BH	135/138 (98%)	120 (89%)	12 (9%)	3 (2%)	5 19
41	DH	135/138 (98%)	121 (90%)	12 (9%)	2 (2%)	8 28
42	BI	125/128 (98%)	111 (89%)	10 (8%)	4 (3%)	3 11
42	DI	125/128 (98%)	111 (89%)	12 (10%)	2 (2%)	7 27
43	BJ	95/105 (90%)	81 (85%)	9 (10%)	5 (5%)	1 5
43	DJ	94/105 (90%)	77 (82%)	10 (11%)	7 (7%)	1 2
44	BK	112/129 (87%)	102 (91%)	8 (7%)	2 (2%)	6 23
44	DK	112/129 (87%)	98 (88%)	10 (9%)	4 (4%)	2 10
45	BL	120/132 (91%)	106 (88%)	13 (11%)	1 (1%)	16 44
45	DL	120/132 (91%)	109 (91%)	11 (9%)	0	100 100
46	BM	121/126 (96%)	101 (84%)	17 (14%)	3 (2%)	4 16
46	DM	120/126 (95%)	98 (82%)	13 (11%)	9 (8%)	1 2
47	BN	58/61 (95%)	49 (84%)	8 (14%)	1 (2%)	7 25
47	DN	58/61 (95%)	53 (91%)	4 (7%)	1 (2%)	7 25
48	BO	86/89 (97%)	77 (90%)	7 (8%)	2 (2%)	5 18
48	DO	86/89 (97%)	72 (84%)	12 (14%)	2 (2%)	5 18
49	BP	80/88 (91%)	66 (82%)	12 (15%)	2 (2%)	4 16

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
49	DP	80/88 (91%)	66 (82%)	13 (16%)	1 (1%)	9 31
50	BQ	97/105 (92%)	87 (90%)	9 (9%)	1 (1%)	12 38
50	DQ	97/105 (92%)	85 (88%)	12 (12%)	0	100 100
51	BR	66/88 (75%)	61 (92%)	4 (6%)	1 (2%)	8 28
51	DR	66/88 (75%)	61 (92%)	5 (8%)	0	100 100
52	BS	82/93 (88%)	73 (89%)	9 (11%)	0	100 100
52	DS	81/93 (87%)	67 (83%)	12 (15%)	2 (2%)	4 16
53	BT	94/106 (89%)	78 (83%)	10 (11%)	6 (6%)	1 3
53	DT	94/106 (89%)	78 (83%)	12 (13%)	4 (4%)	2 7
54	BU	21/27 (78%)	18 (86%)	3 (14%)	0	100 100
54	DU	21/27 (78%)	19 (90%)	1 (5%)	1 (5%)	2 6
59	BZ	722/758 (95%)	598 (83%)	92 (13%)	32 (4%)	2 7
59	DZ	726/758 (96%)	594 (82%)	97 (13%)	35 (5%)	2 6
All	All	13220/14444 (92%)	11544 (87%)	1298 (10%)	378 (3%)	3 13

All (378) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	AC	42	VAL
3	AC	47	LYS
3	AC	68	GLY
3	AC	180	SER
3	AC	181	PHE
4	AD	275	LYS
7	AG	43	LEU
7	AG	47	LYS
7	AG	50	ALA
7	AG	126	ASP
9	AK	56	ASN
9	AK	71	LEU
9	AK	74	LEU
9	AK	75	GLN
9	AK	77	PRO
9	AK	80	VAL
9	AK	85	ASP
9	AK	104	ILE
9	AK	105	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	AK	107	VAL
9	AK	128	LEU
10	AL	115	LEU
16	AS	59	LYS
28	A4	45	GLY
28	A4	49	PHE
28	A4	59	PHE
28	A4	62	ARG
35	BB	17	PHE
35	BB	125	PRO
35	BB	231	GLU
36	BC	65	ALA
36	BC	66	VAL
37	BD	42	GLN
38	BE	98	THR
40	BG	79	ARG
40	BG	80	VAL
41	BH	133	LEU
42	BI	41	VAL
42	BI	44	VAL
42	BI	54	ASP
43	BJ	79	ARG
53	BT	10	LEU
53	BT	100	ILE
59	BZ	-57	GLU
59	BZ	-33	GLY
59	BZ	88	VAL
59	BZ	97	SER
59	BZ	98	MET
59	BZ	171	GLU
59	BZ	183	MET
59	BZ	404	VAL
59	BZ	405	PRO
59	BZ	472	VAL
59	BZ	481	VAL
3	CC	42	VAL
3	CC	47	LYS
3	CC	68	GLY
3	CC	180	SER
3	CC	181	PHE
6	CF	130	ALA
7	CG	14	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	CG	51	ARG
7	CG	81	LYS
8	CH	92	ILE
8	CH	126	PRO
8	CH	143	GLN
8	CH	144	VAL
9	CK	69	PRO
9	CK	70	GLU
9	CK	71	LEU
9	CK	74	LEU
9	CK	75	GLN
9	CK	77	PRO
9	CK	80	VAL
9	CK	85	ASP
9	CK	105	PRO
9	CK	107	VAL
10	CL	87	GLY
13	CP	38	GLN
21	CX	94	GLY
28	C4	62	ARG
28	C4	63	TYR
31	C7	46	VAL
35	DB	10	LEU
35	DB	17	PHE
36	DC	98	ASN
40	DG	55	GLY
42	DI	54	ASP
43	DJ	56	HIS
43	DJ	79	ARG
46	DM	4	ILE
48	DO	19	PRO
53	DT	10	LEU
53	DT	100	ILE
59	DZ	-65	LYS
59	DZ	-57	GLU
59	DZ	85	PRO
59	DZ	117	GLN
59	DZ	160	ARG
59	DZ	183	MET
59	DZ	290	LYS
59	DZ	472	VAL
3	AC	53	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	AC	161	ARG
3	AC	179	ALA
4	AD	3	VAL
9	AK	91	LYS
9	AK	93	LEU
9	AK	125	LEU
9	AK	132	ASP
10	AL	82	ALA
15	AR	2	ARG
19	AV	79	VAL
21	AX	94	GLY
23	AZ	105	VAL
28	A4	63	TYR
35	BB	10	LEU
35	BB	19	HIS
36	BC	101	LEU
37	BD	179	GLU
39	BF	70	ASP
43	BJ	31	GLY
43	BJ	56	HIS
50	BQ	49	GLU
53	BT	47	GLY
59	BZ	85	PRO
59	BZ	92	ILE
59	BZ	114	VAL
59	BZ	400	GLU
59	BZ	402	ILE
59	BZ	418	LYS
59	BZ	688	ILE
3	CC	53	ARG
3	CC	161	ARG
3	CC	179	ALA
4	CD	3	VAL
6	CF	195	ASP
7	CG	96	ARG
9	CK	84	GLU
9	CK	93	LEU
23	CZ	105	VAL
28	C4	11	PRO
28	C4	45	GLY
35	DB	106	LYS
35	DB	123	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	DC	95	THR
37	DD	10	ARG
38	DE	140	ARG
40	DG	80	VAL
41	DH	133	LEU
43	DJ	75	ILE
44	DK	49	GLY
44	DK	117	ASN
46	DM	67	GLU
46	DM	106	ASN
52	DS	12	ASP
53	DT	46	GLU
54	DU	3	LYS
59	DZ	39	ILE
59	DZ	92	ILE
59	DZ	402	ILE
59	DZ	403	GLU
59	DZ	404	VAL
59	DZ	479	PRO
59	DZ	481	VAL
59	DZ	600	VAL
3	AC	30	VAL
3	AC	43	GLU
3	AC	52	PRO
3	AC	69	LEU
3	AC	184	GLU
3	AC	202	PRO
3	AC	209	PHE
4	AD	125	ILE
7	AG	51	ARG
9	AK	20	ALA
9	AK	22	GLY
9	AK	39	ALA
9	AK	69	PRO
9	AK	101	PRO
10	AL	89	HIS
12	AO	5	GLN
13	AP	36	LYS
22	AY	54	LYS
23	AZ	65	GLN
36	BC	51	GLY
43	BJ	77	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
44	BK	105	VAL
46	BM	67	GLU
46	BM	113	PRO
48	BO	19	PRO
48	BO	86	GLY
51	BR	41	LYS
53	BT	71	THR
53	BT	102	GLY
59	BZ	115	GLU
59	BZ	170	ARG
59	BZ	315	LYS
59	BZ	320	PRO
3	CC	30	VAL
3	CC	43	GLU
3	CC	52	PRO
3	CC	69	LEU
3	CC	184	GLU
3	CC	202	PRO
3	CC	209	PHE
4	CD	239	ARG
5	CE	52	LEU
6	CF	21	ALA
7	CG	52	ILE
9	CK	86	PRO
9	CK	128	LEU
9	CK	132	ASP
10	CL	89	HIS
11	CN	23	LEU
13	CP	122	PRO
16	CS	89	ARG
19	CV	24	LYS
23	CZ	31	ARG
23	CZ	114	GLY
25	C1	3	LYS
28	C4	46	GLN
31	C7	45	ALA
35	DB	8	LYS
35	DB	16	HIS
35	DB	121	LEU
35	DB	125	PRO
35	DB	213	LEU
37	DD	47	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
43	DJ	36	GLY
43	DJ	55	LYS
43	DJ	77	PRO
44	DK	105	VAL
46	DM	5	ALA
46	DM	6	GLY
46	DM	101	GLN
46	DM	108	ARG
48	DO	88	ARG
52	DS	24	ALA
53	DT	102	GLY
59	DZ	-25	SER
59	DZ	20	HIS
59	DZ	170	ARG
59	DZ	400	GLU
59	DZ	418	LYS
59	DZ	598	ASP
59	DZ	599	PRO
59	DZ	651	GLU
3	AC	16	ASP
5	AE	52	LEU
9	AK	33	PRO
9	AK	86	PRO
9	AK	114	GLY
10	AL	81	ALA
24	A0	57	PHE
35	BB	9	GLU
35	BB	16	HIS
35	BB	131	PRO
36	BC	50	ALA
38	BE	86	ALA
41	BH	51	VAL
42	BI	96	LEU
44	BK	49	GLY
59	BZ	172	ASP
59	BZ	469	GLU
59	BZ	596	LYS
59	BZ	641	GLN
59	BZ	671	MET
3	CC	16	ASP
4	CD	125	ILE
5	CE	74	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	CH	119	GLU
9	CK	91	LYS
9	CK	104	ILE
11	CN	2	LYS
15	CR	45	ARG
16	CS	84	GLN
19	CV	79	VAL
22	CY	78	ALA
27	C3	59	VAL
32	C8	57	ARG
35	DB	20	GLU
35	DB	131	PRO
37	DD	22	LYS
37	DD	171	GLY
38	DE	96	PRO
38	DE	104	ALA
38	DE	107	ARG
42	DI	34	ASN
43	DJ	78	ASN
46	DM	35	GLU
47	DN	27	CYS
49	DP	53	VAL
59	DZ	-33	GLY
59	DZ	416	LYS
59	DZ	471	LYS
59	DZ	559	PRO
3	AC	21	TYR
9	AK	120	LYS
9	AK	123	GLU
23	AZ	152	ALA
35	BB	56	ARG
35	BB	195	ASP
36	BC	129	ALA
36	BC	156	ARG
37	BD	178	VAL
46	BM	19	LEU
47	BN	58	LYS
49	BP	49	LEU
59	BZ	322	VAL
59	BZ	324	ARG
59	BZ	416	LYS
59	BZ	479	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	CC	21	TYR
6	CF	60	SER
7	CG	47	LYS
9	CK	119	ALA
10	CL	112	MET
22	CY	43	ASN
22	CY	102	CYS
35	DB	83	MET
37	DD	136	PRO
44	DK	106	LYS
59	DZ	180	VAL
59	DZ	473	ASP
59	DZ	477	GLY
3	AC	221	PRO
8	AH	148	ILE
9	AK	31	GLY
9	AK	119	ALA
28	A4	47	GLN
37	BD	109	GLY
38	BE	68	GLU
39	BF	39	LYS
49	BP	41	PRO
59	BZ	415	PRO
3	CC	221	PRO
8	CH	80	SER
9	CK	101	PRO
13	CP	29	LYS
14	CQ	115	MET
22	CY	51	VAL
35	DB	21	ARG
35	DB	202	PRO
36	DC	108	ASN
37	DD	5	ILE
59	DZ	199	ILE
7	AG	32	PRO
13	AP	122	PRO
23	AZ	158	PRO
35	BB	183	PRO
35	BB	234	PRO
38	BE	69	VAL
43	BJ	75	ILE
53	BT	96	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
59	DZ	116	PRO
35	BB	202	PRO
32	C8	58	ILE
46	DM	85	GLY
9	AK	68	LEU
23	AZ	167	PRO
28	A4	41	PRO
45	BL	125	PRO
14	CQ	27	VAL
35	DB	232	PRO
59	DZ	88	VAL
59	DZ	688	ILE
9	CK	68	LEU
14	CQ	88	GLY
38	DE	69	VAL
41	DH	83	ILE
36	BC	81	GLY
38	BE	85	GLY
41	BH	90	GLY
12	CO	110	GLY
38	DE	105	VAL
39	DF	40	VAL
5	CE	30	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	AC	111/180 (62%)	100 (90%)	11 (10%)	7 24
3	CC	111/180 (62%)	100 (90%)	11 (10%)	7 24
4	AD	215/218 (99%)	180 (84%)	35 (16%)	2 8
4	CD	216/218 (99%)	177 (82%)	39 (18%)	2 6
5	AE	164/166 (99%)	134 (82%)	30 (18%)	2 6
5	CE	164/166 (99%)	135 (82%)	29 (18%)	2 6

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
6	AF	160/166 (96%)	132 (82%)	28 (18%)	2 7
6	CF	159/166 (96%)	130 (82%)	29 (18%)	2 6
7	AG	143/156 (92%)	115 (80%)	28 (20%)	1 5
7	CG	142/156 (91%)	112 (79%)	30 (21%)	1 4
8	AH	144/148 (97%)	124 (86%)	20 (14%)	3 12
8	CH	144/148 (97%)	116 (81%)	28 (19%)	1 5
10	AL	50/111 (45%)	44 (88%)	6 (12%)	5 17
10	CL	50/111 (45%)	43 (86%)	7 (14%)	3 12
11	AN	118/119 (99%)	94 (80%)	24 (20%)	1 4
11	CN	118/119 (99%)	91 (77%)	27 (23%)	1 3
12	AO	100/100 (100%)	83 (83%)	17 (17%)	2 7
12	CO	100/100 (100%)	79 (79%)	21 (21%)	1 4
13	AP	116/116 (100%)	96 (83%)	20 (17%)	2 7
13	CP	115/116 (99%)	93 (81%)	22 (19%)	1 5
14	AQ	111/111 (100%)	91 (82%)	20 (18%)	2 6
14	CQ	111/111 (100%)	93 (84%)	18 (16%)	2 8
15	AR	101/101 (100%)	80 (79%)	21 (21%)	1 4
15	CR	101/101 (100%)	82 (81%)	19 (19%)	1 5
16	AS	87/88 (99%)	69 (79%)	18 (21%)	1 4
16	CS	85/88 (97%)	66 (78%)	19 (22%)	1 3
17	AT	115/127 (91%)	92 (80%)	23 (20%)	1 4
17	CT	113/127 (89%)	91 (80%)	22 (20%)	1 5
18	AU	93/94 (99%)	76 (82%)	17 (18%)	2 6
18	CU	93/94 (99%)	80 (86%)	13 (14%)	3 12
19	AV	80/82 (98%)	63 (79%)	17 (21%)	1 4
19	CV	80/82 (98%)	65 (81%)	15 (19%)	1 5
20	AW	90/92 (98%)	78 (87%)	12 (13%)	4 14
20	CW	90/92 (98%)	78 (87%)	12 (13%)	4 14
21	AX	77/78 (99%)	69 (90%)	8 (10%)	7 22
21	CX	77/78 (99%)	70 (91%)	7 (9%)	9 28
22	AY	85/91 (93%)	73 (86%)	12 (14%)	3 12

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
22	CY	85/91 (93%)	74 (87%)	11 (13%)	4 14
23	AZ	145/179 (81%)	113 (78%)	32 (22%)	1 3
23	CZ	145/179 (81%)	120 (83%)	25 (17%)	2 7
24	A0	65/67 (97%)	62 (95%)	3 (5%)	24 58
24	C0	65/67 (97%)	59 (91%)	6 (9%)	8 27
25	A1	80/83 (96%)	70 (88%)	10 (12%)	4 15
25	C1	80/83 (96%)	66 (82%)	14 (18%)	2 7
26	A2	65/67 (97%)	50 (77%)	15 (23%)	1 3
26	C2	65/67 (97%)	53 (82%)	12 (18%)	1 6
27	A3	51/52 (98%)	43 (84%)	8 (16%)	2 9
27	C3	50/52 (96%)	40 (80%)	10 (20%)	1 4
28	A4	60/63 (95%)	47 (78%)	13 (22%)	1 3
28	C4	53/63 (84%)	42 (79%)	11 (21%)	1 4
29	A5	50/52 (96%)	43 (86%)	7 (14%)	3 12
29	C5	50/52 (96%)	44 (88%)	6 (12%)	5 17
30	A6	51/52 (98%)	37 (72%)	14 (28%)	0 1
30	C6	50/52 (96%)	44 (88%)	6 (12%)	5 17
31	A7	41/42 (98%)	35 (85%)	6 (15%)	3 11
31	C7	41/42 (98%)	37 (90%)	4 (10%)	7 25
32	A8	54/55 (98%)	43 (80%)	11 (20%)	1 4
32	C8	54/55 (98%)	47 (87%)	7 (13%)	4 14
33	A9	34/34 (100%)	30 (88%)	4 (12%)	5 17
33	C9	34/34 (100%)	30 (88%)	4 (12%)	5 17
35	BB	192/220 (87%)	144 (75%)	48 (25%)	0 2
35	DB	187/220 (85%)	154 (82%)	33 (18%)	2 7
36	BC	143/188 (76%)	121 (85%)	22 (15%)	2 10
36	DC	141/188 (75%)	114 (81%)	27 (19%)	1 5
37	BD	170/181 (94%)	145 (85%)	25 (15%)	3 10
37	DD	174/181 (96%)	151 (87%)	23 (13%)	4 14
38	BE	113/123 (92%)	103 (91%)	10 (9%)	9 29
38	DE	114/123 (93%)	92 (81%)	22 (19%)	1 5

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
39	BF	84/90 (93%)	72 (86%)	12 (14%)	3 11
39	DF	86/90 (96%)	73 (85%)	13 (15%)	3 10
40	BG	119/127 (94%)	97 (82%)	22 (18%)	1 6
40	DG	120/127 (94%)	112 (93%)	8 (7%)	15 42
41	BH	114/119 (96%)	95 (83%)	19 (17%)	2 8
41	DH	114/119 (96%)	90 (79%)	24 (21%)	1 4
42	BI	91/99 (92%)	73 (80%)	18 (20%)	1 5
42	DI	89/99 (90%)	72 (81%)	17 (19%)	1 5
43	BJ	66/92 (72%)	57 (86%)	9 (14%)	3 13
43	DJ	69/92 (75%)	57 (83%)	12 (17%)	2 7
44	BK	83/99 (84%)	70 (84%)	13 (16%)	2 9
44	DK	83/99 (84%)	74 (89%)	9 (11%)	6 21
45	BL	97/109 (89%)	87 (90%)	10 (10%)	7 23
45	DL	97/109 (89%)	86 (89%)	11 (11%)	5 19
46	BM	95/101 (94%)	80 (84%)	15 (16%)	2 9
46	DM	92/101 (91%)	75 (82%)	17 (18%)	1 6
47	BN	49/50 (98%)	39 (80%)	10 (20%)	1 4
47	DN	49/50 (98%)	40 (82%)	9 (18%)	1 6
48	BO	78/80 (98%)	63 (81%)	15 (19%)	1 5
48	DO	78/80 (98%)	65 (83%)	13 (17%)	2 8
49	BP	69/74 (93%)	57 (83%)	12 (17%)	2 7
49	DP	68/74 (92%)	56 (82%)	12 (18%)	2 7
50	BQ	94/97 (97%)	78 (83%)	16 (17%)	2 7
50	DQ	94/97 (97%)	81 (86%)	13 (14%)	3 12
51	BR	59/77 (77%)	45 (76%)	14 (24%)	1 3
51	DR	59/77 (77%)	51 (86%)	8 (14%)	3 13
52	BS	70/80 (88%)	61 (87%)	9 (13%)	4 14
52	DS	67/80 (84%)	59 (88%)	8 (12%)	5 17
53	BT	70/82 (85%)	58 (83%)	12 (17%)	2 7
53	DT	71/82 (87%)	58 (82%)	13 (18%)	2 6
54	BU	18/22 (82%)	16 (89%)	2 (11%)	6 20

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
54	DU	18/22 (82%)	16 (89%)	2 (11%)	6 20
59	BZ	604/636 (95%)	466 (77%)	138 (23%)	1 3
59	DZ	607/636 (95%)	480 (79%)	127 (21%)	1 4
All	All	10652/11672 (91%)	8806 (83%)	1846 (17%)	2 7

All (1846) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	AC	28	ARG
3	AC	29	LEU
3	AC	32	GLU
3	AC	48	LEU
3	AC	50	ILE
3	AC	54	ARG
3	AC	63	VAL
3	AC	184	GLU
3	AC	203	GLU
3	AC	206	LYS
3	AC	208	THR
4	AD	3	VAL
4	AD	12	SER
4	AD	13	ARG
4	AD	18	VAL
4	AD	38	LYS
4	AD	39	LYS
4	AD	54	ARG
4	AD	61	LEU
4	AD	88	ARG
4	AD	94	LEU
4	AD	99	ASP
4	AD	103	ARG
4	AD	106	ILE
4	AD	113	VAL
4	AD	117	VAL
4	AD	122	ASP
4	AD	126	GLN
4	AD	138	VAL
4	AD	141	VAL
4	AD	142	VAL
4	AD	155	LEU
4	AD	165	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	AD	169	GLU
4	AD	173	VAL
4	AD	175	LEU
4	AD	183	ARG
4	AD	193	VAL
4	AD	211	ARG
4	AD	221	VAL
4	AD	229	VAL
4	AD	242	ARG
4	AD	253	GLN
4	AD	257	LEU
4	AD	259	THR
4	AD	260	ARG
5	AE	7	VAL
5	AE	9	VAL
5	AE	21	VAL
5	AE	33	VAL
5	AE	34	VAL
5	AE	39	PRO
5	AE	40	GLU
5	AE	47	VAL
5	AE	48	GLN
5	AE	49	LEU
5	AE	75	VAL
5	AE	78	LEU
5	AE	81	ILE
5	AE	82	ARG
5	AE	93	VAL
5	AE	97	LYS
5	AE	111	ARG
5	AE	116	VAL
5	AE	119	ARG
5	AE	136	ARG
5	AE	144	ARG
5	AE	154	LYS
5	AE	163	GLU
5	AE	167	VAL
5	AE	170	LEU
5	AE	175	VAL
5	AE	178	GLU
5	AE	179	GLU
5	AE	181	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	AE	183	LEU
6	AF	12	LEU
6	AF	19	GLU
6	AF	24	LEU
6	AF	33	LEU
6	AF	53	THR
6	AF	57	VAL
6	AF	64	ILE
6	AF	74	ARG
6	AF	82	ILE
6	AF	88	VAL
6	AF	95	ARG
6	AF	106	ARG
6	AF	110	LEU
6	AF	119	ARG
6	AF	125	LEU
6	AF	127	GLU
6	AF	132	VAL
6	AF	137	LYS
6	AF	140	LEU
6	AF	158	THR
6	AF	161	GLU
6	AF	162	LEU
6	AF	169	ASN
6	AF	170	LEU
6	AF	183	VAL
6	AF	192	LEU
6	AF	195	ASP
6	AF	201	VAL
7	AG	5	VAL
7	AG	7	LEU
7	AG	21	ARG
7	AG	28	VAL
7	AG	31	VAL
7	AG	37	VAL
7	AG	41	GLN
7	AG	43	LEU
7	AG	45	GLU
7	AG	58	GLN
7	AG	60	LEU
7	AG	63	ILE
7	AG	79	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	AG	81	LYS
7	AG	82	LEU
7	AG	84	LYS
7	AG	86	MET
7	AG	91	ARG
7	AG	128	ARG
7	AG	135	LEU
7	AG	138	GLN
7	AG	140	ILE
7	AG	143	GLU
7	AG	159	VAL
7	AG	173	LEU
7	AG	174	GLU
7	AG	175	LEU
7	AG	181	ARG
8	AH	3	ARG
8	AH	4	ILE
8	AH	6	ARG
8	AH	13	LYS
8	AH	15	VAL
8	AH	24	VAL
8	AH	25	LYS
8	AH	49	VAL
8	AH	57	ASP
8	AH	62	LYS
8	AH	69	ARG
8	AH	71	LEU
8	AH	81	GLU
8	AH	97	ARG
8	AH	116	GLU
8	AH	122	THR
8	AH	125	VAL
8	AH	134	SER
8	AH	139	GLN
8	AH	162	ILE
10	AL	77	LEU
10	AL	86	LYS
10	AL	100	THR
10	AL	105	LEU
10	AL	116	ASN
10	AL	136	VAL
11	AN	5	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	AN	9	VAL
11	AN	14	VAL
11	AN	15	LEU
11	AN	21	LYS
11	AN	28	THR
11	AN	33	LEU
11	AN	34	LEU
11	AN	39	ARG
11	AN	48	MET
11	AN	61	ARG
11	AN	62	VAL
11	AN	65	LYS
11	AN	67	LEU
11	AN	73	THR
11	AN	84	LYS
11	AN	87	LEU
11	AN	97	ARG
11	AN	99	LEU
11	AN	120	LEU
11	AN	133	GLN
11	AN	137	LYS
11	AN	138	LEU
11	AN	140	VAL
12	AO	2	ILE
12	AO	8	LEU
12	AO	10	VAL
12	AO	20	MET
12	AO	23	ARG
12	AO	24	VAL
12	AO	28	SER
12	AO	35	VAL
12	AO	47	ILE
12	AO	52	VAL
12	AO	53	LYS
12	AO	80	ASP
12	AO	91	LEU
12	AO	92	GLU
12	AO	94	ARG
12	AO	98	VAL
12	AO	113	LYS
13	AP	21	ARG
13	AP	42	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	AP	55	ARG
13	AP	59	LEU
13	AP	68	GLN
13	AP	70	GLN
13	AP	71	VAL
13	AP	74	GLU
13	AP	83	VAL
13	AP	98	GLU
13	AP	99	LEU
13	AP	106	LEU
13	AP	112	LEU
13	AP	126	VAL
13	AP	135	LEU
13	AP	138	LEU
13	AP	139	LYS
13	AP	147	LEU
13	AP	148	LEU
13	AP	149	GLU
14	AQ	2	LEU
14	AQ	7	MET
14	AQ	8	LYS
14	AQ	16	ARG
14	AQ	21	THR
14	AQ	22	LYS
14	AQ	35	VAL
14	AQ	42	ILE
14	AQ	45	GLN
14	AQ	54	MET
14	AQ	55	VAL
14	AQ	75	THR
14	AQ	76	LYS
14	AQ	85	LYS
14	AQ	98	LYS
14	AQ	109	VAL
14	AQ	110	THR
14	AQ	115	MET
14	AQ	133	ARG
14	AQ	134	ARG
15	AR	6	SER
15	AR	9	LYS
15	AR	18	LEU
15	AR	27	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
15	AR	28	LEU
15	AR	29	LEU
15	AR	30	THR
15	AR	33	ARG
15	AR	36	THR
15	AR	44	LEU
15	AR	45	ARG
15	AR	54	LEU
15	AR	59	ASP
15	AR	60	LEU
15	AR	65	LEU
15	AR	67	LEU
15	AR	79	LEU
15	AR	91	GLN
15	AR	96	ARG
15	AR	102	GLU
15	AR	111	LEU
16	AS	3	ARG
16	AS	4	LEU
16	AS	14	VAL
16	AS	19	LYS
16	AS	20	ARG
16	AS	25	ARG
16	AS	36	TYR
16	AS	46	VAL
16	AS	48	LEU
16	AS	49	VAL
16	AS	50	SER
16	AS	57	LYS
16	AS	65	VAL
16	AS	69	VAL
16	AS	83	LYS
16	AS	85	VAL
16	AS	93	LYS
16	AS	110	LEU
17	AT	6	LEU
17	AT	13	ARG
17	AT	17	THR
17	AT	23	ARG
17	AT	28	VAL
17	AT	30	VAL
17	AT	34	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
17	AT	40	THR
17	AT	42	ILE
17	AT	49	VAL
17	AT	59	THR
17	AT	65	LYS
17	AT	67	SER
17	AT	74	ARG
17	AT	78	LEU
17	AT	85	LYS
17	AT	89	VAL
17	AT	96	ARG
17	AT	108	ARG
17	AT	112	ARG
17	AT	118	ARG
17	AT	125	ARG
17	AT	128	GLU
18	AU	5	LYS
18	AU	8	VAL
18	AU	13	LYS
18	AU	16	LYS
18	AU	19	LYS
18	AU	20	LEU
18	AU	36	ARG
18	AU	52	ARG
18	AU	60	LEU
18	AU	74	LEU
18	AU	77	SER
18	AU	83	LEU
18	AU	92	ARG
18	AU	95	LEU
18	AU	104	GLN
18	AU	108	GLU
18	AU	112	ARG
19	AV	18	LEU
19	AV	20	LEU
19	AV	21	ARG
19	AV	28	GLU
19	AV	35	LEU
19	AV	43	GLU
19	AV	46	VAL
19	AV	51	VAL
19	AV	52	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
19	AV	61	VAL
19	AV	62	LEU
19	AV	72	VAL
19	AV	79	VAL
19	AV	85	LYS
19	AV	92	THR
19	AV	95	LEU
19	AV	100	ARG
20	AW	4	LYS
20	AW	11	ARG
20	AW	12	ILE
20	AW	15	ARG
20	AW	17	VAL
20	AW	19	LEU
20	AW	24	ILE
20	AW	51	LEU
20	AW	63	ASP
20	AW	96	ILE
20	AW	98	LYS
20	AW	107	LEU
21	AX	45	THR
21	AX	52	VAL
21	AX	57	LEU
21	AX	65	ARG
21	AX	70	LEU
21	AX	76	ARG
21	AX	81	VAL
21	AX	92	LEU
22	AY	7	VAL
22	AY	23	ARG
22	AY	47	LYS
22	AY	55	TYR
22	AY	61	ILE
22	AY	72	VAL
22	AY	73	ARG
22	AY	85	VAL
22	AY	90	LEU
22	AY	91	GLU
22	AY	92	ASN
22	AY	106	LEU
23	AZ	5	LEU
23	AZ	6	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
23	AZ	18	LEU
23	AZ	19	ARG
23	AZ	31	ARG
23	AZ	33	LEU
23	AZ	41	LEU
23	AZ	42	VAL
23	AZ	50	GLN
23	AZ	58	VAL
23	AZ	61	LEU
23	AZ	71	VAL
23	AZ	72	ARG
23	AZ	76	LEU
23	AZ	84	GLU
23	AZ	86	VAL
23	AZ	91	LEU
23	AZ	98	MET
23	AZ	102	LEU
23	AZ	117	LEU
23	AZ	119	GLU
23	AZ	120	ILE
23	AZ	126	VAL
23	AZ	128	VAL
23	AZ	129	SER
23	AZ	141	VAL
23	AZ	146	ILE
23	AZ	149	SER
23	AZ	154	ASP
23	AZ	155	LEU
23	AZ	161	VAL
23	AZ	170	THR
24	A0	20	ARG
24	A0	55	ARG
24	A0	63	VAL
25	A1	21	ARG
25	A1	30	VAL
25	A1	40	ARG
25	A1	46	LEU
25	A1	51	VAL
25	A1	59	THR
25	A1	80	LEU
25	A1	83	GLU
25	A1	89	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
25	A1	95	LEU
26	A2	1	MET
26	A2	3	LEU
26	A2	19	VAL
26	A2	20	GLU
26	A2	28	LYS
26	A2	30	ARG
26	A2	32	LEU
26	A2	45	SER
26	A2	53	LEU
26	A2	59	ARG
26	A2	62	THR
26	A2	65	ASN
26	A2	67	LYS
26	A2	68	ARG
26	A2	70	GLN
27	A3	3	ARG
27	A3	6	VAL
27	A3	8	LEU
27	A3	23	LEU
27	A3	29	ARG
27	A3	54	VAL
27	A3	58	VAL
27	A3	60	GLU
28	A4	1	MET
28	A4	3	GLU
28	A4	5	ILE
28	A4	8	LYS
28	A4	34	GLU
28	A4	46	GLN
28	A4	49	PHE
28	A4	50	VAL
28	A4	56	VAL
28	A4	59	PHE
28	A4	60	GLN
28	A4	63	TYR
28	A4	68	ARG
29	A5	6	VAL
29	A5	16	ARG
29	A5	26	THR
29	A5	29	THR
29	A5	40	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
29	A5	55	ARG
29	A5	56	LYS
30	A6	3	SER
30	A6	4	GLU
30	A6	5	VAL
30	A6	6	ARG
30	A6	7	ILE
30	A6	9	LEU
30	A6	14	THR
30	A6	35	GLU
30	A6	38	LYS
30	A6	44	ARG
30	A6	47	THR
30	A6	48	VAL
30	A6	50	ARG
30	A6	52	VAL
31	A7	9	ARG
31	A7	24	THR
31	A7	32	LYS
31	A7	41	ARG
31	A7	43	THR
31	A7	46	VAL
32	A8	6	THR
32	A8	14	VAL
32	A8	15	LYS
32	A8	21	LYS
32	A8	23	VAL
32	A8	30	ARG
32	A8	32	LEU
32	A8	37	SER
32	A8	41	ILE
32	A8	46	ARG
32	A8	59	LYS
33	A9	4	ARG
33	A9	17	ILE
33	A9	19	ARG
33	A9	36	GLN
35	BB	8	LYS
35	BB	11	LEU
35	BB	15	VAL
35	BB	17	PHE
35	BB	20	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	BB	21	ARG
35	BB	23	ARG
35	BB	35	GLU
35	BB	37	ASN
35	BB	45	GLN
35	BB	48	MET
35	BB	58	ILE
35	BB	60	ASP
35	BB	67	THR
35	BB	75	LYS
35	BB	76	GLN
35	BB	80	ILE
35	BB	83	MET
35	BB	84	GLU
35	BB	87	ARG
35	BB	93	VAL
35	BB	96	ARG
35	BB	111	ARG
35	BB	112	VAL
35	BB	117	GLU
35	BB	126	GLU
35	BB	137	ARG
35	BB	145	LEU
35	BB	147	LYS
35	BB	150	SER
35	BB	153	ARG
35	BB	156	LYS
35	BB	158	LEU
35	BB	160	ASP
35	BB	168	THR
35	BB	169	LYS
35	BB	170	GLU
35	BB	178	ARG
35	BB	185	ILE
35	BB	187	LEU
35	BB	196	LEU
35	BB	197	VAL
35	BB	200	ILE
35	BB	208	ILE
35	BB	217	ARG
35	BB	221	LEU
35	BB	229	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	BB	230	VAL
36	BC	3	ASN
36	BC	27	LYS
36	BC	28	GLN
36	BC	37	GLN
36	BC	38	ARG
36	BC	44	GLU
36	BC	45	LYS
36	BC	49	SER
36	BC	52	LEU
36	BC	70	VAL
36	BC	77	ILE
36	BC	103	VAL
36	BC	115	LEU
36	BC	118	GLN
36	BC	131	ARG
36	BC	182	ILE
36	BC	188	LEU
36	BC	191	THR
36	BC	196	LEU
36	BC	202	ILE
36	BC	206	GLU
36	BC	207	VAL
37	BD	5	ILE
37	BD	11	LEU
37	BD	15	GLU
37	BD	19	LEU
37	BD	28	SER
37	BD	31	CYS
37	BD	49	ARG
37	BD	57	ARG
37	BD	58	LEU
37	BD	65	ARG
37	BD	86	LYS
37	BD	100	ARG
37	BD	108	LEU
37	BD	118	ARG
37	BD	127	THR
37	BD	134	ASP
37	BD	135	LEU
37	BD	141	ARG
37	BD	157	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
37	BD	158	ILE
37	BD	168	ARG
37	BD	178	VAL
37	BD	188	LEU
37	BD	190	ASP
37	BD	196	LEU
38	BE	10	MET
38	BE	12	LEU
38	BE	13	ILE
38	BE	41	VAL
38	BE	47	LYS
38	BE	67	VAL
38	BE	79	GLU
38	BE	87	SER
38	BE	91	LEU
38	BE	120	THR
39	BF	40	VAL
39	BF	45	LEU
39	BF	55	ASP
39	BF	61	LEU
39	BF	69	GLU
39	BF	71	ARG
39	BF	72	VAL
39	BF	73	ASN
39	BF	75	LEU
39	BF	82	ARG
39	BF	89	MET
39	BF	91	VAL
40	BG	8	GLU
40	BG	12	LEU
40	BG	16	LEU
40	BG	21	VAL
40	BG	27	ILE
40	BG	31	MET
40	BG	38	LEU
40	BG	50	ILE
40	BG	51	GLN
40	BG	56	GLN
40	BG	73	MET
40	BG	76	ARG
40	BG	78	ARG
40	BG	79	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
40	BG	91	VAL
40	BG	104	LEU
40	BG	113	GLU
40	BG	114	ARG
40	BG	131	LYS
40	BG	139	GLU
40	BG	140	ASP
40	BG	155	ARG
41	BH	2	LEU
41	BH	6	ILE
41	BH	21	LYS
41	BH	23	SER
41	BH	26	VAL
41	BH	37	ARG
41	BH	38	ILE
41	BH	50	ARG
41	BH	51	VAL
41	BH	60	ARG
41	BH	63	LEU
41	BH	68	ARG
41	BH	78	GLN
41	BH	83	ILE
41	BH	91	ARG
41	BH	99	GLU
41	BH	112	LEU
41	BH	115	SER
41	BH	121	ASP
42	BI	3	GLN
42	BI	7	THR
42	BI	17	VAL
42	BI	23	ASN
42	BI	27	THR
42	BI	56	LEU
42	BI	64	THR
42	BI	65	VAL
42	BI	81	ILE
42	BI	87	GLN
42	BI	97	LYS
42	BI	102	LEU
42	BI	104	ARG
42	BI	108	VAL
42	BI	109	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
42	BI	111	ARG
42	BI	121	ARG
42	BI	128	ARG
43	BJ	5	ARG
43	BJ	7	LYS
43	BJ	16	LEU
43	BJ	23	ILE
43	BJ	44	VAL
43	BJ	49	VAL
43	BJ	67	THR
43	BJ	92	THR
43	BJ	96	ILE
44	BK	41	THR
44	BK	48	ILE
44	BK	51	LYS
44	BK	63	LEU
44	BK	83	ILE
44	BK	84	VAL
44	BK	96	ARG
44	BK	98	LEU
44	BK	104	GLN
44	BK	105	VAL
44	BK	106	LYS
44	BK	109	VAL
44	BK	114	VAL
45	BL	23	LYS
45	BL	27	LEU
45	BL	33	ARG
45	BL	42	THR
45	BL	55	VAL
45	BL	60	LEU
45	BL	83	VAL
45	BL	84	LEU
45	BL	86	ARG
45	BL	97	ARG
46	BM	4	ILE
46	BM	15	VAL
46	BM	17	VAL
46	BM	19	LEU
46	BM	20	THR
46	BM	39	ILE
46	BM	43	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
46	BM	50	GLU
46	BM	56	LEU
46	BM	63	THR
46	BM	70	LEU
46	BM	102	ARG
46	BM	109	THR
46	BM	110	ARG
46	BM	121	LYS
47	BN	3	ARG
47	BN	6	LEU
47	BN	7	ILE
47	BN	9	LYS
47	BN	18	VAL
47	BN	32	SER
47	BN	33	VAL
47	BN	41	ARG
47	BN	44	LEU
47	BN	60	SER
48	BO	3	ILE
48	BO	5	LYS
48	BO	6	GLU
48	BO	7	GLU
48	BO	14	GLU
48	BO	22	THR
48	BO	26	GLU
48	BO	34	LEU
48	BO	35	ARG
48	BO	39	LEU
48	BO	41	GLU
48	BO	66	LEU
48	BO	83	GLU
48	BO	87	ILE
48	BO	88	ARG
49	BP	2	VAL
49	BP	6	LEU
49	BP	11	SER
49	BP	19	ILE
49	BP	20	VAL
49	BP	27	LYS
49	BP	36	ILE
49	BP	50	LYS
49	BP	60	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
49	BP	62	VAL
49	BP	67	THR
49	BP	69	THR
50	BQ	6	LEU
50	BQ	9	VAL
50	BQ	34	LYS
50	BQ	36	ILE
50	BQ	57	VAL
50	BQ	60	ILE
50	BQ	63	ARG
50	BQ	68	ARG
50	BQ	72	ARG
50	BQ	77	VAL
50	BQ	78	GLU
50	BQ	86	GLU
50	BQ	90	ILE
50	BQ	91	ARG
50	BQ	92	ARG
50	BQ	97	SER
51	BR	26	LEU
51	BR	31	LEU
51	BR	32	ARG
51	BR	35	ARG
51	BR	37	VAL
51	BR	38	GLU
51	BR	45	SER
51	BR	46	GLU
51	BR	47	THR
51	BR	55	ARG
51	BR	58	LEU
51	BR	65	ILE
51	BR	68	LYS
51	BR	76	LEU
52	BS	12	ASP
52	BS	28	LYS
52	BS	37	ARG
52	BS	38	SER
52	BS	62	ILE
52	BS	65	ASN
52	BS	78	ARG
52	BS	81	ARG
52	BS	85	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
53	BT	8	ARG
53	BT	10	LEU
53	BT	13	LEU
53	BT	24	LEU
53	BT	43	LEU
53	BT	45	GLN
53	BT	56	MET
53	BT	58	LYS
53	BT	60	GLU
53	BT	62	LEU
53	BT	84	LEU
53	BT	100	ILE
54	BU	9	ARG
54	BU	10	ARG
59	BZ	-64	VAL
59	BZ	-61	LEU
59	BZ	-58	LEU
59	BZ	-52	VAL
59	BZ	-30	VAL
59	BZ	-29	LEU
59	BZ	-23	LEU
59	BZ	-20	LEU
59	BZ	-19	GLU
59	BZ	-16	ILE
59	BZ	-10	ARG
59	BZ	-6	ARG
59	BZ	-1	GLU
59	BZ	4	ILE
59	BZ	7	ASN
59	BZ	12	LEU
59	BZ	13	ARG
59	BZ	15	ILE
59	BZ	21	ILE
59	BZ	25	LYS
59	BZ	30	GLU
59	BZ	33	LEU
59	BZ	69	VAL
59	BZ	71	THR
59	BZ	75	LYS
59	BZ	76	ASP
59	BZ	78	ARG
59	BZ	87	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
59	BZ	89	ASP
59	BZ	92	ILE
59	BZ	99	ARG
59	BZ	102	ASP
59	BZ	105	ILE
59	BZ	107	VAL
59	BZ	112	GLN
59	BZ	121	VAL
59	BZ	130	VAL
59	BZ	132	ARG
59	BZ	139	MET
59	BZ	146	LEU
59	BZ	148	LEU
59	BZ	152	THR
59	BZ	156	ARG
59	BZ	160	ARG
59	BZ	166	LEU
59	BZ	172	ASP
59	BZ	180	VAL
59	BZ	196	ILE
59	BZ	198	GLU
59	BZ	203	GLU
59	BZ	207	ASP
59	BZ	208	GLN
59	BZ	222	ASP
59	BZ	225	GLU
59	BZ	228	MET
59	BZ	238	THR
59	BZ	239	GLU
59	BZ	240	GLU
59	BZ	247	ARG
59	BZ	255	ILE
59	BZ	260	LEU
59	BZ	267	LYS
59	BZ	269	VAL
59	BZ	282	SER
59	BZ	284	LEU
59	BZ	286	ILE
59	BZ	289	ILE
59	BZ	290	LYS
59	BZ	295	GLU
59	BZ	298	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
59	BZ	312	LEU
59	BZ	315	LYS
59	BZ	328	ILE
59	BZ	329	ARG
59	BZ	331	TYR
59	BZ	336	THR
59	BZ	339	SER
59	BZ	349	LYS
59	BZ	350	GLU
59	BZ	352	VAL
59	BZ	354	ARG
59	BZ	355	LEU
59	BZ	356	LEU
59	BZ	362	HIS
59	BZ	363	ARG
59	BZ	368	GLU
59	BZ	369	LEU
59	BZ	374	LEU
59	BZ	377	VAL
59	BZ	381	LYS
59	BZ	382	GLU
59	BZ	389	LEU
59	BZ	396	ARG
59	BZ	397	VAL
59	BZ	399	LEU
59	BZ	402	ILE
59	BZ	406	GLU
59	BZ	409	ILE
59	BZ	418	LYS
59	BZ	421	GLN
59	BZ	422	GLU
59	BZ	431	LEU
59	BZ	433	GLU
59	BZ	437	THR
59	BZ	442	THR
59	BZ	446	THR
59	BZ	457	LEU
59	BZ	464	ASP
59	BZ	466	LEU
59	BZ	468	ARG
59	BZ	473	ASP
59	BZ	484	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
59	BZ	485	GLU
59	BZ	486	THR
59	BZ	504	ARG
59	BZ	510	VAL
59	BZ	512	ILE
59	BZ	515	GLU
59	BZ	530	VAL
59	BZ	533	VAL
59	BZ	572	TYR
59	BZ	600	VAL
59	BZ	607	ARG
59	BZ	614	GLU
59	BZ	617	MET
59	BZ	630	GLN
59	BZ	634	MET
59	BZ	644	ARG
59	BZ	647	VAL
59	BZ	651	GLU
59	BZ	659	LEU
59	BZ	670	VAL
59	BZ	679	VAL
59	BZ	681	LYS
59	BZ	683	VAL
59	BZ	684	GLN
59	BZ	686	LYS
59	BZ	689	LYS
3	CC	28	ARG
3	CC	29	LEU
3	CC	32	GLU
3	CC	48	LEU
3	CC	50	ILE
3	CC	54	ARG
3	CC	63	VAL
3	CC	184	GLU
3	CC	203	GLU
3	CC	206	LYS
3	CC	208	THR
4	CD	3	VAL
4	CD	5	LYS
4	CD	12	SER
4	CD	13	ARG
4	CD	14	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	CD	26	LYS
4	CD	54	ARG
4	CD	61	LEU
4	CD	71	ASP
4	CD	89	SER
4	CD	94	LEU
4	CD	99	ASP
4	CD	101	GLU
4	CD	103	ARG
4	CD	106	ILE
4	CD	111	LEU
4	CD	113	VAL
4	CD	134	ARG
4	CD	138	VAL
4	CD	141	VAL
4	CD	142	VAL
4	CD	165	ILE
4	CD	169	GLU
4	CD	173	VAL
4	CD	185	VAL
4	CD	193	VAL
4	CD	211	ARG
4	CD	212	SER
4	CD	217	ARG
4	CD	221	VAL
4	CD	229	VAL
4	CD	253	GLN
4	CD	257	LEU
4	CD	259	THR
4	CD	260	ARG
4	CD	262	ARG
4	CD	264	LYS
4	CD	270	ILE
4	CD	276	LYS
5	CE	9	VAL
5	CE	12	THR
5	CE	21	VAL
5	CE	33	VAL
5	CE	34	VAL
5	CE	40	GLU
5	CE	45	THR
5	CE	49	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	CE	58	ARG
5	CE	61	ARG
5	CE	75	VAL
5	CE	77	ILE
5	CE	78	LEU
5	CE	79	ARG
5	CE	82	ARG
5	CE	89	ASP
5	CE	91	VAL
5	CE	111	ARG
5	CE	116	VAL
5	CE	119	ARG
5	CE	134	ILE
5	CE	144	ARG
5	CE	154	LYS
5	CE	170	LEU
5	CE	175	VAL
5	CE	181	LEU
5	CE	184	VAL
5	CE	195	LEU
5	CE	202	LYS
6	CF	17	ARG
6	CF	19	GLU
6	CF	20	LEU
6	CF	24	LEU
6	CF	33	LEU
6	CF	40	GLN
6	CF	50	SER
6	CF	53	THR
6	CF	57	VAL
6	CF	70	THR
6	CF	74	ARG
6	CF	77	ASP
6	CF	88	VAL
6	CF	95	ARG
6	CF	106	ARG
6	CF	107	LYS
6	CF	110	LEU
6	CF	135	LYS
6	CF	140	LEU
6	CF	157	VAL
6	CF	158	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	CF	169	ASN
6	CF	170	LEU
6	CF	175	THR
6	CF	183	VAL
6	CF	186	ILE
6	CF	192	LEU
6	CF	196	LEU
6	CF	201	VAL
7	CG	3	LEU
7	CG	4	ASP
7	CG	5	VAL
7	CG	16	ARG
7	CG	18	GLU
7	CG	28	VAL
7	CG	31	VAL
7	CG	33	ARG
7	CG	35	GLU
7	CG	43	LEU
7	CG	49	ASP
7	CG	60	LEU
7	CG	70	VAL
7	CG	71	THR
7	CG	79	ASN
7	CG	80	PHE
7	CG	91	ARG
7	CG	111	LEU
7	CG	115	ARG
7	CG	130	ASN
7	CG	136	ARG
7	CG	140	ILE
7	CG	143	GLU
7	CG	145	THR
7	CG	148	MET
7	CG	152	LEU
7	CG	159	VAL
7	CG	162	THR
7	CG	165	THR
7	CG	170	ARG
8	CH	3	ARG
8	CH	7	LEU
8	CH	19	VAL
8	CH	27	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	CH	33	LEU
8	CH	37	VAL
8	CH	41	MET
8	CH	44	VAL
8	CH	45	VAL
8	CH	69	ARG
8	CH	81	GLU
8	CH	84	SER
8	CH	88	LEU
8	CH	89	ILE
8	CH	98	LEU
8	CH	104	GLU
8	CH	106	THR
8	CH	110	SER
8	CH	114	VAL
8	CH	122	THR
8	CH	124	GLU
8	CH	129	THR
8	CH	136	ILE
8	CH	139	GLN
8	CH	140	LYS
8	CH	147	ASN
8	CH	171	LEU
8	CH	172	LYS
10	CL	77	LEU
10	CL	78	ILE
10	CL	86	LYS
10	CL	96	VAL
10	CL	105	LEU
10	CL	112	MET
10	CL	117	THR
11	CN	2	LYS
11	CN	3	THR
11	CN	5	VAL
11	CN	15	LEU
11	CN	16	ILE
11	CN	28	THR
11	CN	33	LEU
11	CN	34	LEU
11	CN	43	THR
11	CN	46	VAL
11	CN	48	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	CN	60	ILE
11	CN	61	ARG
11	CN	62	VAL
11	CN	82	LEU
11	CN	87	LEU
11	CN	97	ARG
11	CN	99	LEU
11	CN	103	VAL
11	CN	104	LYS
11	CN	115	ARG
11	CN	120	LEU
11	CN	127	ASP
11	CN	133	GLN
11	CN	137	LYS
11	CN	138	LEU
11	CN	140	VAL
12	CO	1	MET
12	CO	5	GLN
12	CO	10	VAL
12	CO	14	THR
12	CO	23	ARG
12	CO	24	VAL
12	CO	28	SER
12	CO	35	VAL
12	CO	66	LYS
12	CO	69	ILE
12	CO	77	ILE
12	CO	78	ARG
12	CO	85	VAL
12	CO	86	ILE
12	CO	91	LEU
12	CO	92	GLU
12	CO	94	ARG
12	CO	98	VAL
12	CO	108	GLU
12	CO	113	LYS
12	CO	117	LEU
13	CP	2	LYS
13	CP	3	LEU
13	CP	21	ARG
13	CP	38	GLN
13	CP	39	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	CP	40	SER
13	CP	42	SER
13	CP	45	LEU
13	CP	55	ARG
13	CP	56	SER
13	CP	59	LEU
13	CP	64	LYS
13	CP	65	ARG
13	CP	75	ILE
13	CP	83	VAL
13	CP	95	VAL
13	CP	98	GLU
13	CP	106	LEU
13	CP	125	VAL
13	CP	131	SER
13	CP	147	LEU
13	CP	148	LEU
14	CQ	1	MET
14	CQ	2	LEU
14	CQ	3	MET
14	CQ	7	MET
14	CQ	8	LYS
14	CQ	12	GLN
14	CQ	16	ARG
14	CQ	21	THR
14	CQ	22	LYS
14	CQ	35	VAL
14	CQ	45	GLN
14	CQ	60	ARG
14	CQ	75	THR
14	CQ	109	VAL
14	CQ	110	THR
14	CQ	115	MET
14	CQ	128	LYS
14	CQ	131	ILE
15	CR	1	MET
15	CR	18	LEU
15	CR	24	GLN
15	CR	27	SER
15	CR	28	LEU
15	CR	29	LEU
15	CR	30	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
15	CR	36	THR
15	CR	44	LEU
15	CR	60	LEU
15	CR	65	LEU
15	CR	67	LEU
15	CR	73	VAL
15	CR	75	LEU
15	CR	79	LEU
15	CR	96	ARG
15	CR	100	LEU
15	CR	111	LEU
15	CR	114	VAL
16	CS	8	GLU
16	CS	14	VAL
16	CS	19	LYS
16	CS	20	ARG
16	CS	25	ARG
16	CS	35	ILE
16	CS	36	TYR
16	CS	39	ILE
16	CS	48	LEU
16	CS	49	VAL
16	CS	58	LEU
16	CS	64	GLU
16	CS	67	ARG
16	CS	68	GLN
16	CS	69	VAL
16	CS	78	LEU
16	CS	80	LEU
16	CS	103	GLU
16	CS	110	LEU
17	CT	6	LEU
17	CT	8	LYS
17	CT	13	ARG
17	CT	18	ASP
17	CT	28	VAL
17	CT	34	VAL
17	CT	49	VAL
17	CT	51	ARG
17	CT	53	ARG
17	CT	59	THR
17	CT	64	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
17	CT	74	ARG
17	CT	78	LEU
17	CT	85	LYS
17	CT	89	VAL
17	CT	93	ARG
17	CT	96	ARG
17	CT	113	LYS
17	CT	115	ARG
17	CT	118	ARG
17	CT	123	GLN
17	CT	124	ASP
18	CU	6	THR
18	CU	8	VAL
18	CU	13	LYS
18	CU	31	SER
18	CU	60	LEU
18	CU	74	LEU
18	CU	83	LEU
18	CU	88	ILE
18	CU	92	ARG
18	CU	93	LYS
18	CU	100	VAL
18	CU	101	ARG
18	CU	104	GLN
19	CV	1	MET
19	CV	6	LYS
19	CV	15	GLU
19	CV	18	LEU
19	CV	19	LYS
19	CV	24	LYS
19	CV	46	VAL
19	CV	51	VAL
19	CV	52	VAL
19	CV	61	VAL
19	CV	62	LEU
19	CV	66	ARG
19	CV	73	SER
19	CV	79	VAL
19	CV	95	LEU
20	CW	11	ARG
20	CW	14	PRO
20	CW	15	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
20	CW	17	VAL
20	CW	19	LEU
20	CW	23	LEU
20	CW	37	ARG
20	CW	51	LEU
20	CW	63	ASP
20	CW	100	THR
20	CW	101	SER
20	CW	107	LEU
21	CX	35	THR
21	CX	45	THR
21	CX	57	LEU
21	CX	60	ARG
21	CX	76	ARG
21	CX	87	GLN
21	CX	92	LEU
22	CY	7	VAL
22	CY	9	LYS
22	CY	14	LEU
22	CY	21	LYS
22	CY	37	VAL
22	CY	43	ASN
22	CY	49	VAL
22	CY	70	SER
22	CY	73	ARG
22	CY	91	GLU
22	CY	102	CYS
23	CZ	5	LEU
23	CZ	18	LEU
23	CZ	33	LEU
23	CZ	41	LEU
23	CZ	56	VAL
23	CZ	61	LEU
23	CZ	66	SER
23	CZ	71	VAL
23	CZ	86	VAL
23	CZ	90	VAL
23	CZ	91	LEU
23	CZ	97	GLU
23	CZ	102	LEU
23	CZ	107	THR
23	CZ	120	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
23	CZ	124	ILE
23	CZ	126	VAL
23	CZ	128	VAL
23	CZ	129	SER
23	CZ	136	PHE
23	CZ	141	VAL
23	CZ	144	LEU
23	CZ	146	ILE
23	CZ	161	VAL
23	CZ	170	THR
24	C0	3	HIS
24	C0	19	LYS
24	C0	20	ARG
24	C0	36	ILE
24	C0	44	ARG
24	C0	49	LYS
25	C1	6	GLU
25	C1	21	ARG
25	C1	35	THR
25	C1	40	ARG
25	C1	51	VAL
25	C1	52	ARG
25	C1	59	THR
25	C1	70	VAL
25	C1	80	LEU
25	C1	86	SER
25	C1	89	GLU
25	C1	95	LEU
25	C1	97	LEU
25	C1	98	LEU
26	C2	2	LYS
26	C2	19	VAL
26	C2	32	LEU
26	C2	35	LEU
26	C2	40	SER
26	C2	41	ILE
26	C2	44	LEU
26	C2	53	LEU
26	C2	64	LEU
26	C2	66	GLU
26	C2	67	LYS
26	C2	70	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
27	C3	3	ARG
27	C3	5	LYS
27	C3	6	VAL
27	C3	8	LEU
27	C3	18	ASP
27	C3	23	LEU
27	C3	24	LYS
27	C3	31	LEU
27	C3	54	VAL
27	C3	56	VAL
28	C4	1	MET
28	C4	3	GLU
28	C4	5	ILE
28	C4	10	VAL
28	C4	14	ILE
28	C4	34	GLU
28	C4	50	VAL
28	C4	56	VAL
28	C4	61	ARG
28	C4	63	TYR
28	C4	68	ARG
29	C5	6	VAL
29	C5	16	ARG
29	C5	29	THR
29	C5	35	GLU
29	C5	48	GLU
29	C5	58	LEU
30	C6	5	VAL
30	C6	9	LEU
30	C6	23	THR
30	C6	44	ARG
30	C6	47	THR
30	C6	48	VAL
31	C7	1	MET
31	C7	9	ARG
31	C7	14	LYS
31	C7	43	THR
32	C8	4	MET
32	C8	14	VAL
32	C8	16	ILE
32	C8	26	LYS
32	C8	30	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	C8	36	LYS
32	C8	59	LYS
33	C9	4	ARG
33	C9	17	ILE
33	C9	19	ARG
33	C9	26	ILE
35	DB	7	VAL
35	DB	10	LEU
35	DB	15	VAL
35	DB	23	ARG
35	DB	44	LEU
35	DB	50	GLU
35	DB	51	LEU
35	DB	67	THR
35	DB	71	VAL
35	DB	80	ILE
35	DB	95	GLN
35	DB	98	LEU
35	DB	108	ILE
35	DB	115	LEU
35	DB	116	GLU
35	DB	117	GLU
35	DB	128	GLU
35	DB	135	GLN
35	DB	154	LEU
35	DB	155	LEU
35	DB	157	ARG
35	DB	158	LEU
35	DB	162	ILE
35	DB	169	LYS
35	DB	179	LYS
35	DB	185	ILE
35	DB	187	LEU
35	DB	189	ASP
35	DB	212	GLN
35	DB	214	ILE
35	DB	215	LEU
35	DB	217	ARG
35	DB	229	VAL
36	DC	3	ASN
36	DC	12	LEU
36	DC	14	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	DC	15	THR
36	DC	21	ARG
36	DC	29	TYR
36	DC	30	ARG
36	DC	47	LEU
36	DC	49	SER
36	DC	52	LEU
36	DC	91	LEU
36	DC	101	LEU
36	DC	104	GLN
36	DC	108	ASN
36	DC	115	LEU
36	DC	116	VAL
36	DC	128	PHE
36	DC	140	ARG
36	DC	152	ILE
36	DC	153	VAL
36	DC	154	SER
36	DC	165	THR
36	DC	178	LEU
36	DC	190	ARG
36	DC	191	THR
36	DC	192	THR
36	DC	195	VAL
37	DD	3	ARG
37	DD	5	ILE
37	DD	31	CYS
37	DD	34	GLU
37	DD	47	ARG
37	DD	57	ARG
37	DD	58	LEU
37	DD	61	LYS
37	DD	63	LYS
37	DD	65	ARG
37	DD	96	LEU
37	DD	108	LEU
37	DD	127	THR
37	DD	135	LEU
37	DD	137	SER
37	DD	150	GLU
37	DD	155	LEU
37	DD	178	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
37	DD	187	ARG
37	DD	188	LEU
37	DD	200	GLU
37	DD	203	VAL
37	DD	208	SER
38	DE	10	MET
38	DE	16	THR
38	DE	18	ARG
38	DE	31	LEU
38	DE	41	VAL
38	DE	47	LYS
38	DE	53	LEU
38	DE	68	GLU
38	DE	71	LEU
38	DE	75	THR
38	DE	76	ILE
38	DE	79	GLU
38	DE	82	VAL
38	DE	87	SER
38	DE	89	ILE
38	DE	91	LEU
38	DE	96	PRO
38	DE	101	ILE
38	DE	117	ASP
38	DE	120	THR
38	DE	137	GLU
38	DE	150	ARG
39	DF	1	MET
39	DF	10	LEU
39	DF	21	LEU
39	DF	27	GLN
39	DF	28	ARG
39	DF	40	VAL
39	DF	65	VAL
39	DF	69	GLU
39	DF	72	VAL
39	DF	75	LEU
39	DF	82	ARG
39	DF	87	ARG
39	DF	93	SER
40	DG	32	ARG
40	DG	52	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
40	DG	75	VAL
40	DG	98	SER
40	DG	104	LEU
40	DG	114	ARG
40	DG	115	ARG
40	DG	155	ARG
41	DH	2	LEU
41	DH	3	THR
41	DH	9	MET
41	DH	24	THR
41	DH	26	VAL
41	DH	39	LEU
41	DH	51	VAL
41	DH	52	ASP
41	DH	60	ARG
41	DH	63	LEU
41	DH	65	TYR
41	DH	78	GLN
41	DH	84	ARG
41	DH	85	ARG
41	DH	98	LYS
41	DH	109	ILE
41	DH	111	ILE
41	DH	112	LEU
41	DH	115	SER
41	DH	119	LEU
41	DH	120	THR
41	DH	125	ARG
41	DH	127	LEU
41	DH	133	LEU
42	DI	14	VAL
42	DI	23	ASN
42	DI	27	THR
42	DI	31	GLN
42	DI	41	VAL
42	DI	53	VAL
42	DI	64	THR
42	DI	65	VAL
42	DI	85	LEU
42	DI	89	ASN
42	DI	92	TYR
42	DI	102	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
42	DI	108	VAL
42	DI	109	VAL
42	DI	113	LYS
42	DI	124	GLN
42	DI	128	ARG
43	DJ	6	ILE
43	DJ	21	GLN
43	DJ	30	SER
43	DJ	34	VAL
43	DJ	43	ARG
43	DJ	46	ARG
43	DJ	62	HIS
43	DJ	67	THR
43	DJ	72	VAL
43	DJ	85	LEU
43	DJ	95	GLU
43	DJ	96	ILE
44	DK	14	VAL
44	DK	18	ARG
44	DK	30	VAL
44	DK	33	THR
44	DK	51	LYS
44	DK	54	ARG
44	DK	92	GLU
44	DK	109	VAL
44	DK	126	ARG
45	DL	7	ILE
45	DL	33	ARG
45	DL	42	THR
45	DL	47	LYS
45	DL	52	LEU
45	DL	66	VAL
45	DL	75	HIS
45	DL	85	ILE
45	DL	89	ARG
45	DL	102	ARG
45	DL	104	VAL
46	DM	3	ARG
46	DM	8	GLU
46	DM	11	ARG
46	DM	15	VAL
46	DM	27	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
46	DM	29	ARG
46	DM	52	GLU
46	DM	66	LEU
46	DM	70	LEU
46	DM	73	GLU
46	DM	77	ASN
46	DM	90	LEU
46	DM	92	HIS
46	DM	98	VAL
46	DM	106	ASN
46	DM	110	ARG
46	DM	121	LYS
47	DN	3	ARG
47	DN	6	LEU
47	DN	13	THR
47	DN	18	VAL
47	DN	22	THR
47	DN	33	VAL
47	DN	44	LEU
47	DN	46	GLU
47	DN	56	VAL
48	DO	3	ILE
48	DO	4	THR
48	DO	5	LYS
48	DO	7	GLU
48	DO	12	ILE
48	DO	22	THR
48	DO	26	GLU
48	DO	38	ARG
48	DO	39	LEU
48	DO	48	LYS
48	DO	64	ARG
48	DO	66	LEU
48	DO	87	ILE
49	DP	2	VAL
49	DP	4	ILE
49	DP	5	ARG
49	DP	20	VAL
49	DP	21	VAL
49	DP	25	ARG
49	DP	29	ASP
49	DP	45	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
49	DP	53	VAL
49	DP	60	LEU
49	DP	62	VAL
49	DP	74	LEU
50	DQ	6	LEU
50	DQ	9	VAL
50	DQ	50	LYS
50	DQ	52	LYS
50	DQ	61	GLU
50	DQ	63	ARG
50	DQ	69	LYS
50	DQ	72	ARG
50	DQ	74	LEU
50	DQ	79	SER
50	DQ	86	GLU
50	DQ	96	GLU
50	DQ	98	LEU
51	DR	32	ARG
51	DR	37	VAL
51	DR	41	LYS
51	DR	42	ARG
51	DR	53	ARG
51	DR	65	ILE
51	DR	76	LEU
51	DR	85	LEU
52	DS	6	LYS
52	DS	12	ASP
52	DS	22	LEU
52	DS	33	THR
52	DS	43	GLU
52	DS	65	ASN
52	DS	78	ARG
52	DS	83	HIS
53	DT	10	LEU
53	DT	25	ARG
53	DT	36	LEU
53	DT	46	GLU
53	DT	56	MET
53	DT	61	SER
53	DT	62	LEU
53	DT	71	THR
53	DT	79	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
53	DT	80	ARG
53	DT	84	LEU
53	DT	89	ARG
53	DT	93	GLU
54	DU	10	ARG
54	DU	15	ARG
59	DZ	-65	LYS
59	DZ	-58	LEU
59	DZ	-55	LEU
59	DZ	-53	ASP
59	DZ	-47	ASP
59	DZ	-29	LEU
59	DZ	-20	LEU
59	DZ	-19	GLU
59	DZ	-13	GLN
59	DZ	-10	ARG
59	DZ	-6	ARG
59	DZ	-5	LYS
59	DZ	4	ILE
59	DZ	7	ASN
59	DZ	8	ASP
59	DZ	9	LEU
59	DZ	12	LEU
59	DZ	15	ILE
59	DZ	21	ILE
59	DZ	25	LYS
59	DZ	26	THR
59	DZ	30	GLU
59	DZ	31	ARG
59	DZ	33	LEU
59	DZ	69	VAL
59	DZ	70	THR
59	DZ	75	LYS
59	DZ	78	ARG
59	DZ	79	ILE
59	DZ	92	ILE
59	DZ	93	GLU
59	DZ	98	MET
59	DZ	100	VAL
59	DZ	105	ILE
59	DZ	107	VAL
59	DZ	112	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
59	DZ	117	GLN
59	DZ	120	THR
59	DZ	121	VAL
59	DZ	130	VAL
59	DZ	132	ARG
59	DZ	146	LEU
59	DZ	163	VAL
59	DZ	170	ARG
59	DZ	196	ILE
59	DZ	204	GLU
59	DZ	215	LYS
59	DZ	219	VAL
59	DZ	228	MET
59	DZ	232	LEU
59	DZ	236	GLU
59	DZ	240	GLU
59	DZ	255	ILE
59	DZ	264	LEU
59	DZ	277	VAL
59	DZ	285	ASP
59	DZ	286	ILE
59	DZ	289	ILE
59	DZ	292	THR
59	DZ	297	GLU
59	DZ	299	VAL
59	DZ	302	HIS
59	DZ	312	LEU
59	DZ	315	LYS
59	DZ	322	VAL
59	DZ	325	LEU
59	DZ	326	THR
59	DZ	328	ILE
59	DZ	334	THR
59	DZ	341	VAL
59	DZ	352	VAL
59	DZ	355	LEU
59	DZ	356	LEU
59	DZ	363	ARG
59	DZ	369	LEU
59	DZ	377	VAL
59	DZ	382	GLU
59	DZ	384	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
59	DZ	385	THR
59	DZ	396	ARG
59	DZ	399	LEU
59	DZ	403	GLU
59	DZ	409	ILE
59	DZ	418	LYS
59	DZ	422	GLU
59	DZ	426	GLN
59	DZ	437	THR
59	DZ	442	THR
59	DZ	445	GLU
59	DZ	446	THR
59	DZ	462	ILE
59	DZ	471	LYS
59	DZ	473	ASP
59	DZ	475	ASN
59	DZ	488	THR
59	DZ	498	ILE
59	DZ	504	ARG
59	DZ	512	ILE
59	DZ	526	VAL
59	DZ	536	LYS
59	DZ	537	GLU
59	DZ	556	ILE
59	DZ	572	TYR
59	DZ	578	SER
59	DZ	590	ILE
59	DZ	594	VAL
59	DZ	598	ASP
59	DZ	600	VAL
59	DZ	601	ILE
59	DZ	602	LEU
59	DZ	605	ILE
59	DZ	612	THR
59	DZ	614	GLU
59	DZ	621	ILE
59	DZ	623	ASP
59	DZ	624	LEU
59	DZ	630	GLN
59	DZ	631	ILE
59	DZ	649	LEU
59	DZ	651	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
59	DZ	659	LEU
59	DZ	660	ARG
59	DZ	668	SER
59	DZ	679	VAL
59	DZ	681	LYS
59	DZ	686	LYS
59	DZ	689	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (188) such sidechains are listed below:

Mol	Chain	Res	Type
3	AC	18	ASN
3	AC	67	HIS
3	AC	189	ASN
3	AC	200	HIS
4	AD	126	GLN
4	AD	129	ASN
4	AD	253	GLN
5	AE	85	ASN
5	AE	192	ASN
6	AF	169	ASN
6	AF	203	GLN
7	AG	26	GLN
7	AG	40	ASN
7	AG	41	GLN
10	AL	103	GLN
10	AL	116	ASN
11	AN	131	GLN
13	AP	38	GLN
13	AP	84	ASN
14	AQ	89	ASN
15	AR	31	HIS
15	AR	71	GLN
16	AS	95	HIS
17	AT	43	GLN
17	AT	90	GLN
18	AU	72	HIS
18	AU	94	ASN
21	AX	31	HIS
21	AX	82	GLN
22	AY	92	ASN
23	AZ	34	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
23	AZ	118	GLN
24	A0	17	GLN
26	A2	9	GLN
26	A2	65	ASN
27	A3	32	GLN
33	A9	36	GLN
35	BB	16	HIS
35	BB	45	GLN
35	BB	212	GLN
36	BC	6	HIS
36	BC	28	GLN
36	BC	118	GLN
36	BC	136	GLN
36	BC	170	GLN
36	BC	181	ASN
37	BD	45	GLN
37	BD	119	GLN
37	BD	123	HIS
37	BD	125	HIS
37	BD	160	GLN
37	BD	161	ASN
38	BE	38	GLN
38	BE	56	GLN
39	BF	94	GLN
39	BF	100	ASN
40	BG	28	ASN
40	BG	51	GLN
40	BG	64	GLN
42	BI	23	ASN
42	BI	31	GLN
42	BI	89	ASN
42	BI	124	GLN
43	BJ	56	HIS
44	BK	104	GLN
45	BL	78	GLN
45	BL	80	HIS
46	BM	77	ASN
47	BN	49	HIS
48	BO	9	GLN
48	BO	28	GLN
48	BO	50	HIS
50	BQ	16	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
52	BS	65	ASN
52	BS	69	HIS
53	BT	26	ASN
53	BT	45	GLN
53	BT	73	HIS
53	BT	75	ASN
59	BZ	-50	GLN
59	BZ	-13	GLN
59	BZ	77	HIS
59	BZ	112	GLN
59	BZ	154	GLN
59	BZ	208	GLN
59	BZ	362	HIS
59	BZ	475	ASN
59	BZ	506	GLN
59	BZ	641	GLN
59	BZ	675	HIS
59	BZ	682	GLN
59	BZ	684	GLN
3	CC	18	ASN
3	CC	67	HIS
3	CC	173	HIS
3	CC	189	ASN
3	CC	200	HIS
4	CD	87	ASN
4	CD	164	GLN
4	CD	253	GLN
6	CF	69	HIS
6	CF	75	HIS
6	CF	169	ASN
6	CF	203	GLN
7	CG	40	ASN
11	CN	8	GLN
11	CN	133	GLN
12	CO	90	GLN
13	CP	38	GLN
13	CP	128	HIS
14	CQ	45	GLN
15	CR	13	HIS
15	CR	31	HIS
15	CR	61	HIS
16	CS	95	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
17	CT	84	GLN
18	CU	94	ASN
18	CU	104	GLN
20	CW	60	ASN
21	CX	31	HIS
22	CY	43	ASN
22	CY	68	HIS
23	CZ	132	ASN
30	C6	20	ASN
33	C9	36	GLN
35	DB	45	GLN
35	DB	76	GLN
35	DB	94	ASN
35	DB	135	GLN
35	DB	224	GLN
36	DC	3	ASN
36	DC	28	GLN
36	DC	63	ASN
36	DC	104	GLN
36	DC	123	GLN
37	DD	77	ASN
37	DD	123	HIS
37	DD	125	HIS
37	DD	160	GLN
38	DE	73	ASN
38	DE	141	GLN
39	DF	7	ASN
39	DF	18	GLN
39	DF	94	GLN
39	DF	100	ASN
40	DG	28	ASN
40	DG	51	GLN
40	DG	96	GLN
40	DG	97	GLN
40	DG	110	GLN
40	DG	122	HIS
40	DG	148	ASN
41	DH	15	ASN
42	DI	23	ASN
42	DI	31	GLN
42	DI	58	HIS
42	DI	73	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
42	DI	124	GLN
43	DJ	13	HIS
43	DJ	21	GLN
43	DJ	68	HIS
44	DK	93	GLN
44	DK	116	HIS
45	DL	49	ASN
45	DL	75	HIS
45	DL	99	HIS
46	DM	40	ASN
46	DM	92	HIS
48	DO	28	GLN
49	DP	13	HIS
49	DP	16	HIS
50	DQ	16	GLN
51	DR	36	ASN
52	DS	23	ASN
52	DS	56	GLN
52	DS	83	HIS
53	DT	75	ASN
59	DZ	-50	GLN
59	DZ	7	ASN
59	DZ	154	GLN
59	DZ	165	GLN
59	DZ	270	GLN
59	DZ	302	HIS
59	DZ	361	ASN
59	DZ	509	HIS
59	DZ	630	GLN
59	DZ	641	GLN
59	DZ	677	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	2866/2915 (98%)	481 (16%)	41 (1%)
1	CA	2860/2915 (98%)	523 (18%)	37 (1%)
2	AB	119/121 (98%)	11 (9%)	0
2	CB	119/121 (98%)	19 (15%)	0
34	BA	1494/1521 (98%)	265 (17%)	21 (1%)
34	DA	1501/1521 (98%)	285 (18%)	23 (1%)

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
55	BV	12/24 (50%)	3 (25%)	0
55	DV	11/24 (45%)	1 (9%)	0
56	BW	71/76 (93%)	18 (25%)	1 (1%)
56	DW	68/76 (89%)	22 (32%)	2 (2%)
57	BX	74/77 (96%)	10 (13%)	0
57	DX	74/77 (96%)	13 (17%)	0
58	BY	72/76 (94%)	20 (27%)	2 (2%)
58	DY	71/76 (93%)	21 (29%)	0
All	All	9412/9620 (97%)	1692 (17%)	127 (1%)

All (1692) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	12	U
1	AA	13	A
1	AA	34	C
1	AA	45	C
1	AA	62	U
1	AA	70	A
1	AA	71	U
1	AA	73	A
1	AA	74	G
1	AA	83	A
1	AA	91	G
1	AA	94	G
1	AA	99	G
1	AA	116	A
1	AA	117	A
1	AA	118	U
1	AA	120	G
1	AA	137	G
1	AA	149	A
1	AA	185	A
1	AA	186	A
1	AA	188	A
1	AA	189	U
1	AA	190	C
1	AA	194	G
1	AA	203	G
1	AA	204	G
1	AA	205	A
1	AA	210	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	AA	211	A
1	AA	217	A
1	AA	218	A
1	AA	222	A
1	AA	237	G
1	AA	239	G
1	AA	262	C
1	AA	269	G
1	AA	271	U
1	AA	272	U
1	AA	273	G
1	AA	274	U
1	AA	276	C
1	AA	279	G
1	AA	289	G
1	AA	299	G
1	AA	303	C
1	AA	311	C
1	AA	335	A
1	AA	348	A
1	AA	353	G
1	AA	354	A
1	AA	376	G
1	AA	387	G
1	AA	407	U
1	AA	413	G
1	AA	423	G
1	AA	434	G
1	AA	438	G
1	AA	439	A
1	AA	455	A
1	AA	469	A
1	AA	470	C
1	AA	474	U
1	AA	477	C
1	AA	482	C
1	AA	483	A
1	AA	496	A
1	AA	501	U
1	AA	505	A
1	AA	507	G
1	AA	519	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	AA	529	U
1	AA	530	A
1	AA	534	C
1	AA	551	A
1	AA	553	A
1	AA	555	G
1	AA	556	C
1	AA	557	A
1	AA	558	G
1	AA	569	G
1	AA	573	G
1	AA	574	G
1	AA	586	G
1	AA	596	G
1	AA	598	A
1	AA	609	A
1	AA	616	G
1	AA	626	A
1	AA	627	G
1	AA	630	U
1	AA	633	G
1	AA	639	G
1	AA	641	G
1	AA	644	G
1	AA	659	C
1	AA	662	A
1	AA	670	C
1	AA	671	A
1	AA	692	C
1	AA	693	G
1	AA	697	C
1	AA	716	G
1	AA	717	A
1	AA	733	G
1	AA	762	G
1	AA	777	C
1	AA	785	G
1	AA	787	U
1	AA	793	A
1	AA	794	U
1	AA	811	A
1	AA	812	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	AA	822	G
1	AA	823	G
1	AA	829	A
1	AA	831	A
1	AA	832	G
1	AA	837	C
1	AA	839	G
1	AA	852	G
1	AA	859	C
1	AA	866	A
1	AA	867	A
1	AA	874	U
1	AA	875	U
1	AA	877	G
1	AA	888	A
1	AA	906	G
1	AA	924	U
1	AA	927	G
1	AA	931	C
1	AA	932	C
1	AA	933	C
1	AA	934	A
1	AA	935	C
1	AA	936	C
1	AA	937	A
1	AA	938	G
1	AA	939	C
1	AA	940	C
1	AA	942	A
1	AA	943	C
1	AA	945	A
1	AA	946	A
1	AA	953	U
1	AA	956	A
1	AA	957	A
1	AA	960	C
1	AA	972	A
1	AA	977	G
1	AA	986	A
1	AA	990	A
1	AA	991	G
1	AA	1003	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	AA	1004	A
1	AA	1006	C
1	AA	1019	G
1	AA	1020	C
1	AA	1029	A
1	AA	1036	A
1	AA	1042	A
1	AA	1051	C
1	AA	1054	C
1	AA	1058	U
1	AA	1059	C
1	AA	1068	G
1	AA	1072	U
1	AA	1077	G
1	AA	1079	U
1	AA	1084	C
1	AA	1092	A
1	AA	1093	G
1	AA	1096	A
1	AA	1099	C
1	AA	1100	A
1	AA	1101	G
1	AA	1105	G
1	AA	1106	U
1	AA	1107	U
1	AA	1108	G
1	AA	1111	U
1	AA	1112	U
1	AA	1116	A
1	AA	1121	C
1	AA	1122	C
1	AA	1125	C
1	AA	1126	C
1	AA	1129	U
1	AA	1134	A
1	AA	1136	U
1	AA	1139	G
1	AA	1154	U
1	AA	1155	C
1	AA	1156	G
1	AA	1174	A
1	AA	1180	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	AA	1181	G
1	AA	1184	G
1	AA	1196	C
1	AA	1197	G
1	AA	1210	G
1	AA	1217	G
1	AA	1218	G
1	AA	1219	A
1	AA	1220	U
1	AA	1221	G
1	AA	1222	A
1	AA	1223	C
1	AA	1255	A
1	AA	1256	U
1	AA	1265	A
1	AA	1287	A
1	AA	1290	G
1	AA	1294	G
1	AA	1299	A
1	AA	1302	G
1	AA	1317	G
1	AA	1318	A
1	AA	1322	A
1	AA	1346	U
1	AA	1347	A
1	AA	1348	A
1	AA	1349	G
1	AA	1367	A
1	AA	1391	C
1	AA	1405	A
1	AA	1406	A
1	AA	1411	A
1	AA	1425	A
1	AA	1426	G
1	AA	1430	A
1	AA	1431	G
1	AA	1462	G
1	AA	1463	C
1	AA	1466	U
1	AA	1467	G
1	AA	1468	G
1	AA	1473	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	AA	1474	C
1	AA	1491	A
1	AA	1496	A
1	AA	1497	G
1	AA	1500	A
1	AA	1502	G
1	AA	1508	G
1	AA	1514	C
1	AA	1518	A
1	AA	1525	G
1	AA	1529	G
1	AA	1539	C
1	AA	1554	A
1	AA	1555	C
1	AA	1556	A
1	AA	1578	C
1	AA	1587	U
1	AA	1589	A
1	AA	1590	C
1	AA	1605	A
1	AA	1607	G
1	AA	1613	A
1	AA	1616	A
1	AA	1625	U
1	AA	1627	A
1	AA	1628	G
1	AA	1630	A
1	AA	1631	C
1	AA	1632	A
1	AA	1654	A
1	AA	1655	A
1	AA	1656	A
1	AA	1695	C
1	AA	1721	G
1	AA	1743	G
1	AA	1747	A
1	AA	1764	G
1	AA	1767	A
1	AA	1776	G
1	AA	1787	G
1	AA	1788	U
1	AA	1793	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	AA	1794	G
1	AA	1795	G
1	AA	1804	A
1	AA	1811	A
1	AA	1813	C
1	AA	1822	A
1	AA	1831	C
1	AA	1833	A
1	AA	1847	G
1	AA	1850	A
1	AA	1870	G
1	AA	1878	A
1	AA	1889	G
1	AA	1890	A
1	AA	1892	G
1	AA	1898	A
1	AA	1900	G
1	AA	1911	A
1	AA	1922	A
1	AA	1928	G
1	AA	1935	A
1	AA	1941	A
1	AA	1951	G
1	AA	1952	G
1	AA	1953	U
1	AA	1956	C
1	AA	1960	A
1	AA	1977	U
1	AA	1985	U
1	AA	1987	C
1	AA	1989	C
1	AA	1992	A
1	AA	1993	A
1	AA	1994	A
1	AA	2003	A
1	AA	2014	G
1	AA	2015	U
1	AA	2019	G
1	AA	2028	C
1	AA	2042	A
1	AA	2045	G
1	AA	2053	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	AA	2055	A
1	AA	2065	C
1	AA	2073	A
1	AA	2077	C
1	AA	2078	G
1	AA	2082	A
1	AA	2083	G
1	AA	2084	A
1	AA	2091	G
1	AA	2123	G
1	AA	2132	G
1	AA	2133	C
1	AA	2141	A
1	AA	2143	G
1	AA	2144	U
1	AA	2149	G
1	AA	2152	U
1	AA	2153	G
1	AA	2154	U
1	AA	2155	G
1	AA	2156	A
1	AA	2157	A
1	AA	2158	C
1	AA	2159	C
1	AA	2160	C
1	AA	2162	C
1	AA	2163	G
1	AA	2164	C
1	AA	2165	C
1	AA	2169	G
1	AA	2173	G
1	AA	2175	G
1	AA	2179	G
1	AA	2180	A
1	AA	2181	G
1	AA	2182	G
1	AA	2188	G
1	AA	2190	G
1	AA	2191	A
1	AA	2194	U
1	AA	2195	A
1	AA	2196	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	AA	2198	A
1	AA	2199	C
1	AA	2200	C
1	AA	2203	G
1	AA	2204	G
1	AA	2205	C
1	AA	2206	G
1	AA	2210	C
1	AA	2211	U
1	AA	2213	G
1	AA	2214	G
1	AA	2220	A
1	AA	2221	A
1	AA	2227	G
1	AA	2228	G
1	AA	2229	A
1	AA	2237	A
1	AA	2251	G
1	AA	2252	C
1	AA	2280	A
1	AA	2285	A
1	AA	2287	C
1	AA	2295	C
1	AA	2298	A
1	AA	2299	A
1	AA	2317	A
1	AA	2319	G
1	AA	2320	G
1	AA	2321	A
1	AA	2324	U
1	AA	2332	A
1	AA	2337	G
1	AA	2346	G
1	AA	2348	A
1	AA	2352	G
1	AA	2359	C
1	AA	2362	C
1	AA	2366	G
1	AA	2373	A
1	AA	2391	G
1	AA	2395	G
1	AA	2397	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	AA	2418	U
1	AA	2419	G
1	AA	2426	G
1	AA	2436	C
1	AA	2437	A
1	AA	2441	G
1	AA	2442	A
1	AA	2443	U
1	AA	2446	A
1	AA	2447	A
1	AA	2451	A
1	AA	2452	C
1	AA	2453	C
1	AA	2459	G
1	AA	2460	A
1	AA	2461	U
1	AA	2471	A
1	AA	2488	A
1	AA	2490	A
1	AA	2506	G
1	AA	2514	G
1	AA	2517	G
1	AA	2530	A
1	AA	2541	G
1	AA	2566	U
1	AA	2567	U
1	AA	2578	A
1	AA	2579	G
1	AA	2585	C
1	AA	2594	G
1	AA	2614	A
1	AA	2621	U
1	AA	2623	U
1	AA	2624	C
1	AA	2640	C
1	AA	2641	A
1	AA	2642	G
1	AA	2644	A
1	AA	2653	G
1	AA	2658	C
1	AA	2666	A
1	AA	2675	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	AA	2701	U
1	AA	2702	C
1	AA	2714	U
1	AA	2715	C
1	AA	2725	A
1	AA	2726	A
1	AA	2727	G
1	AA	2739	U
1	AA	2740	G
1	AA	2746	A
1	AA	2752	U
1	AA	2768	C
1	AA	2771	A
1	AA	2774	G
1	AA	2778	A
1	AA	2779	G
1	AA	2791	A
1	AA	2803	A
1	AA	2804	C
1	AA	2813	G
1	AA	2828	G
1	AA	2830	A
1	AA	2831	A
1	AA	2843	G
1	AA	2845	A
1	AA	2847	G
1	AA	2871	G
1	AA	2882	G
1	AA	2883	A
1	AA	2890	C
1	AA	2902	G
1	AA	2903	G
2	AB	2	C
2	AB	9	G
2	AB	12	C
2	AB	21	G
2	AB	45	A
2	AB	47	C
2	AB	56	G
2	AB	67	G
2	AB	73	A
2	AB	110	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	AB	116	G
34	BA	5	U
34	BA	7	G
34	BA	9	G
34	BA	29	G
34	BA	30	U
34	BA	32	A
34	BA	39	G
34	BA	47	C
34	BA	48	C
34	BA	50	A
34	BA	51	A
34	BA	58	C
34	BA	61	G
34	BA	69	G
34	BA	77	G
34	BA	79	G
34	BA	91	C
34	BA	97	G
34	BA	101	A
34	BA	115	G
34	BA	116	A
34	BA	121	C
34	BA	129(A)	G
34	BA	131	C
34	BA	139	G
34	BA	161	A
34	BA	163	C
34	BA	174	C
34	BA	182	U
34	BA	189(D)	C
34	BA	189(F)	U
34	BA	195	A
34	BA	197	A
34	BA	199	G
34	BA	202	U
34	BA	204	U
34	BA	216	G
34	BA	222	U
34	BA	247	G
34	BA	251	G
34	BA	266	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	BA	267	C
34	BA	289	G
34	BA	301	G
34	BA	321	A
34	BA	328	C
34	BA	332	G
34	BA	342	C
34	BA	343	U
34	BA	346	G
34	BA	347	G
34	BA	348	G
34	BA	351	G
34	BA	352	C
34	BA	353	A
34	BA	354	G
34	BA	355	C
34	BA	365	U
34	BA	367	U
34	BA	372	C
34	BA	373	A
34	BA	383	A
34	BA	384	G
34	BA	388	G
34	BA	397	A
34	BA	398	C
34	BA	406	G
34	BA	412	A
34	BA	413	G
34	BA	424	G
34	BA	429	U
34	BA	439	A
34	BA	442	C
34	BA	452	A
34	BA	470	C
34	BA	485	G
34	BA	496	A
34	BA	498	U
34	BA	505	G
34	BA	509	A
34	BA	510	A
34	BA	511	C
34	BA	513	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	BA	518	C
34	BA	524	G
34	BA	527	G
34	BA	531	U
34	BA	532	A
34	BA	533	A
34	BA	536	C
34	BA	547	A
34	BA	559	A
34	BA	561	U
34	BA	572	A
34	BA	573	A
34	BA	576	G
34	BA	577	G
34	BA	596	C
34	BA	607	A
34	BA	616	G
34	BA	618	C
34	BA	630	G
34	BA	631	G
34	BA	632	A
34	BA	634	C
34	BA	653	A
34	BA	661	G
34	BA	665	A
34	BA	666	G
34	BA	667	G
34	BA	671	G
34	BA	673	G
34	BA	687	A
34	BA	688	G
34	BA	695	A
34	BA	723	U
34	BA	724	G
34	BA	728	A
34	BA	731	G
34	BA	749	C
34	BA	755	G
34	BA	765	G
34	BA	786	G
34	BA	788	U
34	BA	792	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	BA	793	U
34	BA	794	A
34	BA	815	A
34	BA	817	C
34	BA	828	A
34	BA	832	C
34	BA	840	C
34	BA	841	U
34	BA	848	C
34	BA	851	G
34	BA	859	A
34	BA	860	A
34	BA	874	G
34	BA	875	C
34	BA	876	G
34	BA	902	G
34	BA	908	A
34	BA	914	A
34	BA	926	G
34	BA	927	G
34	BA	932	C
34	BA	934	C
34	BA	935	A
34	BA	942	G
34	BA	960	U
34	BA	961	U
34	BA	968	A
34	BA	969	A
34	BA	971	G
34	BA	972	C
34	BA	974	A
34	BA	975	A
34	BA	976	G
34	BA	977	A
34	BA	982	U
34	BA	992	U
34	BA	993	G
34	BA	1000	U
34	BA	1003	G
34	BA	1004	A
34	BA	1005	A
34	BA	1008	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	BA	1009	G
34	BA	1016	A
34	BA	1019	C
34	BA	1022	G
34	BA	1023	G
34	BA	1025	U
34	BA	1027	C
34	BA	1028	C
34	BA	1030	C
34	BA	1030(A)	G
34	BA	1030(C)	G
34	BA	1031	G
34	BA	1033	G
34	BA	1045	C
34	BA	1054	C
34	BA	1065	U
34	BA	1066	C
34	BA	1068	G
34	BA	1070	U
34	BA	1081	G
34	BA	1094	G
34	BA	1095	U
34	BA	1101	A
34	BA	1108	G
34	BA	1123	A
34	BA	1124	G
34	BA	1125	U
34	BA	1126	U
34	BA	1134	G
34	BA	1136	U
34	BA	1137	C
34	BA	1138	G
34	BA	1139	G
34	BA	1140	C
34	BA	1141	C
34	BA	1145	C
34	BA	1146	A
34	BA	1152	A
34	BA	1159	U
34	BA	1166	G
34	BA	1183	A
34	BA	1184	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	BA	1187	G
34	BA	1189	C
34	BA	1196	U
34	BA	1197	G
34	BA	1202	G
34	BA	1212	U
34	BA	1213	A
34	BA	1227	A
34	BA	1236	A
34	BA	1238	A
34	BA	1240	U
34	BA	1253	G
34	BA	1256	A
34	BA	1257	U
34	BA	1258	G
34	BA	1260	C
34	BA	1270	C
34	BA	1273	G
34	BA	1278	U
34	BA	1279	A
34	BA	1280	A
34	BA	1286	A
34	BA	1287	A
34	BA	1299	A
34	BA	1300	G
34	BA	1302	U
34	BA	1321	C
34	BA	1335	C
34	BA	1336	C
34	BA	1338	G
34	BA	1340	A
34	BA	1347	G
34	BA	1353	G
34	BA	1359	C
34	BA	1360	A
34	BA	1363	C
34	BA	1364	U
34	BA	1370	G
34	BA	1397	C
34	BA	1419	G
34	BA	1442	G
34	BA	1442(A)	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	BA	1447	A
34	BA	1452	C
34	BA	1492	A
34	BA	1494	G
34	BA	1502	A
34	BA	1503	A
34	BA	1504	G
34	BA	1506	U
34	BA	1516	G
34	BA	1517	G
34	BA	1519	A
34	BA	1529	G
34	BA	1530	G
34	BA	1531	A
55	BV	13	A
55	BV	23	A
55	BV	24	A
56	BW	3	C
56	BW	8	4SU
56	BW	9	A
56	BW	13	C
56	BW	14	A
56	BW	19	G
56	BW	20	U
56	BW	21	A
56	BW	24	G
56	BW	45	U
56	BW	46	7MG
56	BW	47	U
56	BW	48	C
56	BW	49	C
56	BW	64	A
56	BW	68	C
56	BW	73	A
56	BW	74	C
57	BX	13	C
57	BX	19	G
57	BX	21	A
57	BX	34	C
57	BX	42	G
57	BX	47	U
57	BX	49	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
57	BX	56	C
57	BX	58	A
57	BX	68	C
58	BY	5	G
58	BY	6	G
58	BY	9	A
58	BY	13	C
58	BY	14	A
58	BY	20	U
58	BY	21	A
58	BY	26	A
58	BY	36	A
58	BY	41	C
58	BY	42	C
58	BY	44	G
58	BY	45	U
58	BY	46	7MG
58	BY	47	U
58	BY	48	C
58	BY	57	G
58	BY	59	U
58	BY	60	U
58	BY	68	C
1	CA	12	U
1	CA	13	A
1	CA	34	C
1	CA	36	G
1	CA	41	C
1	CA	45	C
1	CA	64	A
1	CA	71	A
1	CA	74	A
1	CA	75	G
1	CA	84	A
1	CA	90	U
1	CA	95	G
1	CA	100	G
1	CA	102	G
1	CA	118	A
1	CA	119	A
1	CA	120	U
1	CA	141	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	CA	154(A)	C
1	CA	157	U
1	CA	173	G
1	CA	196	A
1	CA	197	A
1	CA	205	G
1	CA	214	G
1	CA	215	G
1	CA	216	A
1	CA	221	A
1	CA	222	A
1	CA	225	A
1	CA	228	A
1	CA	229	A
1	CA	248	G
1	CA	250	G
1	CA	271(I)	G
1	CA	271(K)	U
1	CA	271(L)	U
1	CA	271(M)	G
1	CA	271(N)	U
1	CA	271(O)	C
1	CA	272(A)	U
1	CA	272(B)	G
1	CA	277	C
1	CA	278	A
1	CA	283	A
1	CA	294	A
1	CA	299	A
1	CA	304	G
1	CA	310	A
1	CA	311	A
1	CA	329	G
1	CA	330	A
1	CA	338	G
1	CA	342	G
1	CA	345	A
1	CA	352	G
1	CA	357	A
1	CA	362	U
1	CA	363	G
1	CA	363(B)	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	CA	363(C)	G
1	CA	363(F)	A
1	CA	386	G
1	CA	395	U
1	CA	407	G
1	CA	411	G
1	CA	412	A
1	CA	422	A
1	CA	428	A
1	CA	443	A
1	CA	444	C
1	CA	455	C
1	CA	456	C
1	CA	457	A
1	CA	470	A
1	CA	471	A
1	CA	481	G
1	CA	501	A
1	CA	504	U
1	CA	505	A
1	CA	509	C
1	CA	528	A
1	CA	529	A
1	CA	530	G
1	CA	531	C
1	CA	532	A
1	CA	533	G
1	CA	545	G
1	CA	563	G
1	CA	573	G
1	CA	575	A
1	CA	586	A
1	CA	587	C
1	CA	588	U
1	CA	599	G
1	CA	603	A
1	CA	604	G
1	CA	606	U
1	CA	607	U
1	CA	614(B)	G
1	CA	614(C)	A
1	CA	615	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	CA	616	G
1	CA	627	A
1	CA	631	A
1	CA	637	A
1	CA	645	C
1	CA	646	A
1	CA	652(A)	A
1	CA	652(B)	A
1	CA	652(C)	G
1	CA	652(U)	G
1	CA	668	G
1	CA	669	G
1	CA	686	G
1	CA	709	U
1	CA	730	C
1	CA	752	A
1	CA	753	C
1	CA	764	A
1	CA	765	G
1	CA	774	A
1	CA	775	G
1	CA	776	G
1	CA	782	A
1	CA	784	A
1	CA	785	G
1	CA	790	C
1	CA	792	G
1	CA	805	G
1	CA	812	C
1	CA	819	A
1	CA	827	U
1	CA	828	U
1	CA	857	C
1	CA	859	G
1	CA	866	A
1	CA	879	G
1	CA	880	G
1	CA	884	C
1	CA	886	C
1	CA	887	A
1	CA	888	C
1	CA	889	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	CA	890	A
1	CA	893	C
1	CA	896	A
1	CA	897	C
1	CA	898	C
1	CA	900	A
1	CA	901	A
1	CA	902	C
1	CA	910	A
1	CA	917	A
1	CA	931	G
1	CA	932	G
1	CA	938	G
1	CA	941	A
1	CA	945	A
1	CA	946	G
1	CA	958	U
1	CA	959	A
1	CA	961	C
1	CA	968	G
1	CA	974	G
1	CA	975	C
1	CA	983	A
1	CA	996	A
1	CA	1002	G
1	CA	1005	C
1	CA	1012	U
1	CA	1013	C
1	CA	1016	G
1	CA	1022	G
1	CA	1033	U
1	CA	1036	G
1	CA	1038	C
1	CA	1039	G
1	CA	1042	G
1	CA	1046	A
1	CA	1047	G
1	CA	1048	A
1	CA	1053	C
1	CA	1054	A
1	CA	1055	G
1	CA	1058	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	CA	1059	G
1	CA	1060	U
1	CA	1061	U
1	CA	1062	G
1	CA	1063	G
1	CA	1064	C
1	CA	1069	A
1	CA	1070	A
1	CA	1073	A
1	CA	1076	C
1	CA	1081	U
1	CA	1083	U
1	CA	1088	A
1	CA	1090	U
1	CA	1100	C
1	CA	1101	U
1	CA	1107	G
1	CA	1109	C
1	CA	1110	G
1	CA	1111	A
1	CA	1112	G
1	CA	1113	U
1	CA	1116	C
1	CA	1119	C
1	CA	1128	A
1	CA	1135	C
1	CA	1136	G
1	CA	1139	G
1	CA	1151	G
1	CA	1155	A
1	CA	1204	A
1	CA	1210	A
1	CA	1211	U
1	CA	1220	A
1	CA	1241	A
1	CA	1252	G
1	CA	1253	A
1	CA	1256	G
1	CA	1271	G
1	CA	1272	A
1	CA	1273	U
1	CA	1287	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	CA	1300	U
1	CA	1301	A
1	CA	1302	A
1	CA	1308	A
1	CA	1314	C
1	CA	1327	C
1	CA	1342	A
1	CA	1359	A
1	CA	1360	A
1	CA	1365	A
1	CA	1368	G
1	CA	1370	C
1	CA	1379	A
1	CA	1384	A
1	CA	1385	G
1	CA	1386	C
1	CA	1395	A
1	CA	1416	G
1	CA	1417	C
1	CA	1419	A
1	CA	1420	U
1	CA	1421	G
1	CA	1427	A
1	CA	1428	C
1	CA	1436	G
1	CA	1437	C
1	CA	1445	A
1	CA	1449	A
1	CA	1450	G
1	CA	1455	G
1	CA	1459	G
1	CA	1465	G
1	CA	1467	C
1	CA	1471	A
1	CA	1482	G
1	CA	1490	A
1	CA	1493	C
1	CA	1494	A
1	CA	1496	A
1	CA	1497	U
1	CA	1509	C
1	CA	1509(A)	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	CA	1525	G
1	CA	1531	C
1	CA	1532	C
1	CA	1533	G
1	CA	1542	A
1	CA	1547	C
1	CA	1554	A
1	CA	1558	A
1	CA	1559	G
1	CA	1560	G
1	CA	1566	A
1	CA	1569	A
1	CA	1578	U
1	CA	1582	C
1	CA	1584	C
1	CA	1586	A
1	CA	1608	A
1	CA	1609	A
1	CA	1616	A
1	CA	1648	C
1	CA	1653	G
1	CA	1654	A
1	CA	1674	G
1	CA	1676	A
1	CA	1696	G
1	CA	1700	A
1	CA	1701	A
1	CA	1703	G
1	CA	1722	A
1	CA	1739	U
1	CA	1756	G
1	CA	1763	G
1	CA	1764	G
1	CA	1773	A
1	CA	1780	A
1	CA	1791	A
1	CA	1800	C
1	CA	1801	G
1	CA	1812	A
1	CA	1816	G
1	CA	1829	A
1	CA	1835	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	CA	1847	A
1	CA	1848	A
1	CA	1866	C
1	CA	1877	A
1	CA	1878	G
1	CA	1883	G
1	CA	1889	A
1	CA	1900	A
1	CA	1906	G
1	CA	1913	A
1	CA	1914	C
1	CA	1929	G
1	CA	1930	G
1	CA	1934	C
1	CA	1952	A
1	CA	1955	U
1	CA	1963	U
1	CA	1967	C
1	CA	1970	A
1	CA	1971	A
1	CA	1972	A
1	CA	1983	C
1	CA	1992	G
1	CA	1993	U
1	CA	1997	G
1	CA	2005	A
1	CA	2020	A
1	CA	2023	G
1	CA	2031	A
1	CA	2032	G
1	CA	2033	A
1	CA	2038	G
1	CA	2043	C
1	CA	2046	G
1	CA	2055	C
1	CA	2056	G
1	CA	2060	A
1	CA	2061	G
1	CA	2062	A
1	CA	2063	C
1	CA	2069	G
1	CA	2082	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	CA	2096	U
1	CA	2102	U
1	CA	2106	G
1	CA	2110	G
1	CA	2111	C
1	CA	2112	G
1	CA	2113	U
1	CA	2115	G
1	CA	2116	G
1	CA	2117	A
1	CA	2119	A
1	CA	2122	U
1	CA	2124	G
1	CA	2126	A
1	CA	2127	G
1	CA	2130	U
1	CA	2131	G
1	CA	2132	U
1	CA	2133	G
1	CA	2134	A
1	CA	2135	A
1	CA	2136	C
1	CA	2137	C
1	CA	2142	C
1	CA	2144	U
1	CA	2146	C
1	CA	2148	G
1	CA	2150	U
1	CA	2153	G
1	CA	2154	G
1	CA	2157	G
1	CA	2158	A
1	CA	2161	C
1	CA	2162	G
1	CA	2164	C
1	CA	2165	G
1	CA	2166	G
1	CA	2167	U
1	CA	2168	G
1	CA	2169	A
1	CA	2170	A
1	CA	2172	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	CA	2173	A
1	CA	2178	C
1	CA	2181	G
1	CA	2185	C
1	CA	2186	G
1	CA	2188	C
1	CA	2189	U
1	CA	2192	G
1	CA	2198	A
1	CA	2206	G
1	CA	2207	G
1	CA	2208	A
1	CA	2218	U
1	CA	2225	A
1	CA	2238	G
1	CA	2239	G
1	CA	2240	C
1	CA	2248	C
1	CA	2268	A
1	CA	2269	A
1	CA	2275	C
1	CA	2278	A
1	CA	2279	G
1	CA	2283	C
1	CA	2287	A
1	CA	2289	G
1	CA	2294	C
1	CA	2305	A
1	CA	2308	G
1	CA	2312	U
1	CA	2319	G
1	CA	2320	A
1	CA	2321	G
1	CA	2325	G
1	CA	2334	G
1	CA	2336	A
1	CA	2343	C
1	CA	2347	C
1	CA	2350	C
1	CA	2354	G
1	CA	2376	A
1	CA	2383	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	CA	2385	C
1	CA	2406	U
1	CA	2407	G
1	CA	2410	G
1	CA	2423	U
1	CA	2424	C
1	CA	2425	A
1	CA	2428	G
1	CA	2429	G
1	CA	2430	A
1	CA	2435	A
1	CA	2439	A
1	CA	2440	C
1	CA	2441	C
1	CA	2448	A
1	CA	2452	C
1	CA	2474	C
1	CA	2476	A
1	CA	2491	U
1	CA	2492	U
1	CA	2494	G
1	CA	2498	C
1	CA	2502	G
1	CA	2505	G
1	CA	2506	U
1	CA	2518	A
1	CA	2520	C
1	CA	2529	G
1	CA	2554	U
1	CA	2564	A
1	CA	2566	A
1	CA	2567	G
1	CA	2573	C
1	CA	2582	G
1	CA	2602	A
1	CA	2611	U
1	CA	2612	C
1	CA	2629	A
1	CA	2630	G
1	CA	2632	A
1	CA	2636	U
1	CA	2654	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	CA	2663	G
1	CA	2669	G
1	CA	2673	G
1	CA	2689	U
1	CA	2690	C
1	CA	2703	C
1	CA	2712(A)	A
1	CA	2713	A
1	CA	2718	G
1	CA	2721	A
1	CA	2726	U
1	CA	2727	G
1	CA	2733	A
1	CA	2739	U
1	CA	2744	G
1	CA	2748	A
1	CA	2751	G
1	CA	2757	A
1	CA	2758	A
1	CA	2761	G
1	CA	2764	A
1	CA	2765	A
1	CA	2766	G
1	CA	2778	A
1	CA	2793	G
1	CA	2794	C
1	CA	2802	G
1	CA	2808	U
1	CA	2818	G
1	CA	2820	A
1	CA	2821	A
1	CA	2833	G
1	CA	2835	A
1	CA	2839	G
1	CA	2872	G
1	CA	2876	G
1	CA	2880	C
1	CA	2892	A
1	CA	2893	G
1	CA	2894	G
1	CA	2896	C
1	CA	2897	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	CB	2	C
2	CB	7	G
2	CB	8	U
2	CB	12	C
2	CB	13	A
2	CB	15	A
2	CB	25	A
2	CB	28	C
2	CB	30	C
2	CB	32	C
2	CB	42	C
2	CB	52	A
2	CB	56	G
2	CB	58	A
2	CB	73	A
2	CB	85	G
2	CB	95	C
2	CB	106	G
2	CB	110	G
34	DA	5	U
34	DA	9	G
34	DA	22	G
34	DA	26	A
34	DA	32	A
34	DA	39	G
34	DA	47	C
34	DA	48	C
34	DA	50	A
34	DA	51	A
34	DA	60	A
34	DA	61	G
34	DA	65	U
34	DA	66	G
34	DA	73	G
34	DA	80	G
34	DA	88	A
34	DA	89	C
34	DA	97	G
34	DA	98	G
34	DA	101	A
34	DA	115	G
34	DA	116	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	DA	121	C
34	DA	122	G
34	DA	129(A)	G
34	DA	131	C
34	DA	144	G
34	DA	151	A
34	DA	163	C
34	DA	180	U
34	DA	182	U
34	DA	189(E)	U
34	DA	189(F)	U
34	DA	189(K)	U
34	DA	195	A
34	DA	197	A
34	DA	201	C
34	DA	203	U
34	DA	204	U
34	DA	216	G
34	DA	221	C
34	DA	231	G
34	DA	247	G
34	DA	251	G
34	DA	258	G
34	DA	266	G
34	DA	267	C
34	DA	269	C
34	DA	281	G
34	DA	289	G
34	DA	301	G
34	DA	317	G
34	DA	321	A
34	DA	328	C
34	DA	332	G
34	DA	344	A
34	DA	352	C
34	DA	353	A
34	DA	354	G
34	DA	355	C
34	DA	367	U
34	DA	372	C
34	DA	373	A
34	DA	384	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	DA	398	C
34	DA	406	G
34	DA	410	G
34	DA	412	A
34	DA	413	G
34	DA	423	G
34	DA	424	G
34	DA	429	U
34	DA	430	A
34	DA	439	A
34	DA	442	C
34	DA	452	A
34	DA	461	A
34	DA	485	G
34	DA	496	A
34	DA	498	U
34	DA	505	G
34	DA	509	A
34	DA	510	A
34	DA	511	C
34	DA	513	C
34	DA	518	C
34	DA	527	G
34	DA	531	U
34	DA	532	A
34	DA	533	A
34	DA	547	A
34	DA	559	A
34	DA	561	U
34	DA	563	A
34	DA	564	C
34	DA	571	U
34	DA	572	A
34	DA	573	A
34	DA	576	G
34	DA	577	G
34	DA	581	G
34	DA	596	C
34	DA	601	C
34	DA	607	A
34	DA	620	C
34	DA	630	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	DA	632	A
34	DA	651	C
34	DA	653	A
34	DA	654	G
34	DA	665	A
34	DA	671	G
34	DA	687	A
34	DA	688	G
34	DA	695	A
34	DA	703	G
34	DA	720	C
34	DA	723	U
34	DA	724	G
34	DA	731	G
34	DA	749	C
34	DA	753	A
34	DA	755	G
34	DA	777	A
34	DA	792	A
34	DA	793	U
34	DA	794	A
34	DA	802	A
34	DA	817	C
34	DA	819	A
34	DA	821	G
34	DA	828	A
34	DA	829	G
34	DA	833	U
34	DA	836	G
34	DA	840	C
34	DA	841	U
34	DA	848	C
34	DA	851	G
34	DA	853	G
34	DA	859	A
34	DA	874	G
34	DA	902	G
34	DA	914	A
34	DA	916	G
34	DA	922	G
34	DA	926	G
34	DA	927	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	DA	934	C
34	DA	935	A
34	DA	960	U
34	DA	961	U
34	DA	968	A
34	DA	969	A
34	DA	971	G
34	DA	972	C
34	DA	974	A
34	DA	975	A
34	DA	976	G
34	DA	977	A
34	DA	984	C
34	DA	989	C
34	DA	991	U
34	DA	992	U
34	DA	993	G
34	DA	999	C
34	DA	1002	G
34	DA	1003	G
34	DA	1005	A
34	DA	1006	C
34	DA	1017	G
34	DA	1022	G
34	DA	1023	G
34	DA	1024	G
34	DA	1025	U
34	DA	1026	G
34	DA	1027	C
34	DA	1028	C
34	DA	1030	C
34	DA	1030(A)	G
34	DA	1030(B)	C
34	DA	1030(C)	G
34	DA	1038	C
34	DA	1041	A
34	DA	1046	A
34	DA	1052	U
34	DA	1054	C
34	DA	1065	U
34	DA	1066	C
34	DA	1081	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	DA	1089	G
34	DA	1094	G
34	DA	1095	U
34	DA	1100	C
34	DA	1101	A
34	DA	1117	G
34	DA	1121	U
34	DA	1122	U
34	DA	1124	G
34	DA	1125	U
34	DA	1129	C
34	DA	1130	A
34	DA	1136	U
34	DA	1137	C
34	DA	1138	G
34	DA	1139	G
34	DA	1146	A
34	DA	1152	A
34	DA	1154	G
34	DA	1157	A
34	DA	1159	U
34	DA	1166	G
34	DA	1181	G
34	DA	1183	A
34	DA	1184	G
34	DA	1196	U
34	DA	1202	G
34	DA	1211	U
34	DA	1212	U
34	DA	1213	A
34	DA	1220	G
34	DA	1227	A
34	DA	1228	C
34	DA	1238	A
34	DA	1240	U
34	DA	1241	G
34	DA	1253	G
34	DA	1254	C
34	DA	1256	A
34	DA	1257	U
34	DA	1258	G
34	DA	1260	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	DA	1273	G
34	DA	1275	A
34	DA	1278	U
34	DA	1279	A
34	DA	1280	A
34	DA	1281	U
34	DA	1282	C
34	DA	1285	A
34	DA	1287	A
34	DA	1299	A
34	DA	1300	G
34	DA	1305	G
34	DA	1317	C
34	DA	1319	A
34	DA	1322	C
34	DA	1338	G
34	DA	1340	A
34	DA	1346	A
34	DA	1347	G
34	DA	1353	G
34	DA	1358	U
34	DA	1360	A
34	DA	1363	C
34	DA	1368	G
34	DA	1370	G
34	DA	1379	G
34	DA	1381	U
34	DA	1397	C
34	DA	1401	G
34	DA	1419	G
34	DA	1442	G
34	DA	1442(A)	G
34	DA	1442(B)	A
34	DA	1446	U
34	DA	1447	A
34	DA	1452	C
34	DA	1456	G
34	DA	1487	G
34	DA	1492	A
34	DA	1493	A
34	DA	1494	G
34	DA	1497	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	DA	1502	A
34	DA	1503	A
34	DA	1504	G
34	DA	1506	U
34	DA	1517	G
34	DA	1520	G
34	DA	1529	G
34	DA	1530	G
34	DA	1531	A
34	DA	1532	U
55	DV	24	A
56	DW	3	C
56	DW	7	A
56	DW	8	4SU
56	DW	9	A
56	DW	13	C
56	DW	14	A
56	DW	15	G
56	DW	19	G
56	DW	22	G
56	DW	23	A
56	DW	46	7MG
56	DW	47	U
56	DW	48	C
56	DW	49	C
56	DW	50	U
56	DW	61	C
56	DW	62	C
56	DW	67	C
56	DW	68	C
56	DW	70	G
56	DW	73	A
56	DW	74	C
57	DX	13	C
57	DX	18	G
57	DX	19	G
57	DX	20	U
57	DX	21	A
57	DX	22	G
57	DX	30	G
57	DX	47	U
57	DX	48	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
57	DX	59	A
57	DX	61	C
57	DX	68	C
57	DX	75	C
58	DY	9	A
58	DY	13	C
58	DY	14	A
58	DY	19	G
58	DY	21	A
58	DY	26	A
58	DY	34	G
58	DY	37	MIA
58	DY	39	PSU
58	DY	45	U
58	DY	46	7MG
58	DY	47	U
58	DY	48	C
58	DY	49	C
58	DY	54	5MU
58	DY	55	PSU
58	DY	57	G
58	DY	58	A
58	DY	59	U
58	DY	65	G
58	DY	70	G

All (127) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	AA	185	A
1	AA	188	A
1	AA	271	U
1	AA	302	A
1	AA	334	A
1	AA	572	A
1	AA	641	G
1	AA	716	G
1	AA	793	A
1	AA	811	A
1	AA	821	A
1	AA	945	A
1	AA	1019	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	AA	1098	C
1	AA	1154	U
1	AA	1188	A
1	AA	1219	A
1	AA	1220	U
1	AA	1221	G
1	AA	1255	A
1	AA	1286	U
1	AA	1321	A
1	AA	1347	A
1	AA	1425	A
1	AA	1442	U
1	AA	1466	U
1	AA	1654	A
1	AA	1655	A
1	AA	1793	A
1	AA	2014	G
1	AA	2148	A
1	AA	2203	G
1	AA	2209	G
1	AA	2320	G
1	AA	2345	A
1	AA	2418	U
1	AA	2442	A
1	AA	2451	A
1	AA	2623	U
1	AA	2701	U
1	AA	2902	G
34	BA	115	G
34	BA	243	A
34	BA	266	G
34	BA	347	G
34	BA	353	A
34	BA	509	A
34	BA	560	U
34	BA	687	A
34	BA	748	C
34	BA	793	U
34	BA	839	U
34	BA	913	A
34	BA	991	U
34	BA	1065	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	BA	1067	A
34	BA	1165	C
34	BA	1201	A
34	BA	1285	A
34	BA	1335	C
34	BA	1442	G
34	BA	1530	G
56	BW	13	C
58	BY	19	G
58	BY	58	A
1	CA	195	A
1	CA	196	A
1	CA	249	C
1	CA	271(K)	U
1	CA	271(M)	G
1	CA	277	C
1	CA	310	A
1	CA	529	A
1	CA	685	A
1	CA	752	A
1	CA	764	A
1	CA	774	A
1	CA	776	G
1	CA	856	C
1	CA	900	A
1	CA	1057	A
1	CA	1063	G
1	CA	1210	A
1	CA	1301	A
1	CA	1420	U
1	CA	1427	A
1	CA	1558	A
1	CA	1608	A
1	CA	1653	G
1	CA	1913	A
1	CA	1992	G
1	CA	1997	G
1	CA	2110	G
1	CA	2126	A
1	CA	2318	G
1	CA	2406	U
1	CA	2439	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	CA	2581	G
1	CA	2611	U
1	CA	2689	U
1	CA	2726	U
1	CA	2756	U
34	DA	60	A
34	DA	65	U
34	DA	115	G
34	DA	243	A
34	DA	266	G
34	DA	353	A
34	DA	429	U
34	DA	509	A
34	DA	532	A
34	DA	560	U
34	DA	687	A
34	DA	748	C
34	DA	793	U
34	DA	840	C
34	DA	913	A
34	DA	991	U
34	DA	992	U
34	DA	1064	G
34	DA	1065	U
34	DA	1183	A
34	DA	1201	A
34	DA	1442	G
34	DA	1492	A
56	DW	13	C
56	DW	14	A

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

40 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	$\#\|Z\|>2$
56	5MU	BW	54	56	19,22,23	1.50	4 (21%)	27,32,35	2.06	8 (29%)
56	4SU	BW	8	56	18,21,22	1.80	4 (22%)	25,30,33	2.20	5 (20%)
57	5MC	BX	32	57	19,22,23	1.37	3 (15%)	26,32,35	1.32	3 (11%)
56	PSU	DW	32	56	18,21,22	1.41	3 (16%)	21,30,33	2.00	3 (14%)
56	MIA	DW	37	56	21,24,32	1.60	4 (19%)	30,35,47	2.02	7 (23%)
56	PSU	DW	55	56	18,21,22	1.42	2 (11%)	21,30,33	1.97	3 (14%)
58	5MU	BY	54	58	19,22,23	1.52	4 (21%)	27,32,35	2.19	9 (33%)
58	5MU	DY	54	58	19,22,23	1.44	6 (31%)	27,32,35	2.07	6 (22%)
58	7MG	BY	46	58	23,26,27	1.29	4 (17%)	27,39,42	2.68	7 (25%)
58	PSU	DY	32	58	18,21,22	1.36	2 (11%)	21,30,33	1.94	3 (14%)
58	PSU	BY	32	58	18,21,22	1.40	3 (16%)	21,30,33	1.90	4 (19%)
56	4SU	DW	8	56	18,21,22	1.77	5 (27%)	25,30,33	2.21	5 (20%)
57	5MU	BX	54	60,57	19,22,23	1.54	5 (26%)	27,32,35	2.06	8 (29%)
57	4SU	BX	8	57	18,21,22	1.48	3 (16%)	25,30,33	2.27	5 (20%)
57	PSU	BX	55	57	18,21,22	1.28	2 (11%)	21,30,33	2.12	5 (23%)
56	PSU	DW	39	56	18,21,22	1.30	2 (11%)	21,30,33	1.93	3 (14%)
57	5MU	DX	54	57	19,22,23	1.43	5 (26%)	27,32,35	2.22	8 (29%)
56	7MG	BW	46	56	23,26,27	1.35	3 (13%)	27,39,42	2.59	7 (25%)
56	PSU	BW	39	56	18,21,22	1.37	3 (16%)	21,30,33	2.11	4 (19%)
57	4SU	DX	8	57	18,21,22	1.88	4 (22%)	25,30,33	2.43	4 (16%)
56	PSU	BW	32	56,60	18,21,22	1.37	2 (11%)	21,30,33	1.94	3 (14%)
56	7MG	DW	46	56	23,26,27	1.31	3 (13%)	27,39,42	2.56	7 (25%)
58	MIA	DY	37	58	21,24,32	1.58	4 (19%)	30,35,47	2.03	8 (26%)
57	31H	BX	76	60,57	31,34,35	1.39	4 (12%)	35,47,50	2.31	11 (31%)
56	F3N	DW	76	1,56	33,36,37	1.44	5 (15%)	41,51,54	1.81	10 (24%)
58	MIA	BY	37	58	21,24,32	1.67	4 (19%)	30,35,47	2.03	9 (30%)
56	5MU	DW	54	56	19,22,23	1.41	5 (26%)	27,32,35	2.02	8 (29%)
57	31H	DX	76	60,57	31,34,35	1.38	4 (12%)	35,47,50	2.31	11 (31%)
57	5MC	DX	32	57	19,22,23	1.94	2 (10%)	26,32,35	1.38	4 (15%)
57	PSU	DX	55	57	18,21,22	1.39	2 (11%)	21,30,33	1.90	4 (19%)
58	4SU	DY	8	58	18,21,22	1.84	4 (22%)	25,30,33	2.39	5 (20%)
58	PSU	BY	55	58	18,21,22	1.37	2 (11%)	21,30,33	1.95	3 (14%)
58	PSU	DY	55	58	18,21,22	1.45	2 (11%)	21,30,33	2.03	4 (19%)
56	F3N	BW	76	1,56	33,36,37	1.36	5 (15%)	41,51,54	1.74	8 (19%)
56	MIA	BW	37	56	28,31,32	2.44	6 (21%)	38,44,47	2.78	14 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
58	7MG	DY	46	58	23,26,27	1.29	3 (13%)	27,39,42	2.79	7 (25%)
58	4SU	BY	8	58	18,21,22	1.85	4 (22%)	25,30,33	2.23	5 (20%)
58	PSU	BY	39	58	18,21,22	1.37	2 (11%)	21,30,33	1.99	3 (14%)
58	PSU	DY	39	58	18,21,22	1.43	1 (5%)	21,30,33	1.99	4 (19%)
56	PSU	BW	55	56	18,21,22	1.44	3 (16%)	21,30,33	2.06	4 (19%)

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
56	5MU	BW	54	56	-	0/7/25/26	0/2/2/2
56	4SU	BW	8	56	-	0/7/25/26	0/2/2/2
57	5MC	BX	32	57	-	0/7/25/26	0/2/2/2
56	PSU	DW	32	56	-	0/7/25/26	0/2/2/2
56	MIA	DW	37	56	-	0/7/25/34	0/3/3/3
56	PSU	DW	55	56	-	0/7/25/26	0/2/2/2
58	5MU	BY	54	58	-	1/7/25/26	0/2/2/2
58	5MU	DY	54	58	-	2/7/25/26	0/2/2/2
58	7MG	BY	46	58	-	5/7/37/38	0/3/3/3
58	PSU	DY	32	58	-	0/7/25/26	0/2/2/2
58	PSU	BY	32	58	-	0/7/25/26	0/2/2/2
56	4SU	DW	8	56	-	0/7/25/26	0/2/2/2
57	5MU	BX	54	60,57	-	0/7/25/26	0/2/2/2
57	4SU	BX	8	57	-	0/7/25/26	0/2/2/2
57	PSU	BX	55	57	-	0/7/25/26	0/2/2/2
56	PSU	DW	39	56	-	0/7/25/26	0/2/2/2
57	5MU	DX	54	57	-	0/7/25/26	0/2/2/2
56	7MG	BW	46	56	-	3/7/37/38	0/3/3/3
56	PSU	BW	39	56	-	0/7/25/26	0/2/2/2
57	4SU	DX	8	57	-	0/7/25/26	0/2/2/2
56	PSU	BW	32	56,60	-	0/7/25/26	0/2/2/2
56	7MG	DW	46	56	-	2/7/37/38	0/3/3/3
58	MIA	DY	37	58	-	2/7/25/34	0/3/3/3
57	31H	BX	76	60,57	-	8/22/40/41	0/3/3/3
56	F3N	DW	76	1,56	-	0/19/37/38	0/4/4/4
58	MIA	BY	37	58	-	2/7/25/34	0/3/3/3
56	5MU	DW	54	56	-	0/7/25/26	0/2/2/2
57	31H	DX	76	60,57	-	8/22/40/41	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	5MC	DX	32	57	-	0/7/25/26	0/2/2/2
57	PSU	DX	55	57	-	1/7/25/26	0/2/2/2
58	4SU	DY	8	58	-	1/7/25/26	0/2/2/2
58	PSU	BY	55	58	-	1/7/25/26	0/2/2/2
58	PSU	DY	55	58	-	3/7/25/26	0/2/2/2
56	F3N	BW	76	1,56	-	1/19/37/38	0/4/4/4
56	MIA	BW	37	56	-	3/15/33/34	0/3/3/3
58	7MG	DY	46	58	-	3/7/37/38	0/3/3/3
58	4SU	BY	8	58	-	1/7/25/26	0/2/2/2
58	PSU	BY	39	58	-	0/7/25/26	0/2/2/2
58	PSU	DY	39	58	-	2/7/25/26	0/2/2/2
56	PSU	BW	55	56	-	0/7/25/26	0/2/2/2

All (138) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	BW	37	MIA	C2-S10	-7.77	1.69	1.75
57	DX	32	5MC	C5-C4	7.07	1.49	1.44
56	BW	37	MIA	C13-C14	7.05	1.53	1.32
58	BY	37	MIA	C5-C4	5.28	1.48	1.39
57	DX	8	4SU	C4-S4	-5.11	1.59	1.68
56	DW	37	MIA	C5-C4	5.08	1.48	1.39
58	DY	37	MIA	C5-C4	5.06	1.48	1.39
58	BY	8	4SU	C4-S4	-4.98	1.59	1.68
58	DY	8	4SU	C4-S4	-4.89	1.60	1.68
56	BW	8	4SU	C4-S4	-4.87	1.60	1.68
56	DW	8	4SU	C4-S4	-4.75	1.60	1.68
56	BW	37	MIA	C5-C4	4.70	1.47	1.39
56	DW	55	PSU	C6-C5	4.23	1.40	1.35
57	BX	8	4SU	C4-S4	-4.18	1.61	1.68
56	DW	76	F3N	CB-CG	-4.03	1.41	1.51
56	DW	32	PSU	C6-C5	4.00	1.39	1.35
57	DX	55	PSU	C6-C5	3.95	1.39	1.35
58	DY	39	PSU	C6-C5	3.93	1.39	1.35
56	DW	76	F3N	C5-N7	-3.92	1.31	1.39
58	BY	32	PSU	C6-C5	3.91	1.39	1.35
58	DY	32	PSU	C6-C5	3.87	1.39	1.35
57	BX	76	31H	C5-N7	-3.85	1.32	1.39
57	DX	76	31H	C5-N7	-3.85	1.32	1.39
56	BW	55	PSU	C6-C5	3.84	1.39	1.35
56	BW	32	PSU	C6-C5	3.82	1.39	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	BW	76	F3N	C5-N7	-3.76	1.32	1.39
58	BY	39	PSU	C6-C5	3.73	1.39	1.35
57	BX	32	5MC	C5-C4	3.72	1.46	1.44
56	BW	76	F3N	CB-CG	-3.71	1.42	1.51
58	BY	55	PSU	C6-C5	3.69	1.39	1.35
57	BX	76	31H	C5-C4	-3.65	1.32	1.39
57	DX	32	5MC	C6-C5	3.63	1.40	1.34
57	DX	76	31H	C5-C4	-3.63	1.32	1.39
56	BW	54	5MU	C4-C5	3.62	1.50	1.44
57	DX	8	4SU	C4-N3	-3.61	1.33	1.37
56	BW	39	PSU	C6-C5	3.56	1.39	1.35
58	DY	46	7MG	C5-C4	3.50	1.48	1.37
58	DY	55	PSU	C6-C5	3.48	1.39	1.35
56	BW	46	7MG	C4-N9	-3.41	1.33	1.37
58	BY	54	5MU	C2-N1	3.40	1.43	1.38
56	DW	46	7MG	C4-N9	-3.34	1.33	1.37
58	BY	46	7MG	C5-C4	3.31	1.47	1.37
56	BW	46	7MG	C5-C4	3.29	1.47	1.37
57	BX	55	PSU	C6-C5	3.26	1.38	1.35
57	BX	54	5MU	C4-C5	3.22	1.50	1.44
56	DW	46	7MG	C5-C4	3.19	1.47	1.37
57	BX	54	5MU	C6-C5	3.15	1.39	1.34
56	BW	37	MIA	C5-C6	3.14	1.49	1.41
58	BY	8	4SU	C4-N3	-3.14	1.34	1.37
56	DW	39	PSU	C6-C5	3.13	1.38	1.35
56	DW	8	4SU	C4-N3	-3.13	1.34	1.37
56	BW	8	4SU	C4-N3	-3.08	1.34	1.37
56	BW	54	5MU	C6-C5	3.04	1.39	1.34
57	BX	32	5MC	C6-C5	3.03	1.39	1.34
58	BY	54	5MU	C6-C5	3.03	1.39	1.34
57	DX	76	31H	C3'-N3'	3.01	1.50	1.45
57	BX	76	31H	C3'-N3'	3.01	1.50	1.45
57	BX	32	5MC	C6-N1	-3.00	1.32	1.38
58	BY	37	MIA	C5-C6	2.98	1.49	1.41
56	DW	54	5MU	C4-C5	2.97	1.49	1.44
58	BY	8	4SU	C5-C4	-2.97	1.39	1.42
57	DX	8	4SU	C5-C4	-2.96	1.39	1.42
58	DY	8	4SU	C4-N3	-2.94	1.34	1.37
56	DW	54	5MU	C6-C5	2.90	1.39	1.34
58	DY	8	4SU	C2-N1	2.87	1.43	1.38
58	DY	8	4SU	C5-C4	-2.82	1.39	1.42
56	DW	37	MIA	C5-C6	2.82	1.48	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	DX	8	4SU	C2-N3	-2.76	1.33	1.38
56	BW	8	4SU	C5-C4	-2.76	1.39	1.42
58	DY	55	PSU	C4-N3	-2.72	1.33	1.38
57	BX	54	5MU	C4-N3	-2.72	1.33	1.38
57	DX	76	31H	C5-C6	-2.71	1.33	1.41
57	DX	54	5MU	C4-N3	-2.71	1.33	1.38
58	DY	37	MIA	C5-C6	2.71	1.48	1.41
57	BX	76	31H	C5-C6	-2.70	1.33	1.41
58	DY	54	5MU	C6-C5	2.64	1.38	1.34
58	DY	54	5MU	C4-N3	-2.64	1.33	1.38
56	BW	55	PSU	C4-N3	-2.64	1.33	1.38
56	DW	76	F3N	C3'-N3'	2.58	1.49	1.45
58	BY	37	MIA	C8-N7	2.57	1.36	1.31
57	DX	54	5MU	C6-N1	-2.57	1.33	1.38
58	BY	46	7MG	C4-N9	-2.56	1.34	1.37
58	DY	54	5MU	C2-N1	2.53	1.42	1.38
57	DX	54	5MU	C4-C5	2.52	1.48	1.44
56	BW	32	PSU	C4-N3	-2.52	1.34	1.38
56	DW	8	4SU	C5-C4	-2.50	1.39	1.42
58	BY	54	5MU	C4-C5	2.46	1.48	1.44
58	BY	55	PSU	C4-N3	-2.45	1.34	1.38
56	DW	76	F3N	C5-C4	-2.45	1.34	1.39
56	BW	76	F3N	C2'-C3'	-2.45	1.49	1.53
58	BY	39	PSU	C4-N3	-2.44	1.34	1.38
58	BY	54	5MU	C4-N3	-2.44	1.34	1.38
58	BY	32	PSU	C4-N3	-2.43	1.34	1.38
57	DX	54	5MU	C2-N3	-2.41	1.33	1.38
56	DW	55	PSU	C4-N3	-2.41	1.34	1.38
58	DY	54	5MU	C4-C5	2.40	1.48	1.44
57	BX	55	PSU	C4-N3	-2.39	1.34	1.38
56	BW	76	F3N	C5-C4	-2.39	1.34	1.39
56	DW	76	F3N	C5-C6	-2.39	1.34	1.41
57	DX	55	PSU	C4-N3	-2.38	1.34	1.38
58	BY	8	4SU	C2-N1	2.38	1.42	1.38
56	BW	37	MIA	C8-N7	2.37	1.36	1.31
58	DY	37	MIA	C8-N7	2.36	1.36	1.31
56	DW	32	PSU	C4-N3	-2.34	1.34	1.38
57	DX	54	5MU	C6-C5	2.34	1.38	1.34
58	DY	46	7MG	C6-N1	-2.32	1.34	1.38
58	DY	32	PSU	C4-N3	-2.32	1.34	1.38
56	DW	39	PSU	C4-N3	-2.30	1.34	1.38
58	DY	37	MIA	C5-N7	-2.29	1.34	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	BX	8	4SU	C2-N3	-2.26	1.34	1.38
56	DW	8	4SU	C2-N1	2.23	1.42	1.38
56	BW	37	MIA	C4-N9	-2.23	1.33	1.37
56	DW	54	5MU	C4-N3	-2.23	1.34	1.38
56	DW	46	7MG	C6-N1	-2.22	1.34	1.38
58	BY	46	7MG	C6-N1	-2.21	1.34	1.38
58	DY	54	5MU	C6-N1	-2.20	1.34	1.38
56	BW	39	PSU	C2-N1	-2.18	1.33	1.36
57	BX	8	4SU	C4-N3	-2.18	1.35	1.37
56	DW	37	MIA	C5-N7	-2.17	1.35	1.39
57	BX	54	5MU	C6-N1	-2.16	1.34	1.38
56	BW	76	F3N	C5-C6	-2.15	1.35	1.41
56	BW	55	PSU	C2-N3	-2.14	1.33	1.37
56	DW	37	MIA	C8-N7	2.14	1.35	1.31
56	BW	8	4SU	C2-N1	2.14	1.41	1.38
56	BW	54	5MU	C4-N3	-2.13	1.34	1.38
56	BW	46	7MG	C6-N1	-2.12	1.34	1.38
58	DY	54	5MU	C2-N3	-2.10	1.34	1.38
56	DW	32	PSU	C4-C5	2.09	1.50	1.44
56	BW	54	5MU	C6-N1	-2.08	1.34	1.38
58	BY	37	MIA	C5-N7	-2.08	1.35	1.39
58	BY	32	PSU	C4-C5	2.07	1.50	1.44
57	BX	54	5MU	C2-N1	2.06	1.41	1.38
56	DW	54	5MU	C2-N1	2.06	1.41	1.38
56	BW	39	PSU	C4-C5	2.05	1.50	1.44
58	BY	46	7MG	C5-C6	2.05	1.48	1.43
56	DW	54	5MU	C6-N1	-2.02	1.34	1.38
56	DW	8	4SU	C6-C5	2.02	1.39	1.35
58	DY	46	7MG	C4-N9	-2.01	1.35	1.37

All (239) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
58	DY	46	7MG	N9-C4-N3	9.87	139.93	125.46
58	BY	46	7MG	N9-C4-N3	9.18	138.92	125.46
56	BW	37	MIA	C12-C13-C14	-9.10	110.68	127.01
56	BW	46	7MG	N9-C4-N3	8.72	138.23	125.46
56	DW	46	7MG	N9-C4-N3	8.45	137.84	125.46
57	DX	8	4SU	C4-N3-C2	-7.31	120.31	127.31
57	BX	8	4SU	C4-N3-C2	-7.14	120.47	127.31
56	BW	37	MIA	C5-C4-N3	-6.71	120.12	127.18
56	DW	8	4SU	C4-N3-C2	-6.61	120.98	127.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
58	DY	8	4SU	C4-N3-C2	-6.50	121.08	127.31
56	BW	8	4SU	C4-N3-C2	-6.49	121.09	127.31
57	DX	8	4SU	C5-C4-N3	6.42	120.72	114.75
58	BY	39	PSU	N1-C2-N3	6.29	121.81	115.17
57	BX	55	PSU	N1-C2-N3	6.24	121.75	115.17
56	BW	32	PSU	N1-C2-N3	6.22	121.73	115.17
56	DW	32	PSU	N1-C2-N3	6.20	121.71	115.17
58	BY	8	4SU	C4-N3-C2	-6.16	121.41	127.31
58	DY	55	PSU	N1-C2-N3	6.16	121.67	115.17
56	DW	55	PSU	N1-C2-N3	6.06	121.56	115.17
58	BY	55	PSU	N1-C2-N3	6.03	121.53	115.17
58	DY	37	MIA	C5-C4-N3	-5.99	118.47	126.72
58	DY	46	7MG	C5-C4-N3	-5.95	116.96	128.13
58	DY	39	PSU	N1-C2-N3	5.94	121.43	115.17
56	DW	37	MIA	C5-C4-N3	-5.93	118.55	126.72
58	DY	32	PSU	N1-C2-N3	5.93	121.42	115.17
56	BW	55	PSU	N1-C2-N3	5.91	121.41	115.17
57	BX	54	5MU	N3-C2-N1	5.90	122.58	114.89
57	DX	55	PSU	N1-C2-N3	5.85	121.34	115.17
57	BX	76	31H	O4'-C1'-N9	5.78	119.20	108.09
57	DX	76	31H	O4'-C1'-N9	5.78	119.18	108.09
56	DW	76	F3N	N1-C2-N3	-5.76	119.87	128.58
56	DW	39	PSU	N1-C2-N3	5.76	121.24	115.17
56	BW	76	F3N	N1-C2-N3	-5.75	119.87	128.58
57	BX	76	31H	N1-C2-N3	-5.69	119.97	128.58
58	BY	32	PSU	N1-C2-N3	5.67	121.15	115.17
57	DX	76	31H	N1-C2-N3	-5.67	120.00	128.58
58	BY	46	7MG	C5-C4-N3	-5.65	117.52	128.13
56	BW	46	7MG	N9-C8-N7	-5.57	95.49	103.37
56	BW	39	PSU	N1-C2-N3	5.54	121.02	115.17
58	DY	8	4SU	C5-C4-N3	5.51	119.88	114.75
58	BY	37	MIA	C5-C4-N3	-5.49	119.15	126.72
56	BW	8	4SU	C5-C4-N3	5.48	119.85	114.75
57	DX	54	5MU	C4-N3-C2	-5.41	120.25	127.34
56	DW	46	7MG	N9-C8-N7	-5.38	95.76	103.37
58	BY	8	4SU	C5-C4-N3	5.36	119.73	114.75
58	BY	46	7MG	N9-C8-N7	-5.29	95.88	103.37
58	BY	54	5MU	N3-C2-N1	5.26	121.73	114.89
56	DW	8	4SU	C5-C4-N3	5.17	119.56	114.75
56	DW	46	7MG	C5-C4-N3	-5.14	118.48	128.13
56	BW	37	MIA	N3-C4-N9	5.12	133.49	126.99
57	DX	76	31H	C5-C4-N3	-5.05	119.76	126.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	BX	76	31H	C5-C4-N3	-5.04	119.78	126.72
57	BX	8	4SU	C5-C4-N3	5.03	119.42	114.75
56	BW	46	7MG	C5-C4-N3	-4.99	118.76	128.13
58	DY	8	4SU	C5-C4-S4	-4.98	118.62	124.31
58	DY	46	7MG	N9-C8-N7	-4.96	96.36	103.37
58	DY	54	5MU	C4-N3-C2	-4.93	120.88	127.34
56	BW	54	5MU	N3-C2-N1	4.91	121.29	114.89
58	DY	54	5MU	N3-C2-N1	4.87	121.23	114.89
57	BX	54	5MU	C4-N3-C2	-4.87	120.96	127.34
56	DW	37	MIA	N3-C4-N9	4.86	135.43	127.17
56	DW	76	F3N	C5-C4-N3	-4.85	120.04	126.72
56	BW	37	MIA	C11-S10-C2	-4.83	98.62	102.25
58	BY	54	5MU	C4-N3-C2	-4.82	121.02	127.34
58	DY	37	MIA	N3-C4-N9	4.80	135.34	127.17
57	DX	54	5MU	C5-C4-N3	4.80	119.50	115.32
57	DX	54	5MU	N3-C2-N1	4.77	121.10	114.89
56	DW	54	5MU	C4-N3-C2	-4.77	121.09	127.34
56	BW	76	F3N	C5-C4-N3	-4.72	120.22	126.72
56	BW	54	5MU	C4-N3-C2	-4.67	121.22	127.34
58	BY	46	7MG	C2-N3-C4	4.62	120.25	112.30
58	DY	46	7MG	C2-N3-C4	4.60	120.22	112.30
57	BX	8	4SU	N3-C2-N1	4.57	120.84	114.89
56	DW	54	5MU	N3-C2-N1	4.55	120.81	114.89
56	BW	39	PSU	O2-C2-N1	-4.54	118.10	122.79
57	BX	55	PSU	C4-N3-C2	-4.49	120.18	126.37
58	BY	37	MIA	N3-C4-N9	4.44	134.71	127.17
56	DW	46	7MG	C2-N3-C4	4.41	119.90	112.30
56	DW	8	4SU	N3-C2-N1	4.41	120.63	114.89
58	DY	39	PSU	O2-C2-N1	-4.40	118.25	122.79
57	DX	8	4SU	N3-C2-N1	4.36	120.57	114.89
58	BY	8	4SU	C5-C4-S4	-4.33	119.36	124.31
56	BW	54	5MU	O2-C2-N1	-4.31	117.19	122.80
58	BY	54	5MU	O4-C4-C5	-4.29	120.01	124.92
56	BW	46	7MG	C2-N3-C4	4.23	119.58	112.30
56	BW	8	4SU	C5-C4-S4	-4.22	119.48	124.31
56	BW	37	MIA	C6-C5-N7	4.21	137.02	132.43
57	DX	54	5MU	C5-C6-N1	-4.20	118.75	123.31
58	DY	54	5MU	C5-C4-N3	4.20	118.97	115.32
58	DY	55	PSU	C4-N3-C2	-4.12	120.69	126.37
56	BW	39	PSU	C6-C5-C4	-4.10	115.41	118.17
56	DW	54	5MU	C5-C4-N3	4.10	118.88	115.32
57	DX	8	4SU	C5-C4-S4	-4.05	119.67	124.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	DX	55	PSU	C4-N3-C2	-4.05	120.79	126.37
56	BW	55	PSU	C4-N3-C2	-4.04	120.80	126.37
56	DW	8	4SU	C5-C4-S4	-4.02	119.72	124.31
56	BW	8	4SU	N3-C2-N1	3.99	120.08	114.89
57	DX	32	5MC	C5-C4-N3	-3.99	117.67	121.75
58	DY	8	4SU	N3-C2-N1	3.96	120.04	114.89
57	BX	32	5MC	C5-C4-N3	-3.92	117.73	121.75
58	BY	54	5MU	C5-C4-N3	3.92	118.73	115.32
57	BX	8	4SU	C5-C4-S4	-3.91	119.84	124.31
58	BY	39	PSU	C4-N3-C2	-3.91	120.98	126.37
58	BY	8	4SU	N3-C2-N1	3.90	119.97	114.89
58	DY	55	PSU	O2-C2-N1	-3.90	118.77	122.79
56	BW	37	MIA	C4-C5-N7	-3.88	106.15	110.58
57	DX	54	5MU	O4-C4-C5	-3.87	120.49	124.92
56	DW	32	PSU	C4-N3-C2	-3.87	121.04	126.37
58	DY	32	PSU	C4-N3-C2	-3.86	121.05	126.37
56	DW	39	PSU	C4-N3-C2	-3.83	121.09	126.37
58	BY	32	PSU	C4-N3-C2	-3.80	121.13	126.37
58	DY	54	5MU	O4-C4-C5	-3.80	120.57	124.92
58	BY	55	PSU	C4-N3-C2	-3.77	121.18	126.37
56	DW	37	MIA	C2-N3-C4	3.74	120.97	111.83
56	BW	55	PSU	C6-C5-C4	-3.73	115.66	118.17
58	DY	8	4SU	C1'-N1-C2	3.71	124.26	117.59
56	BW	39	PSU	C4-N3-C2	-3.71	121.26	126.37
56	DW	39	PSU	O2-C2-N1	-3.70	118.97	122.79
56	BW	37	MIA	C15-C14-C13	-3.70	111.55	122.66
58	DY	37	MIA	C2-N3-C4	3.70	120.86	111.83
57	BX	76	31H	N9-C8-N7	-3.69	108.70	113.94
56	DW	55	PSU	C4-N3-C2	-3.69	121.28	126.37
57	DX	76	31H	N9-C8-N7	-3.69	108.71	113.94
58	BY	37	MIA	C4-C5-N7	-3.68	106.38	110.58
56	BW	37	MIA	C16-C14-C13	-3.67	111.63	122.66
56	BW	32	PSU	C4-N3-C2	-3.65	121.35	126.37
58	BY	37	MIA	N3-C2-N1	-3.60	123.14	128.58
56	DW	54	5MU	O4-C4-C5	-3.58	120.82	124.92
57	DX	76	31H	C4'-O4'-C1'	-3.58	101.57	109.47
56	DW	37	MIA	N3-C2-N1	-3.57	123.17	128.58
57	BX	76	31H	C4'-O4'-C1'	-3.57	101.59	109.47
58	BY	55	PSU	O2-C2-N1	-3.55	119.13	122.79
58	DY	37	MIA	N3-C2-N1	-3.53	123.23	128.58
58	BY	39	PSU	O2-C2-N1	-3.53	119.15	122.79
58	DY	54	5MU	C5-C6-N1	-3.53	119.48	123.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	DW	32	PSU	O2-C2-N1	-3.52	119.16	122.79
58	BY	37	MIA	C2-N3-C4	3.51	120.41	111.83
58	DY	32	PSU	O2-C2-N1	-3.49	119.19	122.79
56	DW	76	F3N	C2-N3-C4	3.45	120.27	111.83
56	BW	76	F3N	C2-N3-C4	3.43	120.20	111.83
56	DW	55	PSU	O2-C2-N1	-3.42	119.26	122.79
56	BW	54	5MU	C5-C4-N3	3.39	118.27	115.32
57	DX	76	31H	C5-N7-C8	3.38	108.77	103.45
57	BX	76	31H	C5-N7-C8	3.38	108.76	103.45
58	DY	37	MIA	C4-C5-N7	-3.37	106.73	110.58
58	BY	8	4SU	C1'-N1-C2	3.36	123.63	117.59
56	BW	37	MIA	C4-N9-C8	3.35	109.25	105.74
58	DY	39	PSU	C4-N3-C2	-3.33	121.78	126.37
56	DW	76	F3N	N9-C8-N7	-3.33	109.21	113.94
57	DX	76	31H	C2-N3-C4	3.33	119.97	111.83
58	BY	54	5MU	C1'-N1-C2	3.32	123.56	117.59
57	BX	76	31H	C2-N3-C4	3.32	119.94	111.83
56	BW	54	5MU	C5-C6-N1	-3.30	119.73	123.31
56	DW	54	5MU	C5-C6-N1	-3.29	119.74	123.31
56	BW	76	F3N	N9-C8-N7	-3.28	109.28	113.94
56	DW	37	MIA	C4-C5-N7	-3.28	106.84	110.58
57	BX	55	PSU	O2-C2-N1	-3.25	119.44	122.79
57	BX	32	5MC	C5-C6-N1	-3.23	119.81	123.31
57	BX	54	5MU	O2-C2-N1	-3.23	118.60	122.80
56	BW	54	5MU	C5M-C5-C4	3.19	122.19	118.78
56	DW	54	5MU	O2-C2-N1	-3.18	118.65	122.80
57	DX	32	5MC	C5-C6-N1	-3.18	119.86	123.31
57	BX	54	5MU	C5-C4-N3	3.07	117.99	115.32
57	DX	32	5MC	O2-C2-N3	-3.03	117.56	122.33
56	BW	37	MIA	C2-N3-C4	3.02	120.21	112.29
56	DW	76	F3N	C5-N7-C8	2.98	108.14	103.45
57	BX	76	31H	CA-N-CN	-2.98	118.25	122.82
57	BX	54	5MU	C5-C6-N1	-2.95	120.11	123.31
57	DX	76	31H	CA-N-CN	-2.94	118.30	122.82
56	DW	46	7MG	C5-C6-N1	2.94	116.11	110.94
56	BW	37	MIA	C2-N1-C6	2.92	123.09	117.54
56	BW	32	PSU	O2-C2-N1	-2.92	119.78	122.79
58	BY	46	7MG	C5-C6-N1	2.87	115.99	110.94
56	BW	76	F3N	C5-N7-C8	2.85	107.94	103.45
58	BY	32	PSU	O2-C2-N1	-2.83	119.86	122.79
57	BX	55	PSU	C5-C6-N1	-2.82	118.23	122.14
58	BY	37	MIA	C5-N7-C8	2.81	107.87	103.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
58	DY	46	7MG	C5-C6-N1	2.78	115.83	110.94
56	DW	54	5MU	C5M-C5-C4	2.74	121.70	118.78
56	BW	37	MIA	C5-N7-C8	2.71	107.70	103.45
58	BY	37	MIA	C4-N9-C8	2.70	108.57	105.74
57	DX	76	31H	N3-C4-N9	2.68	131.73	127.17
56	DW	76	F3N	O4'-C4'-C3'	2.67	108.01	104.13
56	BW	46	7MG	C5-C6-N1	2.67	115.63	110.94
57	BX	76	31H	N3-C4-N9	2.66	131.70	127.17
58	BY	32	PSU	C6-C5-C4	-2.64	116.39	118.17
56	BW	46	7MG	C5-C4-N9	-2.60	103.00	106.33
58	BY	54	5MU	C5-C6-N1	-2.58	120.52	123.31
57	BX	8	4SU	O2-C2-N1	-2.58	119.44	122.80
58	DY	39	PSU	C6-C5-C4	-2.55	116.45	118.17
56	BW	76	F3N	N3-C4-N9	2.54	131.49	127.17
57	BX	32	5MC	N4-C4-N3	2.53	123.09	118.51
56	DW	76	F3N	N3-C4-N9	2.53	131.47	127.17
58	BY	54	5MU	O2-C2-N3	-2.52	116.84	121.49
58	DY	46	7MG	C5-C4-N9	-2.52	103.11	106.33
57	BX	54	5MU	C5M-C5-C4	2.52	121.47	118.78
58	DY	37	MIA	C5-N7-C8	2.50	107.38	103.45
57	DX	55	PSU	O2-C2-N1	-2.50	120.21	122.79
57	BX	76	31H	C5-C4-N9	2.48	108.52	105.81
57	DX	76	31H	C5-C4-N9	2.48	108.51	105.81
56	DW	76	F3N	C5-C4-N9	2.46	108.49	105.81
57	DX	54	5MU	C5M-C5-C4	2.45	121.40	118.78
56	BW	54	5MU	O4-C4-C5	-2.44	122.13	124.92
56	BW	55	PSU	O2-C2-N1	-2.43	120.28	122.79
56	BW	37	MIA	N9-C8-N7	-2.42	110.50	113.94
58	BY	54	5MU	C1'-N1-C6	-2.42	117.17	121.15
56	DW	37	MIA	C5-N7-C8	2.41	107.24	103.45
56	BW	54	5MU	C5M-C5-C6	-2.39	119.62	122.85
58	BY	37	MIA	C2-N1-C6	2.39	122.65	118.73
57	BX	54	5MU	C5M-C5-C6	-2.38	119.63	122.85
56	DW	37	MIA	C4-N9-C8	2.31	108.16	105.74
57	DX	54	5MU	O2-C2-N1	-2.29	119.82	122.80
56	BW	76	F3N	C5-C4-N9	2.28	108.30	105.81
56	BW	37	MIA	N3-C2-N1	-2.23	122.93	127.00
56	BW	46	7MG	O6-C6-C5	-2.22	122.16	127.62
57	DX	32	5MC	N1-C2-N3	2.20	122.62	118.80
57	DX	55	PSU	C5-C6-N1	-2.18	119.11	122.14
58	DY	46	7MG	O6-C6-C5	-2.17	122.30	127.62
58	DY	37	MIA	C4-N9-C8	2.17	108.01	105.74

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
58	BY	46	7MG	C5-C4-N9	-2.16	103.56	106.33
56	DW	8	4SU	O2-C2-N1	-2.16	119.98	122.80
56	BW	8	4SU	C1'-N1-C2	2.15	121.46	117.59
56	DW	76	F3N	C4-C5-N7	-2.14	108.13	110.58
58	DY	55	PSU	C5-C6-N1	-2.14	119.17	122.14
58	BY	46	7MG	O6-C6-C5	-2.11	122.44	127.62
56	DW	46	7MG	C5-C4-N9	-2.09	103.66	106.33
57	DX	76	31H	C4-C5-N7	-2.08	108.20	110.58
57	BX	76	31H	C4-C5-N7	-2.08	108.20	110.58
56	BW	76	F3N	C4-C5-N7	-2.08	108.20	110.58
58	BY	54	5MU	C6-N1-C2	-2.08	119.23	121.30
57	DX	54	5MU	C5M-C5-C6	-2.06	120.06	122.85
57	BX	55	PSU	O4-C4-C5	-2.06	118.88	124.01
58	DY	37	MIA	C2-N1-C6	2.06	122.12	118.73
56	DW	54	5MU	C5M-C5-C6	-2.06	120.07	122.85
56	DW	46	7MG	O6-C6-C5	-2.05	122.59	127.62
58	DY	54	5MU	C5M-C5-C4	2.04	120.96	118.78
58	BY	37	MIA	N9-C8-N7	-2.03	111.05	113.94
56	DW	76	F3N	C6-C5-C4	2.01	119.93	117.18
57	BX	54	5MU	O4-C4-C5	-2.00	122.62	124.92

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
56	BW	37	MIA	N1-C2-S10-C11
56	BW	37	MIA	N3-C2-S10-C11
56	BW	37	MIA	C12-C13-C14-C16
57	BX	76	31H	C4'-C5'-O5'-P
57	BX	76	31H	C-CA-CB-CG
57	BX	76	31H	N-CA-CB-CG
57	BX	76	31H	OCN-CN-N-CA
58	BY	46	7MG	C4'-C5'-O5'-P
57	DX	76	31H	C4'-C5'-O5'-P
57	DX	76	31H	C-CA-CB-CG
57	DX	76	31H	N-CA-CB-CG
57	DX	76	31H	OCN-CN-N-CA
58	DY	37	MIA	C3'-C4'-C5'-O5'
58	DY	39	PSU	C3'-C4'-C5'-O5'
58	DY	46	7MG	O4'-C4'-C5'-O5'
58	DY	54	5MU	O4'-C4'-C5'-O5'
58	DY	55	PSU	O4'-C1'-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
57	BX	76	31H	C3'-C4'-C5'-O5'
57	DX	76	31H	C3'-C4'-C5'-O5'
58	DY	46	7MG	C3'-C4'-C5'-O5'
57	BX	76	31H	O4'-C4'-C5'-O5'
58	BY	46	7MG	C3'-C4'-C5'-O5'
57	DX	76	31H	O4'-C4'-C5'-O5'
58	DY	37	MIA	O4'-C4'-C5'-O5'
58	DY	39	PSU	O4'-C4'-C5'-O5'
58	BY	37	MIA	C3'-C4'-C5'-O5'
58	DY	54	5MU	C3'-C4'-C5'-O5'
56	BW	46	7MG	C3'-C4'-C5'-O5'
56	BW	46	7MG	O4'-C4'-C5'-O5'
58	BY	46	7MG	C2'-C1'-N9-C8
58	BY	37	MIA	O4'-C4'-C5'-O5'
57	BX	76	31H	O-C-CA-N
57	DX	76	31H	O-C-CA-N
58	BY	46	7MG	O4'-C4'-C5'-O5'
56	DW	46	7MG	C2'-C1'-N9-C8
56	BW	46	7MG	C4'-C5'-O5'-P
58	BY	55	PSU	O4'-C1'-C5-C4
57	DX	55	PSU	O4'-C1'-C5-C4
57	BX	76	31H	N3'-C-CA-N
57	DX	76	31H	N3'-C-CA-N
58	DY	55	PSU	O4'-C4'-C5'-O5'
56	DW	46	7MG	O4'-C1'-N9-C8
58	DY	46	7MG	C2'-C1'-N9-C8
58	BY	46	7MG	O4'-C1'-N9-C8
58	DY	55	PSU	C2'-C1'-C5-C6
58	BY	8	4SU	C2'-C1'-N1-C2
58	BY	54	5MU	C2'-C1'-N1-C2
56	BW	76	F3N	C4'-C5'-O5'-P
58	DY	8	4SU	C2'-C1'-N1-C2

There are no ring outliers.

21 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	BW	8	4SU	1	0
57	BX	32	5MC	1	0
56	DW	32	PSU	1	0
56	DW	37	MIA	1	0
56	DW	55	PSU	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	BX	55	PSU	1	0
56	BW	39	PSU	1	0
57	DX	8	4SU	1	0
56	DW	46	7MG	2	0
58	DY	37	MIA	2	0
56	DW	76	F3N	4	0
56	DW	54	5MU	1	0
57	DX	76	31H	3	0
57	DX	55	PSU	1	0
58	DY	8	4SU	1	0
58	DY	55	PSU	2	0
56	BW	76	F3N	2	0
58	BY	8	4SU	1	0
58	BY	39	PSU	1	0
58	DY	39	PSU	1	0
56	BW	55	PSU	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2073 ligands modelled in this entry, 2069 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
64	GDP	BZ	702	60	29,30,30	1.29	2 (6%)	45,47,47	1.82	7 (15%)
63	SF4	BD	501	37	0,12,12	-	-	-		
64	GDP	DZ	702	60	29,30,30	1.19	3 (10%)	45,47,47	1.72	8 (17%)
63	SF4	DD	501	37	0,12,12	-	-	-		

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
64	GDP	BZ	702	60	-	0/16/32/32	0/3/3/3
64	GDP	DZ	702	60	-	2/16/32/32	0/3/3/3
63	SF4	DD	501	37	-	-	0/6/5/5
63	SF4	BD	501	37	-	-	0/6/5/5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
64	BZ	702	GDP	C5-C4	3.21	1.47	1.38
64	BZ	702	GDP	C5-N7	-3.20	1.32	1.39
64	DZ	702	GDP	C5-C4	3.07	1.47	1.38
64	DZ	702	GDP	C6-N1	-2.90	1.33	1.38
64	DZ	702	GDP	C5-N7	-2.27	1.34	1.39

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
64	BZ	702	GDP	C5-C4-N3	-6.13	118.64	128.39
64	DZ	702	GDP	C5-C4-N3	-5.78	119.18	128.39
64	BZ	702	GDP	N9-C4-N3	4.88	135.71	125.95
64	BZ	702	GDP	C2-N3-C4	4.49	120.04	112.30
64	DZ	702	GDP	N9-C4-N3	4.43	134.80	125.95
64	DZ	702	GDP	C2-N3-C4	4.41	119.90	112.30
64	DZ	702	GDP	C6-C5-N7	2.88	135.53	130.29
64	BZ	702	GDP	O6-C6-C5	-2.79	119.17	126.53
64	DZ	702	GDP	O3'-C3'-C4'	-2.44	104.06	111.08
64	BZ	702	GDP	O2A-PA-O3A	2.33	113.58	107.27
64	DZ	702	GDP	C4-C5-N7	-2.22	107.15	110.67
64	DZ	702	GDP	O4'-C1'-C2'	-2.17	101.96	106.62
64	BZ	702	GDP	C2'-C1'-N9	-2.16	107.22	113.25
64	BZ	702	GDP	O6-C6-N1	2.15	124.16	120.11
64	DZ	702	GDP	O6-C6-C5	-2.13	120.90	126.53

There are no chirality outliers.

All (2) torsion outliers are listed below:

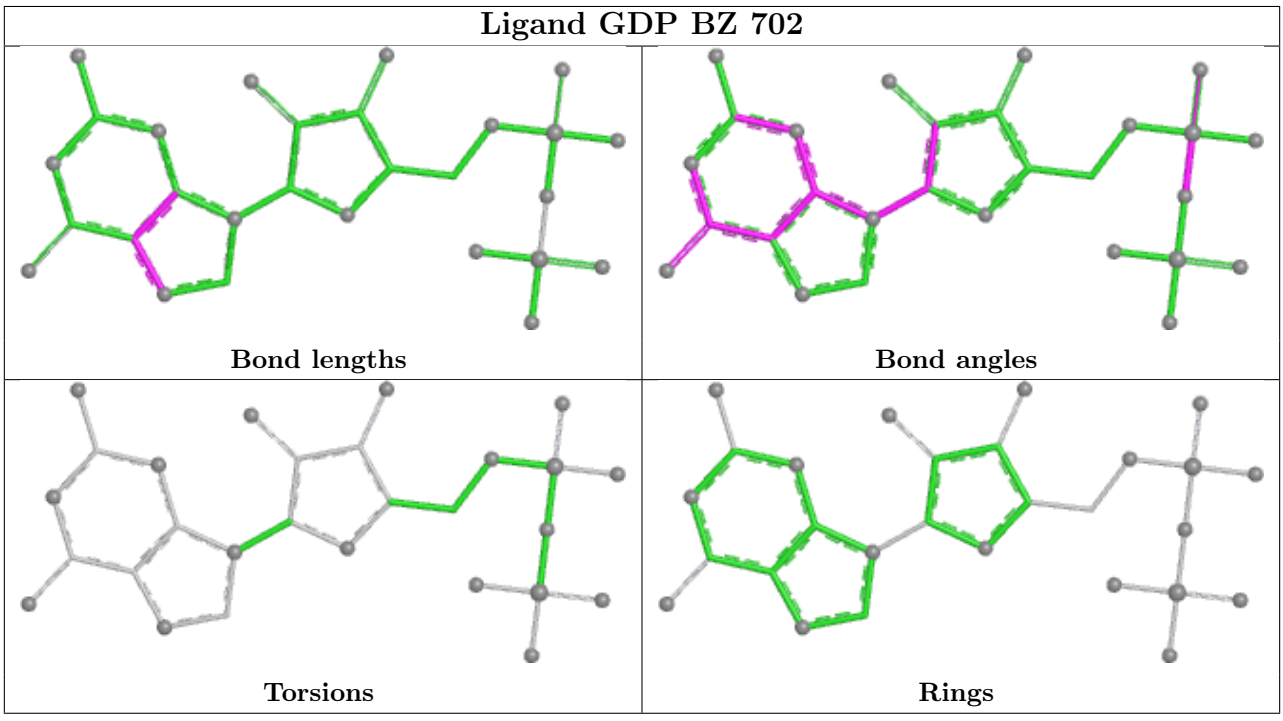
Mol	Chain	Res	Type	Atoms
64	DZ	702	GDP	PA-O3A-PB-O2B
64	DZ	702	GDP	C5'-O5'-PA-O1A

There are no ring outliers.

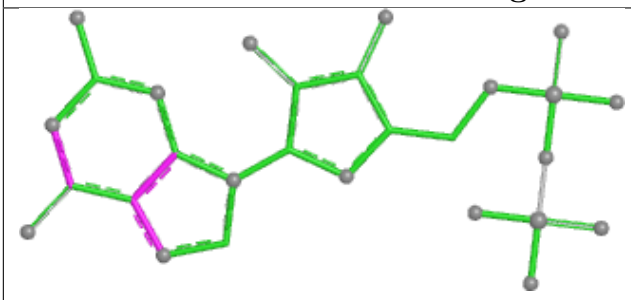
4 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
64	BZ	702	GDP	7	0
63	BD	501	SF4	1	0
64	DZ	702	GDP	7	0
63	DD	501	SF4	1	0

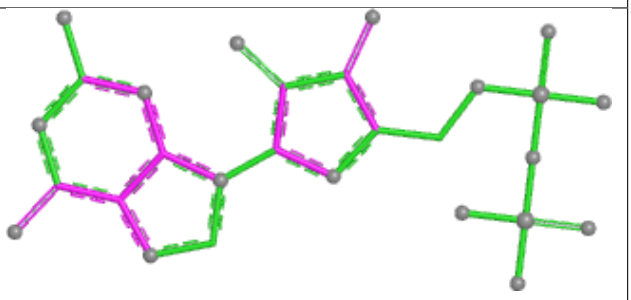
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



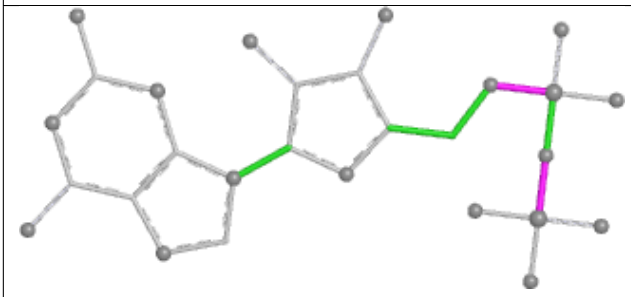
Ligand GDP DZ 702



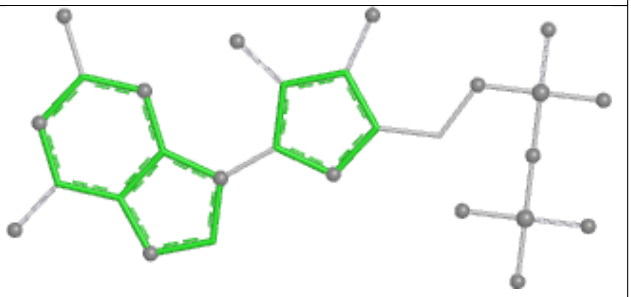
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	AA	2872/2915 (98%)	-0.78	32 (1%) 78 70	16, 35, 152, 288	0
1	CA	2868/2915 (98%)	-0.35	79 (2%) 55 45	24, 53, 186, 314	0
2	AB	120/121 (99%)	-0.55	0 100 100	26, 52, 70, 110	0
2	CB	120/121 (99%)	0.32	1 (0%) 82 75	54, 86, 109, 176	0
3	AC	137/228 (60%)	2.51	91 (66%) 0 0	95, 162, 210, 232	0
3	CC	137/228 (60%)	2.57	90 (65%) 0 0	115, 183, 225, 239	0
4	AD	275/276 (99%)	-0.53	4 (1%) 72 63	16, 35, 58, 111	0
4	CD	275/276 (99%)	-0.17	6 (2%) 62 52	18, 45, 72, 141	0
5	AE	204/206 (99%)	-0.56	0 100 100	8, 35, 66, 99	0
5	CE	204/206 (99%)	-0.14	2 (0%) 79 72	24, 52, 86, 135	0
6	AF	203/210 (96%)	-0.41	1 (0%) 87 82	11, 36, 88, 173	0
6	CF	203/210 (96%)	0.08	3 (1%) 72 63	22, 62, 112, 162	0
7	AG	181/182 (99%)	0.34	5 (2%) 55 45	41, 71, 109, 177	0
7	CG	181/182 (99%)	0.95	18 (9%) 13 9	73, 105, 142, 189	0
8	AH	174/180 (96%)	-0.09	4 (2%) 61 51	30, 51, 79, 171	0
8	CH	174/180 (96%)	0.85	12 (6%) 23 16	44, 93, 139, 208	0
9	AK	130/173 (75%)	1.86	47 (36%) 1 0	62, 123, 186, 226	0
9	CK	130/173 (75%)	2.42	77 (59%) 0 0	103, 170, 203, 226	0
10	AL	66/147 (44%)	2.03	29 (43%) 0 0	133, 179, 216, 233	0
10	CL	66/147 (44%)	2.47	41 (62%) 0 0	115, 192, 239, 248	0
11	AN	140/140 (100%)	-0.51	2 (1%) 73 64	17, 34, 76, 106	0
11	CN	140/140 (100%)	0.13	4 (2%) 53 43	32, 59, 96, 139	0
12	AO	122/122 (100%)	-0.44	0 100 100	20, 39, 65, 93	0
12	CO	122/122 (100%)	-0.15	0 100 100	32, 51, 82, 100	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	AP	149/150 (99%)	-0.32	1 (0%) 84 77	14, 43, 81, 123	0
13	CP	149/150 (99%)	0.26	4 (2%) 56 46	29, 65, 111, 154	0
14	AQ	141/141 (100%)	-0.29	0 100 100	16, 39, 66, 96	0
14	CQ	141/141 (100%)	0.29	5 (3%) 47 38	32, 61, 91, 155	0
15	AR	118/118 (100%)	-0.64	0 100 100	17, 32, 55, 95	0
15	CR	118/118 (100%)	-0.02	1 (0%) 82 75	27, 51, 76, 96	0
16	AS	110/112 (98%)	-0.13	1 (0%) 81 74	32, 53, 79, 101	0
16	CS	110/112 (98%)	0.88	9 (8%) 17 13	52, 82, 110, 143	0
17	AT	131/146 (89%)	-0.07	6 (4%) 37 29	23, 43, 93, 159	0
17	CT	131/146 (89%)	0.11	4 (3%) 51 41	36, 57, 98, 155	0
18	AU	116/118 (98%)	-0.73	1 (0%) 81 74	15, 27, 46, 110	0
18	CU	116/118 (98%)	0.07	2 (1%) 69 60	35, 51, 81, 123	0
19	AV	101/101 (100%)	-0.73	1 (0%) 79 72	18, 34, 60, 117	0
19	CV	101/101 (100%)	0.19	3 (2%) 52 42	32, 72, 106, 137	0
20	AW	112/113 (99%)	-0.61	1 (0%) 81 74	15, 29, 55, 133	0
20	CW	112/113 (99%)	-0.11	2 (1%) 67 58	26, 47, 85, 148	0
21	AX	95/96 (98%)	-0.36	2 (2%) 63 54	22, 38, 68, 123	0
21	CX	95/96 (98%)	0.34	4 (4%) 40 32	39, 60, 92, 134	0
22	AY	107/110 (97%)	-0.06	3 (2%) 55 45	25, 47, 92, 125	0
22	CY	107/110 (97%)	0.76	11 (10%) 12 9	43, 78, 113, 169	0
23	AZ	171/206 (83%)	0.57	22 (12%) 7 6	32, 72, 142, 228	0
23	CZ	174/206 (84%)	1.15	22 (12%) 8 6	59, 106, 172, 238	0
24	A0	83/85 (97%)	-0.24	4 (4%) 35 28	16, 38, 66, 145	0
24	C0	83/85 (97%)	0.55	7 (8%) 17 12	36, 62, 94, 133	0
25	A1	97/98 (98%)	-0.17	2 (2%) 63 54	23, 43, 83, 106	0
25	C1	97/98 (98%)	0.22	3 (3%) 51 41	32, 52, 104, 118	0
26	A2	70/72 (97%)	0.06	4 (5%) 29 22	21, 46, 74, 148	0
26	C2	70/72 (97%)	0.64	4 (5%) 29 22	51, 77, 98, 119	0
27	A3	59/60 (98%)	-0.29	1 (1%) 69 60	17, 33, 62, 112	0
27	C3	59/60 (98%)	0.33	2 (3%) 48 39	42, 61, 105, 167	0
28	A4	69/71 (97%)	0.77	9 (13%) 7 6	59, 99, 181, 193	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
28	C4	69/71 (97%)	1.42	16 (23%) 2 1	87, 137, 192, 210	0
29	A5	59/60 (98%)	-0.76	0 100 100	14, 29, 52, 82	0
29	C5	59/60 (98%)	-0.29	0 100 100	28, 46, 76, 111	0
30	A6	53/54 (98%)	-0.31	1 (1%) 66 57	24, 41, 65, 88	0
30	C6	53/54 (98%)	0.24	1 (1%) 66 57	42, 61, 86, 102	0
31	A7	48/49 (97%)	-0.42	3 (6%) 26 19	13, 25, 62, 124	0
31	C7	48/49 (97%)	0.03	5 (10%) 11 8	25, 37, 80, 105	0
32	A8	64/65 (98%)	-0.49	1 (1%) 70 61	17, 31, 46, 68	0
32	C8	64/65 (98%)	0.06	3 (4%) 36 29	35, 51, 69, 100	0
33	A9	37/37 (100%)	-0.24	1 (2%) 56 46	23, 38, 58, 77	0
33	C9	37/37 (100%)	0.46	3 (8%) 18 13	41, 65, 95, 107	0
34	BA	1497/1521 (98%)	0.12	29 (1%) 66 57	31, 74, 166, 297	0
34	DA	1503/1521 (98%)	0.29	49 (3%) 49 39	39, 82, 173, 313	0
35	BB	231/256 (90%)	1.16	35 (15%) 5 4	61, 108, 165, 196	0
35	DB	231/256 (90%)	1.37	50 (21%) 2 2	77, 128, 182, 226	0
36	BC	206/239 (86%)	1.01	26 (12%) 8 6	59, 102, 137, 192	0
36	DC	206/239 (86%)	1.43	45 (21%) 2 2	77, 125, 169, 191	0
37	BD	208/209 (99%)	0.99	26 (12%) 8 6	50, 81, 119, 168	0
37	DD	208/209 (99%)	0.79	12 (5%) 29 22	46, 79, 111, 161	0
38	BE	148/162 (91%)	0.42	3 (2%) 65 56	47, 72, 109, 140	0
38	DE	148/162 (91%)	0.84	11 (7%) 20 15	45, 88, 128, 150	0
39	BF	100/101 (99%)	0.48	1 (1%) 79 72	45, 79, 116, 136	0
39	DF	100/101 (99%)	0.36	1 (1%) 79 72	48, 79, 103, 120	0
40	BG	155/156 (99%)	0.71	12 (7%) 19 14	57, 88, 131, 172	0
40	DG	155/156 (99%)	0.96	21 (13%) 7 5	66, 102, 142, 188	0
41	BH	137/138 (99%)	0.58	3 (2%) 62 52	44, 75, 105, 134	0
41	DH	137/138 (99%)	1.01	18 (13%) 7 6	54, 88, 126, 168	0
42	BI	127/128 (99%)	1.36	23 (18%) 3 3	50, 101, 139, 163	0
42	DI	127/128 (99%)	1.89	55 (43%) 0 0	65, 117, 158, 198	0
43	BJ	97/105 (92%)	1.73	32 (32%) 1 1	52, 112, 158, 196	0
43	DJ	96/105 (91%)	1.96	40 (41%) 0 0	68, 134, 177, 188	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
44	BK	114/129 (88%)	0.30	5 (4%) 39 31	44, 71, 112, 128	0
44	DK	114/129 (88%)	0.46	9 (7%) 18 13	43, 80, 117, 139	0
45	BL	122/132 (92%)	0.29	4 (3%) 49 39	37, 62, 86, 113	0
45	DL	122/132 (92%)	0.64	9 (7%) 20 15	36, 72, 94, 141	0
46	BM	123/126 (97%)	1.13	12 (9%) 13 9	54, 94, 127, 213	0
46	DM	122/126 (96%)	1.68	35 (28%) 1 1	71, 124, 152, 187	0
47	BN	60/61 (98%)	1.50	15 (25%) 2 1	64, 94, 121, 137	0
47	DN	60/61 (98%)	2.64	43 (71%) 0 0	84, 121, 166, 201	0
48	BO	88/89 (98%)	0.43	4 (4%) 38 30	38, 67, 110, 141	0
48	DO	88/89 (98%)	0.57	3 (3%) 48 39	43, 76, 111, 127	0
49	BP	82/88 (93%)	0.95	8 (9%) 13 9	53, 75, 108, 131	0
49	DP	82/88 (93%)	0.59	3 (3%) 45 36	52, 70, 95, 129	0
50	BQ	99/105 (94%)	0.48	4 (4%) 42 33	42, 69, 96, 110	0
50	DQ	99/105 (94%)	0.57	6 (6%) 27 20	50, 74, 103, 123	0
51	BR	68/88 (77%)	0.39	0 100 100	47, 72, 111, 132	0
51	DR	68/88 (77%)	0.55	2 (2%) 53 43	45, 78, 114, 133	0
52	BS	84/93 (90%)	1.54	24 (28%) 1 1	64, 109, 161, 176	0
52	DS	83/93 (89%)	2.07	37 (44%) 0 0	89, 140, 184, 227	0
53	BT	96/106 (90%)	0.88	14 (14%) 6 4	52, 76, 114, 167	0
53	DT	96/106 (90%)	0.81	10 (10%) 11 8	51, 76, 116, 132	0
54	BU	23/27 (85%)	1.44	7 (30%) 1 1	56, 88, 104, 114	0
54	DU	23/27 (85%)	2.11	11 (47%) 0 0	78, 108, 129, 141	0
55	BV	13/24 (54%)	1.50	6 (46%) 0 0	48, 85, 170, 176	0
55	DV	12/24 (50%)	1.96	5 (41%) 0 0	62, 119, 169, 197	0
56	BW	66/76 (86%)	1.02	7 (10%) 11 8	62, 166, 228, 253	0
56	DW	64/76 (84%)	1.22	7 (10%) 10 8	90, 194, 235, 259	0
57	BX	71/77 (92%)	0.12	1 (1%) 73 64	33, 76, 123, 186	0
57	DX	71/77 (92%)	0.39	2 (2%) 55 45	33, 99, 147, 161	0
58	BY	67/76 (88%)	0.79	8 (11%) 9 7	38, 157, 221, 262	0
58	DY	66/76 (86%)	0.91	9 (13%) 7 5	56, 177, 227, 250	0
59	BZ	728/758 (96%)	1.04	99 (13%) 7 5	40, 106, 190, 249	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
59	DZ	730/758 (96%)	1.09	123 (16%) 4 3	37, 114, 209, 242	0
All	All	22848/24064 (94%)	0.24	1747 (7%) 20 14	8, 67, 175, 314	0

All (1747) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
46	BM	124	PRO	14.9
46	BM	123	ALA	9.3
47	DN	2	ALA	8.4
46	DM	122	LYS	8.3
46	DM	123	ALA	7.6
46	DM	124	PRO	7.5
9	CK	84	GLU	7.2
22	CY	1	MET	7.1
53	BT	9	ASN	7.0
46	BM	122	LYS	6.8
45	DL	18	VAL	6.8
36	BC	2	GLY	6.5
25	C1	2	SER	6.5
52	DS	35	SER	6.5
52	DS	9	VAL	6.4
3	AC	175	PRO	6.4
26	A2	70	GLN	6.4
43	BJ	46	ARG	6.3
59	BZ	502	GLY	6.3
46	DM	121	LYS	6.2
47	BN	2	ALA	6.1
23	CZ	114	GLY	6.1
9	CK	96	PHE	6.0
42	DI	106	ALA	6.0
40	DG	83	ALA	6.0
46	DM	98	VAL	6.0
59	DZ	683	VAL	6.0
55	DV	13	A	5.9
43	DJ	47	PHE	5.8
59	DZ	419	ALA	5.8
47	DN	38	GLY	5.7
24	A0	3	HIS	5.7
9	CK	25	PHE	5.7
42	DI	42	ARG	5.7
3	AC	59	VAL	5.6
42	BI	14	VAL	5.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
8	AH	2	SER	5.5
1	CA	1087	G	5.5
28	C4	66	SER	5.5
9	CK	53	VAL	5.3
9	CK	40	LEU	5.3
22	AY	1	MET	5.2
9	AK	48	GLY	5.2
9	CK	99	SER	5.2
31	C7	48	LYS	5.2
31	A7	47	ARG	5.2
3	CC	175	PRO	5.2
47	DN	13	THR	5.1
4	AD	275	LYS	5.1
59	DZ	429	ALA	5.1
10	CL	138	VAL	5.1
3	CC	33	LEU	5.1
42	BI	106	ALA	5.1
59	DZ	426	GLN	5.1
9	AK	90	ALA	5.1
25	A1	2	SER	5.0
10	CL	127	ILE	5.0
3	AC	69	LEU	5.0
54	DU	4	GLY	5.0
59	DZ	424	LEU	4.9
42	DI	10	ARG	4.9
10	AL	135	GLY	4.9
38	DE	22	GLY	4.9
59	DZ	422	GLU	4.9
9	AK	49	ALA	4.9
45	BL	18	VAL	4.9
42	BI	64	THR	4.9
1	CA	1536	C	4.8
46	DM	118	ALA	4.8
27	C3	2	PRO	4.8
59	DZ	428	LEU	4.8
36	BC	190	ARG	4.8
42	BI	12	GLU	4.8
3	CC	174	ALA	4.8
43	DJ	32	ALA	4.7
16	CS	3	ARG	4.7
42	DI	108	VAL	4.7
24	C0	3	HIS	4.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
52	DS	71	LEU	4.7
3	CC	44	VAL	4.7
1	AA	34	C	4.7
3	CC	221	PRO	4.7
42	BI	2	GLU	4.7
59	BZ	472	VAL	4.7
4	CD	276	LYS	4.7
53	BT	69	GLY	4.7
3	CC	162	ILE	4.7
42	DI	11	LYS	4.6
14	CQ	61	GLY	4.6
10	CL	136	VAL	4.6
54	DU	6	ARG	4.6
23	AZ	144	LEU	4.6
17	CT	130	ALA	4.6
3	CC	59	VAL	4.6
10	AL	120	LEU	4.6
17	AT	130	ALA	4.6
37	DD	23	GLY	4.6
56	BW	1	G	4.6
9	CK	7	VAL	4.6
25	C1	26	ARG	4.5
35	DB	99	GLY	4.5
41	DH	99	GLU	4.5
59	BZ	424	LEU	4.5
4	CD	262	ARG	4.5
46	DM	102	ARG	4.5
9	CK	86	PRO	4.5
8	AH	174	GLY	4.5
52	DS	12	ASP	4.5
10	CL	78	ILE	4.5
3	AC	52	PRO	4.5
47	DN	17	LYS	4.5
3	AC	179	ALA	4.5
42	DI	105	ASP	4.5
59	DZ	160	ARG	4.5
10	CL	126	MET	4.4
1	CA	34	C	4.4
47	DN	6	LEU	4.4
47	DN	39	LEU	4.4
1	CA	1091	G	4.4
4	AD	276	LYS	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
9	CK	89	ALA	4.4
47	DN	10	ALA	4.4
59	BZ	501	THR	4.4
13	CP	76	LYS	4.4
47	DN	15	LYS	4.4
9	AK	51	LEU	4.3
1	CA	1026	U	4.3
3	CC	179	ALA	4.3
59	DZ	593	ALA	4.3
36	DC	188	LEU	4.3
46	BM	121	LYS	4.3
3	CC	190	ILE	4.3
52	DS	75	ALA	4.3
17	AT	131	ALA	4.2
35	DB	170	GLU	4.2
1	CA	1090	U	4.2
40	BG	80	VAL	4.2
59	BZ	481	VAL	4.2
3	AC	159	ALA	4.2
3	CC	12	LEU	4.2
1	CA	1171	G	4.2
43	DJ	76	ASN	4.2
9	AK	53	VAL	4.2
7	AG	50	ALA	4.2
9	CK	85	ASP	4.2
52	BS	13	ASP	4.2
3	AC	48	LEU	4.1
3	CC	15	VAL	4.1
3	CC	176	VAL	4.1
28	C4	56	VAL	4.1
35	DB	187	LEU	4.1
40	BG	83	ALA	4.1
59	BZ	419	ALA	4.1
55	DV	24	A	4.1
10	AL	78	ILE	4.1
9	AK	35	LYS	4.1
37	DD	154	ASN	4.1
47	DN	25	VAL	4.1
9	AK	89	ALA	4.1
59	DZ	688	ILE	4.1
56	BW	73	A	4.1
3	AC	211	ARG	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
9	CK	56	ASN	4.1
35	BB	7	VAL	4.1
52	BS	85	LYS	4.1
55	BV	24	A	4.1
47	DN	33	VAL	4.1
23	AZ	146	ILE	4.1
59	DZ	420	ASP	4.0
7	CG	84	LYS	4.0
54	DU	16	GLY	4.0
3	CC	186	LEU	4.0
43	BJ	77	PRO	4.0
59	DZ	415	PRO	4.0
1	AA	2138	G	4.0
9	CK	28	ASN	4.0
9	AK	83	TYR	4.0
44	DK	25	TYR	4.0
9	CK	57	THR	4.0
35	BB	133	LYS	4.0
3	AC	166	ASN	4.0
37	BD	154	ASN	4.0
4	CD	275	LYS	4.0
9	AK	38	HIS	4.0
3	AC	17	PRO	4.0
59	DZ	680	PRO	4.0
23	AZ	113	ALA	4.0
59	DZ	102	ASP	4.0
24	C0	8	GLY	4.0
36	DC	196	LEU	4.0
3	CC	217	THR	4.0
3	CC	10	ALA	3.9
9	CK	43	ALA	3.9
40	DG	16	LEU	3.9
52	DS	16	LEU	3.9
3	CC	194	ILE	3.9
46	DM	78	ILE	3.9
52	BS	71	LEU	3.9
3	AC	30	VAL	3.9
52	BS	9	VAL	3.9
3	AC	197	LEU	3.9
35	DB	152	PHE	3.9
40	BG	8	GLU	3.9
3	AC	221	PRO	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
48	DO	3	ILE	3.9
38	BE	85	GLY	3.9
3	CC	14	LYS	3.9
59	DZ	212	TYR	3.9
36	DC	189	ALA	3.9
59	DZ	425	SER	3.9
3	AC	49	GLY	3.8
54	BU	16	GLY	3.8
3	CC	210	LEU	3.8
3	AC	57	GLN	3.8
27	A3	2	PRO	3.8
47	DN	31	ARG	3.8
1	CA	2319	G	3.8
22	CY	4	LYS	3.8
3	AC	210	LEU	3.8
10	CL	115	LEU	3.8
43	DJ	65	LEU	3.8
3	CC	30	VAL	3.8
35	DB	136	VAL	3.8
46	DM	88	ARG	3.8
10	CL	130	SER	3.8
44	DK	14	VAL	3.8
59	DZ	227	ILE	3.8
47	DN	32	SER	3.8
3	CC	223	VAL	3.8
59	DZ	594	VAL	3.8
28	C4	65	ASP	3.8
58	DY	34	G	3.8
34	BA	1447	A	3.8
35	BB	12	GLU	3.7
3	AC	168	LYS	3.7
3	CC	4	HIS	3.7
34	DA	1054	C	3.7
35	DB	196	LEU	3.7
40	BG	85	TYR	3.7
59	BZ	91	THR	3.7
9	AK	50	ARG	3.7
3	CC	42	VAL	3.7
3	CC	215	VAL	3.7
35	BB	136	VAL	3.7
3	AC	33	LEU	3.7
47	BN	59	ALA	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
59	DZ	39	ILE	3.7
59	DZ	530	VAL	3.7
36	DC	162	GLN	3.7
3	AC	12	LEU	3.7
10	CL	101	TRP	3.7
3	CC	8	TYR	3.7
35	DB	148	TYR	3.7
52	DS	10	PHE	3.7
59	DZ	268	GLY	3.7
35	DB	21	ARG	3.7
42	DI	128	ARG	3.7
1	AA	2147	G	3.7
59	DZ	421	GLN	3.7
9	AK	88	ALA	3.7
43	BJ	76	ASN	3.7
43	DJ	63	PHE	3.7
9	AK	81	VAL	3.7
59	DZ	404	VAL	3.7
38	DE	21	ALA	3.6
58	BY	34	G	3.6
31	A7	48	LYS	3.6
59	BZ	156	ARG	3.6
52	DS	39	THR	3.6
3	AC	11	LEU	3.6
42	DI	117	HIS	3.6
44	DK	13	GLN	3.6
9	AK	54	ALA	3.6
42	DI	126	SER	3.6
9	CK	55	LYS	3.6
43	DJ	46	ARG	3.6
48	BO	88	ARG	3.6
52	DS	37	ARG	3.6
42	BI	8	GLY	3.6
42	BI	67	GLY	3.6
43	DJ	10	GLY	3.6
42	DI	14	VAL	3.6
59	BZ	242	LEU	3.6
59	BZ	415	PRO	3.6
3	AC	174	ALA	3.6
10	CL	123	ALA	3.6
9	AK	99	SER	3.6
21	CX	68	ARG	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	CC	5	GLY	3.6
52	BS	84	GLY	3.6
1	CA	1095	A	3.6
3	AC	162	ILE	3.6
3	CC	172	ILE	3.6
35	DB	97	TRP	3.6
7	CG	146	TYR	3.6
42	BI	19	LEU	3.6
23	CZ	109	ALA	3.6
36	DC	159	GLY	3.6
36	DC	39	ILE	3.6
40	DG	80	VAL	3.6
10	CL	128	ALA	3.5
1	CA	1078	U	3.5
40	BG	4	ARG	3.5
3	CC	164	PHE	3.5
9	CK	24	PHE	3.5
59	BZ	103	GLY	3.5
10	AL	136	VAL	3.5
35	DB	12	GLU	3.5
59	BZ	463	VAL	3.5
9	CK	111	LEU	3.5
9	AK	6	ASN	3.5
42	DI	7	THR	3.5
43	BJ	100	THR	3.5
9	CK	97	ALA	3.5
35	DB	214	ILE	3.5
59	DZ	601	ILE	3.5
10	CL	137	GLU	3.5
1	CA	1089	G	3.5
58	BY	18	G	3.5
9	CK	29	TYR	3.5
9	CK	6	ASN	3.5
59	DZ	417	THR	3.5
59	DZ	488	THR	3.5
34	DA	1030(B)	C	3.5
34	DA	1531	A	3.5
59	DZ	90	PHE	3.5
59	DZ	629	GLY	3.5
3	CC	20	VAL	3.5
47	DN	34	TYR	3.5
9	CK	100	ASN	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	AC	192	ALA	3.5
37	DD	167	GLY	3.5
55	BV	12	A	3.5
59	BZ	372	GLY	3.5
9	CK	81	VAL	3.5
43	BJ	72	VAL	3.5
59	BZ	422	GLU	3.5
59	DZ	662	LYS	3.5
10	CL	131	ALA	3.5
35	BB	188	ALA	3.5
40	DG	2	ALA	3.5
44	BK	89	ALA	3.5
59	DZ	432	ALA	3.5
42	DI	102	LEU	3.4
3	CC	222	SER	3.4
28	C4	63	TYR	3.4
42	DI	103	THR	3.4
46	BM	2	ALA	3.4
35	DB	95	GLN	3.4
3	AC	71	LYS	3.4
10	CL	135	GLY	3.4
7	CG	53	LEU	3.4
9	CK	44	LEU	3.4
35	DB	165	VAL	3.4
43	DJ	8	LEU	3.4
43	DJ	71	LEU	3.4
23	AZ	112	ARG	3.4
1	AA	12	U	3.4
1	CA	1086	A	3.4
10	AL	75	SER	3.4
3	CC	187	ALA	3.4
3	CC	208	THR	3.4
3	CC	216	THR	3.4
9	AK	130	THR	3.4
9	AK	52	PHE	3.4
10	AL	138	VAL	3.4
40	DG	82	GLY	3.4
47	DN	35	ARG	3.4
43	DJ	37	PRO	3.4
3	AC	190	ILE	3.4
9	CK	42	GLN	3.4
9	CK	106	GLN	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
49	BP	68	ASP	3.4
43	DJ	34	VAL	3.4
59	DZ	158	GLY	3.4
31	C7	47	ARG	3.4
42	DI	12	GLU	3.4
3	CC	27	ALA	3.4
3	AC	172	ILE	3.4
59	DZ	630	GLN	3.4
55	DV	14	A	3.4
9	CK	80	VAL	3.3
34	DA	1224	G	3.3
37	BD	180	GLY	3.3
40	BG	82	GLY	3.3
3	CC	9	ARG	3.3
59	BZ	160	ARG	3.3
59	DZ	614	GLU	3.3
46	DM	92	HIS	3.3
59	DZ	656	ALA	3.3
3	AC	44	VAL	3.3
52	DS	13	ASP	3.3
59	BZ	231	TYR	3.3
46	DM	6	GLY	3.3
46	DM	119	GLY	3.3
3	AC	43	GLU	3.3
3	AC	203	GLU	3.3
46	DM	120	LYS	3.3
36	DC	182	ILE	3.3
3	CC	11	LEU	3.3
42	DI	124	GLN	3.3
59	DZ	431	LEU	3.3
9	AK	7	VAL	3.3
9	AK	23	SER	3.3
36	DC	171	GLY	3.3
37	DD	87	GLY	3.3
59	BZ	86	GLY	3.3
59	DZ	502	GLY	3.3
9	CK	33	PRO	3.3
55	BV	13	A	3.3
58	DY	35	A	3.3
45	DL	126	LYS	3.3
3	AC	219	MET	3.3
34	DA	1320	C	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
9	CK	11	ALA	3.3
9	CK	39	ALA	3.3
59	DZ	631	ILE	3.3
1	CA	1107	G	3.3
3	CC	48	LEU	3.3
3	CC	197	LEU	3.3
59	BZ	428	LEU	3.3
9	AK	30	GLN	3.3
23	AZ	118	GLN	3.3
3	AC	218	THR	3.3
10	CL	118	THR	3.3
42	DI	27	THR	3.3
9	AK	78	SER	3.3
35	BB	97	TRP	3.3
9	CK	127	GLU	3.3
59	BZ	129	LYS	3.3
10	CL	84	LEU	3.3
37	BD	132	ARG	3.3
46	BM	102	ARG	3.3
34	BA	630	G	3.3
34	DA	1202	G	3.3
27	C3	60	GLU	3.2
34	BA	343	U	3.2
59	DZ	433	GLU	3.2
59	DZ	623	ASP	3.2
3	CC	17	PRO	3.2
10	AL	127	ILE	3.2
3	AC	171	ALA	3.2
36	DC	168	ALA	3.2
23	AZ	117	LEU	3.2
23	CZ	117	LEU	3.2
53	DT	10	LEU	3.2
9	AK	82	PHE	3.2
59	BZ	594	VAL	3.2
52	BS	68	GLY	3.2
54	DU	14	TRP	3.2
46	BM	87	TYR	3.2
1	CA	1106	G	3.2
53	DT	9	ASN	3.2
10	AL	131	ALA	3.2
10	CL	81	ALA	3.2
59	BZ	457	LEU	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
24	C0	44	ARG	3.2
3	CC	209	PHE	3.2
36	DC	195	VAL	3.2
58	BY	35	A	3.2
3	CC	177	GLY	3.2
10	CL	94	GLU	3.2
37	BD	163	GLU	3.2
9	CK	78	SER	3.2
9	CK	83	TYR	3.2
9	CK	116	ILE	3.2
42	BI	75	ASP	3.2
59	BZ	92	ILE	3.2
1	AA	1072	U	3.2
43	BJ	40	LEU	3.2
37	BD	153	ARG	3.2
3	AC	176	VAL	3.2
10	CL	96	VAL	3.2
36	DC	207	VAL	3.2
59	DZ	88	VAL	3.2
23	AZ	114	GLY	3.2
9	AK	131	MET	3.2
3	CC	21	TYR	3.2
3	AC	167	ASP	3.2
4	AD	262	ARG	3.2
54	DU	15	ARG	3.2
3	AC	4	HIS	3.2
34	DA	1532	U	3.2
59	DZ	640	ALA	3.2
10	AL	96	VAL	3.2
35	DB	7	VAL	3.2
47	DN	4	LYS	3.2
1	AA	299	G	3.2
3	AC	225	ILE	3.2
38	DE	52	PRO	3.2
47	DN	61	TRP	3.2
59	DZ	487	ILE	3.2
10	CL	76	TYR	3.1
10	CL	105	LEU	3.1
31	C7	23	ARG	3.1
59	BZ	602	LEU	3.1
4	CD	2	ALA	3.1
42	BI	46	ALA	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
59	BZ	435	ASP	3.1
42	DI	101	PHE	3.1
59	BZ	423	LYS	3.1
1	CA	1065	U	3.1
28	A4	50	VAL	3.1
42	DI	109	VAL	3.1
46	BM	24	GLY	3.1
53	BT	102	GLY	3.1
59	DZ	617	MET	3.1
3	AC	216	THR	3.1
59	DZ	486	THR	3.1
21	AX	68	ARG	3.1
43	BJ	85	LEU	3.1
56	DW	15	G	3.1
35	BB	148	TYR	3.1
44	DK	75	TYR	3.1
52	DS	32	LYS	3.1
53	BT	74	LYS	3.1
59	DZ	626	ALA	3.1
55	DV	15	A	3.1
59	DZ	87	HIS	3.1
59	DZ	653	PHE	3.1
9	AK	87	VAL	3.1
59	DZ	472	VAL	3.1
10	AL	134	MET	3.1
59	BZ	684	GLN	3.1
10	AL	77	LEU	3.1
36	DC	12	LEU	3.1
41	DH	2	LEU	3.1
42	DI	125	TYR	3.1
52	DS	14	HIS	3.1
9	AK	85	ASP	3.1
35	BB	229	VAL	3.1
59	DZ	634	MET	3.1
10	CL	129	GLY	3.1
42	DI	30	GLY	3.1
59	BZ	193	GLY	3.1
38	BE	81	GLU	3.1
3	CC	41	THR	3.1
9	CK	37	THR	3.1
37	BD	49	ARG	3.1
42	DI	111	ARG	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
43	DJ	85	LEU	3.1
9	CK	49	ALA	3.1
40	DG	7	ALA	3.1
59	BZ	429	ALA	3.1
59	DZ	463	VAL	3.1
36	DC	155	GLY	3.1
36	DC	194	GLY	3.1
43	DJ	31	GLY	3.1
1	CA	1085	A	3.1
1	CA	2116	G	3.1
23	AZ	2	GLU	3.1
47	DN	46	GLU	3.1
3	AC	37	LYS	3.1
3	AC	41	THR	3.1
10	AL	111	LYS	3.1
35	DB	163	PHE	3.0
35	DB	164	VAL	3.0
45	DL	69	TYR	3.0
47	DN	21	TYR	3.0
52	DS	44	MET	3.0
9	CK	109	SER	3.0
48	DO	89	GLY	3.0
3	CC	69	LEU	3.0
9	AK	36	GLU	3.0
38	DE	81	GLU	3.0
1	CA	1105	U	3.0
17	CT	131	ALA	3.0
8	CH	123	PHE	3.0
3	AC	8	TYR	3.0
52	DS	80	TYR	3.0
8	CH	95	ARG	3.0
40	DG	132	GLY	3.0
42	DI	66	ARG	3.0
43	DJ	50	ILE	3.0
47	DN	28	GLY	3.0
10	CL	95	LYS	3.0
59	BZ	430	ARG	3.0
59	DZ	430	ARG	3.0
1	CA	1088	A	3.0
9	CK	126	ALA	3.0
59	BZ	432	ALA	3.0
3	AC	164	PHE	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
42	BI	53	VAL	3.0
43	BJ	47	PHE	3.0
59	BZ	653	PHE	3.0
34	DA	1190	G	3.0
42	DI	114	TYR	3.0
3	CC	23	ILE	3.0
3	AC	222	SER	3.0
37	BD	87	GLY	3.0
43	DJ	73	ASP	3.0
28	C4	50	VAL	3.0
35	BB	163	PHE	3.0
1	AA	572	A	3.0
52	BS	29	ARG	3.0
59	BZ	498	ILE	3.0
35	BB	72	GLY	3.0
37	DD	2	GLY	3.0
42	DI	115	GLY	3.0
1	CA	1533	G	3.0
10	CL	114	ASP	3.0
35	DB	195	ASP	3.0
35	DB	141	GLU	3.0
31	C7	45	ALA	3.0
37	BD	149	ALA	3.0
3	CC	181	PHE	3.0
52	DS	11	VAL	3.0
59	BZ	440	VAL	3.0
34	BA	1257	U	3.0
35	DB	140	HIS	3.0
32	C8	46	ARG	2.9
44	DK	126	ARG	2.9
59	BZ	504	ARG	2.9
43	BJ	38	ILE	2.9
3	AC	186	LEU	2.9
3	AC	163	GLU	2.9
10	AL	114	ASP	2.9
11	AN	68	GLU	2.9
23	CZ	11	GLU	2.9
37	BD	150	GLU	2.9
42	DI	110	GLU	2.9
59	BZ	401	SER	2.9
34	DA	980	C	2.9
3	CC	71	LYS	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	CA	271(K)	U	2.9
3	CC	211	ARG	2.9
42	DI	104	ARG	2.9
59	DZ	519	ARG	2.9
46	DM	9	ILE	2.9
22	CY	55	TYR	2.9
1	AA	1878	A	2.9
35	BB	202	PRO	2.9
23	AZ	119	GLU	2.9
30	A6	4	GLU	2.9
42	DI	2	GLU	2.9
33	A9	12	ASP	2.9
41	DH	54	ASP	2.9
59	DZ	435	ASP	2.9
9	CK	54	ALA	2.9
23	AZ	107	THR	2.9
59	BZ	90	PHE	2.9
1	CA	1079	C	2.9
40	DG	4	ARG	2.9
52	DS	78	ARG	2.9
59	BZ	631	ILE	2.9
59	DZ	462	ILE	2.9
1	CA	272(A)	U	2.9
43	BJ	31	GLY	2.9
9	CK	65	GLU	2.9
23	AZ	1	MET	2.9
59	BZ	615	GLU	2.9
3	AC	206	LYS	2.9
5	CE	204	ALA	2.9
36	DC	129	ALA	2.9
36	DC	198	VAL	2.9
3	AC	209	PHE	2.9
9	CK	82	PHE	2.9
3	AC	53	ARG	2.9
3	CC	7	ARG	2.9
3	CC	53	ARG	2.9
37	BD	115	ARG	2.9
10	CL	107	ILE	2.9
59	DZ	457	LEU	2.9
1	CA	2145	C	2.9
3	AC	70	GLY	2.9
3	AC	170	GLY	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
43	BJ	36	GLY	2.9
3	AC	214	TYR	2.9
3	AC	198	GLU	2.9
28	A4	57	GLU	2.9
59	DZ	83	ASP	2.9
28	C4	49	PHE	2.9
42	BI	126	SER	2.9
59	BZ	470	PHE	2.9
43	BJ	62	HIS	2.9
46	DM	91	ARG	2.9
54	BU	9	ARG	2.9
3	AC	65	LEU	2.9
3	AC	194	ILE	2.9
24	C0	75	LEU	2.9
36	DC	43	LEU	2.9
13	CP	44	GLY	2.8
59	DZ	379	GLY	2.8
26	C2	70	GLN	2.8
59	BZ	630	GLN	2.8
1	AA	271	U	2.8
1	CA	1104	C	2.8
1	CA	2146	C	2.8
8	AH	58	GLU	2.8
26	A2	12	GLU	2.8
32	C8	56	GLU	2.8
39	BF	54	LYS	2.8
43	BJ	61	GLU	2.8
35	BB	165	VAL	2.8
59	BZ	88	VAL	2.8
59	BZ	408	VAL	2.8
3	CC	193	PHE	2.8
26	A2	69	ARG	2.8
47	BN	3	ARG	2.8
52	BS	48	THR	2.8
59	BZ	687	LEU	2.8
3	AC	204	GLY	2.8
41	DH	70	GLN	2.8
36	BC	167	TRP	2.8
36	DC	161	GLU	2.8
3	AC	7	ARG	2.8
34	DA	1203	C	2.8
36	DC	190	ARG	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
54	BU	24	ARG	2.8
54	DU	24	ARG	2.8
59	DZ	620	VAL	2.8
3	AC	23	ILE	2.8
10	AL	115	LEU	2.8
35	DB	185	ILE	2.8
36	DC	87	LEU	2.8
59	DZ	89	ASP	2.8
1	CA	2147	G	2.8
9	AK	92	THR	2.8
52	DS	38	SER	2.8
34	DA	630	G	2.8
57	DX	2	G	2.8
58	DY	15	G	2.8
1	CA	2062	A	2.8
35	DB	101	MET	2.8
18	AU	117	GLN	2.8
59	DZ	85	PRO	2.8
59	BZ	433	GLU	2.8
3	CC	214	TYR	2.8
52	BS	80	TYR	2.8
59	DZ	279	TYR	2.8
36	DC	187	ALA	2.8
46	DM	5	ALA	2.8
10	AL	99	ILE	2.8
49	BP	19	ILE	2.8
9	CK	47	ASN	2.8
59	BZ	567	LEU	2.8
56	DW	2	C	2.8
9	CK	130	THR	2.8
10	AL	112	MET	2.8
10	CL	80	LYS	2.8
10	CL	111	LYS	2.8
59	DZ	686	LYS	2.8
10	CL	97	GLY	2.8
47	DN	55	GLY	2.8
56	BW	65	G	2.8
59	BZ	680	PRO	2.8
10	AL	101	TRP	2.8
46	DM	64	TRP	2.8
36	BC	207	VAL	2.8
28	A4	63	TYR	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
36	BC	193	TYR	2.8
36	DC	201	TYR	2.8
7	CG	19	LEU	2.8
9	AK	112	LEU	2.8
42	DI	96	LEU	2.8
3	CC	166	ASN	2.8
52	DS	65	ASN	2.8
59	BZ	638	GLY	2.8
40	DG	86	GLN	2.7
43	BJ	33	GLN	2.7
9	CK	36	GLU	2.7
43	BJ	66	ARG	2.7
43	DJ	79	ARG	2.7
10	AL	81	ALA	2.7
36	DC	167	TRP	2.7
9	AK	117	LEU	2.7
34	BA	1190	G	2.7
43	DJ	54	PHE	2.7
59	DZ	584	ILE	2.7
55	DV	22	U	2.7
3	CC	178	LYS	2.7
52	BS	12	ASP	2.7
9	CK	115	GLN	2.7
37	BD	3	ARG	2.7
45	BL	19	ARG	2.7
46	DM	101	GLN	2.7
52	DS	36	ARG	2.7
28	C4	57	GLU	2.7
23	AZ	111	VAL	2.7
59	BZ	670	VAL	2.7
40	BG	16	LEU	2.7
59	DZ	687	LEU	2.7
49	BP	38	TYR	2.7
59	BZ	87	HIS	2.7
16	CS	62	LYS	2.7
34	BA	532	A	2.7
34	DA	1183	A	2.7
43	BJ	55	LYS	2.7
47	BN	15	LYS	2.7
57	BX	47	U	2.7
52	DS	53	ASN	2.7
3	CC	35	THR	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
59	DZ	657	THR	2.7
7	CG	126	ASP	2.7
59	BZ	89	ASP	2.7
59	DZ	520	GLY	2.7
3	AC	60	ARG	2.7
3	CC	182	PRO	2.7
10	CL	93	ARG	2.7
35	BB	125	PRO	2.7
7	CG	76	SER	2.7
37	DD	47	ARG	2.7
40	DG	76	ARG	2.7
53	BT	80	ARG	2.7
9	AK	106	GLN	2.7
9	CK	122	VAL	2.7
23	AZ	116	VAL	2.7
9	CK	79	ALA	2.7
52	BS	40	ILE	2.7
52	DS	49	ILE	2.7
3	CC	6	LYS	2.7
3	CC	168	LYS	2.7
52	DS	34	TRP	2.7
52	DS	70	LYS	2.7
59	BZ	681	LYS	2.7
34	DA	977	A	2.7
40	BG	84	ASN	2.7
7	CG	2	PRO	2.7
9	AK	41	ARG	2.7
10	AL	91	PRO	2.7
10	CL	92	GLY	2.7
47	DN	57	ARG	2.7
52	DS	33	THR	2.7
53	DT	25	ARG	2.7
54	BU	15	ARG	2.7
59	BZ	473	ASP	2.7
1	CA	171	G	2.7
10	AL	133	SER	2.7
52	BS	4	SER	2.7
59	BZ	677	GLN	2.7
59	DZ	521	SER	2.7
59	DZ	677	GLN	2.7
23	CZ	116	VAL	2.7
7	CG	43	LEU	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
52	DS	30	LEU	2.7
42	DI	119	ALA	2.7
22	CY	5	MET	2.7
36	BC	184	TYR	2.7
28	C4	68	ARG	2.7
43	DJ	78	ASN	2.7
45	DL	94	PRO	2.7
46	DM	97	PRO	2.7
1	AA	2135	U	2.7
1	CA	1083	U	2.7
58	DY	36	A	2.7
3	CC	57	GLN	2.7
59	BZ	95	GLU	2.7
59	DZ	440	VAL	2.7
53	BT	11	SER	2.7
10	CL	82	ALA	2.6
23	AZ	136	PHE	2.6
53	DT	21	LYS	2.6
53	DT	74	LYS	2.6
43	BJ	26	ALA	2.6
7	AG	51	ARG	2.6
14	CQ	60	ARG	2.6
47	BN	35	ARG	2.6
34	BA	163	C	2.6
3	CC	52	PRO	2.6
48	BO	2	PRO	2.6
23	CZ	144	LEU	2.6
23	CZ	146	ILE	2.6
35	DB	133	LYS	2.6
36	DC	91	LEU	2.6
42	DI	91	ASP	2.6
46	DM	69	GLU	2.6
59	BZ	119	GLU	2.6
1	CA	896	A	2.6
1	CA	614(B)	G	2.6
3	AC	161	ARG	2.6
9	AK	29	TYR	2.6
34	BA	1002	G	2.6
58	DY	1	G	2.6
58	DY	19	G	2.6
59	DZ	655	TYR	2.6
3	CC	227	PRO	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	CD	238	GLY	2.6
9	CK	31	GLY	2.6
1	CA	2111	C	2.6
16	CS	11	LYS	2.6
3	AC	223	VAL	2.6
8	CH	49	VAL	2.6
16	CS	58	LEU	2.6
34	DA	1066	C	2.6
36	BC	204	LEU	2.6
36	DC	32	LEU	2.6
3	CC	225	ILE	2.6
36	DC	8	ILE	2.6
43	BJ	4	ILE	2.6
46	BM	32	GLU	2.6
15	CR	69	ASP	2.6
22	CY	107	ASP	2.6
35	BB	28	PHE	2.6
35	BB	237	ALA	2.6
35	DB	62	ALA	2.6
42	DI	9	ARG	2.6
49	BP	81	ARG	2.6
49	DP	48	TRP	2.6
10	AL	140	GLY	2.6
36	BC	171	GLY	2.6
37	BD	124	GLY	2.6
52	BS	72	GLY	2.6
19	CV	85	LYS	2.6
59	DZ	681	LYS	2.6
3	AC	215	VAL	2.6
9	CK	27	VAL	2.6
9	CK	51	LEU	2.6
9	CK	125	LEU	2.6
46	DM	70	LEU	2.6
35	DB	222	ILE	2.6
36	DC	64	VAL	2.6
36	BC	206	GLU	2.6
43	BJ	83	GLU	2.6
46	DM	73	GLU	2.6
47	BN	7	ILE	2.6
58	DY	18	G	2.6
14	CQ	1	MET	2.6
26	C2	11	GLU	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
59	BZ	223	PHE	2.6
1	AA	1985	U	2.6
1	CA	614(A)	U	2.6
3	CC	180	SER	2.6
31	C7	41	ARG	2.6
38	DE	18	ARG	2.6
53	BT	8	ARG	2.6
34	DA	1092	A	2.6
21	CX	69	TYR	2.6
35	DB	236	TYR	2.6
47	BN	34	TYR	2.6
47	DN	50	LYS	2.6
53	BT	103	GLY	2.6
10	AL	105	LEU	2.6
3	AC	169	THR	2.6
42	DI	64	THR	2.6
43	DJ	42	THR	2.6
59	BZ	227	ILE	2.6
59	BZ	454	MET	2.6
59	DZ	608	VAL	2.6
37	BD	179	GLU	2.6
3	AC	38	PHE	2.6
10	CL	116	ASN	2.6
3	AC	200	HIS	2.5
36	DC	176	HIS	2.5
42	BI	120	ARG	2.5
1	AA	2183	C	2.5
47	DN	11	LYS	2.5
9	AK	86	PRO	2.5
34	BA	1286	A	2.5
59	BZ	202	PRO	2.5
43	DJ	88	LEU	2.5
52	BS	15	LEU	2.5
53	BT	10	LEU	2.5
59	BZ	647	VAL	2.5
9	CK	92	THR	2.5
52	DS	79	THR	2.5
9	AK	126	ALA	2.5
36	BC	189	ALA	2.5
40	DG	84	ASN	2.5
5	CE	58	ARG	2.5
16	AS	3	ARG	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
35	DB	144	ARG	2.5
37	BD	168	ARG	2.5
47	DN	12	ARG	2.5
20	CW	111	HIS	2.5
36	DC	6	HIS	2.5
3	AC	178	LYS	2.5
45	BL	13	LYS	2.5
47	BN	17	LYS	2.5
1	AA	2134	G	2.5
34	DA	1033	G	2.5
1	AA	2168	C	2.5
56	DW	72	C	2.5
9	AK	31	GLY	2.5
9	CK	58	LEU	2.5
9	CK	77	PRO	2.5
19	CV	71	LEU	2.5
43	DJ	53	PRO	2.5
43	DJ	93	GLY	2.5
38	DE	10	MET	2.5
40	DG	156	TRP	2.5
59	BZ	466	LEU	2.5
35	BB	127	ILE	2.5
36	BC	195	VAL	2.5
34	DA	1447	A	2.5
58	BY	36	A	2.5
9	AK	118	THR	2.5
59	BZ	685	GLU	2.5
42	BI	37	PHE	2.5
45	DL	78	GLN	2.5
3	AC	27	ALA	2.5
16	CS	61	ASN	2.5
52	BS	14	HIS	2.5
35	DB	139	LYS	2.5
59	BZ	175	SER	2.5
9	CK	74	LEU	2.5
25	A1	98	LEU	2.5
52	DS	2	PRO	2.5
59	DZ	517	LEU	2.5
10	AL	92	GLY	2.5
23	AZ	120	ILE	2.5
42	DI	72	GLY	2.5
59	BZ	503	GLY	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
46	DM	117	VAL	2.5
1	CA	1110	G	2.5
56	DW	71	G	2.5
18	CU	89	GLU	2.5
59	BZ	438	PHE	2.5
59	DZ	635	GLU	2.5
3	CC	199	ALA	2.5
9	CK	30	GLN	2.5
23	CZ	118	GLN	2.5
47	DN	22	THR	2.5
53	BT	18	GLN	2.5
1	CA	1098	A	2.5
55	BV	14	A	2.5
7	AG	182	LYS	2.5
42	BI	11	LYS	2.5
45	BL	126	LYS	2.5
41	DH	4	ASP	2.5
3	CC	29	LEU	2.5
35	DB	11	LEU	2.5
13	CP	43	GLY	2.5
30	C6	54	ILE	2.5
47	DN	42	ILE	2.5
58	BY	33	U	2.5
59	DZ	86	GLY	2.5
9	CK	87	VAL	2.5
35	BB	93	VAL	2.5
42	BI	17	VAL	2.5
42	BI	41	VAL	2.5
3	CC	43	GLU	2.5
10	AL	85	GLU	2.5
36	BC	201	TYR	2.5
42	BI	35	GLU	2.5
50	BQ	24	GLU	2.5
59	BZ	212	TYR	2.5
59	DZ	470	PHE	2.5
3	AC	26	ALA	2.5
35	DB	96	ARG	2.5
59	DZ	159	ALA	2.5
59	DZ	501	THR	2.5
47	DN	58	LYS	2.5
53	BT	14	LYS	2.5
34	BA	1001(A)	G	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
34	DA	1184	G	2.5
47	DN	49	HIS	2.5
47	DN	40	CYS	2.5
3	CC	167	ASP	2.4
9	AK	40	LEU	2.4
35	BB	11	LEU	2.4
43	DJ	40	LEU	2.4
46	BM	90	LEU	2.4
46	DM	82	MET	2.4
59	DZ	255	ILE	2.4
3	AC	220	GLY	2.4
40	BG	81	GLY	2.4
10	CL	133	SER	2.4
41	DH	19	VAL	2.4
1	CA	1066	U	2.4
26	C2	12	GLU	2.4
37	BD	47	ARG	2.4
40	DG	32	ARG	2.4
43	BJ	64	GLU	2.4
47	BN	29	ARG	2.4
50	DQ	75	ARG	2.4
54	DU	10	ARG	2.4
10	AL	123	ALA	2.4
10	CL	124	ALA	2.4
3	AC	208	THR	2.4
43	DJ	87	THR	2.4
16	CS	95	HIS	2.4
53	BT	73	HIS	2.4
1	CA	1075	C	2.4
3	CC	189	ASN	2.4
36	DC	34	LEU	2.4
34	DA	1201	A	2.4
1	CA	2148	G	2.4
34	DA	1002	G	2.4
35	BB	159	PRO	2.4
44	DK	36	ASP	2.4
9	CK	22	GLY	2.4
36	DC	197	GLY	2.4
44	DK	46	GLY	2.4
47	BN	51	GLY	2.4
59	BZ	404	VAL	2.4
59	BZ	526	VAL	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
59	BZ	530	VAL	2.4
59	BZ	654	GLY	2.4
35	DB	137	ARG	2.4
46	BM	93	ARG	2.4
52	DS	4	SER	2.4
59	DZ	465	ARG	2.4
10	CL	109	LYS	2.4
32	A8	56	GLU	2.4
35	BB	70	PHE	2.4
36	BC	135	LYS	2.4
41	DH	32	LYS	2.4
50	BQ	100	LYS	2.4
59	DZ	423	LYS	2.4
9	CK	124	ALA	2.4
47	DN	20	ALA	2.4
3	CC	45	HIS	2.4
9	CK	32	LEU	2.4
21	CX	1	MET	2.4
43	BJ	8	LEU	2.4
52	BS	16	LEU	2.4
10	AL	116	ASN	2.4
34	DA	1322	C	2.4
35	BB	197	VAL	2.4
43	BJ	10	GLY	2.4
43	BJ	58	ASP	2.4
59	DZ	163	VAL	2.4
1	CA	1103	A	2.4
34	DA	1044	A	2.4
36	DC	135	LYS	2.4
43	BJ	5	ARG	2.4
47	DN	3	ARG	2.4
49	BP	5	ARG	2.4
59	BZ	471	LYS	2.4
1	CA	1093	G	2.4
3	AC	212	SER	2.4
7	AG	76	SER	2.4
14	CQ	112	GLU	2.4
33	C9	28	GLU	2.4
34	BA	631	G	2.4
34	BA	1003	G	2.4
34	BA	1036	G	2.4
3	AC	187	ALA	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	CC	26	ALA	2.4
35	DB	161	ALA	2.4
9	AK	46	GLN	2.4
44	BK	75	TYR	2.4
54	DU	8	THR	2.4
59	BZ	634	MET	2.4
8	CH	7	LEU	2.4
35	BB	187	LEU	2.4
47	DN	47	LEU	2.4
7	CG	77	ILE	2.4
59	DZ	625	ASN	2.4
23	CZ	111	VAL	2.4
3	CC	37	LYS	2.4
17	AT	107	ASP	2.4
38	DE	27	ARG	2.4
43	BJ	29	ARG	2.4
1	AA	942	A	2.4
3	AC	40	GLU	2.4
23	CZ	13	GLU	2.4
34	BA	160	A	2.4
47	DN	36	PHE	2.4
37	BD	156	GLU	2.4
40	DG	8	GLU	2.4
55	BV	23	A	2.4
43	DJ	27	ALA	2.4
59	DZ	136	ALA	2.4
37	DD	160	GLN	2.4
40	BG	110	GLN	2.4
1	CA	1058	G	2.4
1	CA	2112	G	2.4
3	CC	169	THR	2.4
34	BA	723	U	2.4
34	DA	1017	G	2.4
3	CC	65	LEU	2.4
35	DB	149	LEU	2.4
36	DC	178	LEU	2.4
36	DC	204	LEU	2.4
46	DM	19	LEU	2.4
10	CL	99	ILE	2.4
59	DZ	461	ILE	2.4
3	CC	183	PRO	2.4
23	AZ	95	PRO	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
54	BU	23	PRO	2.4
3	AC	20	VAL	2.3
3	CC	58	ASN	2.3
3	CC	60	ARG	2.3
8	CH	62	LYS	2.3
9	CK	16	ASN	2.3
9	CK	98	LYS	2.3
28	A4	56	VAL	2.3
44	BK	117	ASN	2.3
47	BN	11	LYS	2.3
52	DS	45	VAL	2.3
59	BZ	628	ARG	2.3
59	DZ	514	VAL	2.3
19	CV	42	GLY	2.3
11	CN	68	GLU	2.3
34	DA	1363	C	2.3
49	BP	82	GLN	2.3
56	BW	74	C	2.3
1	CA	1067	A	2.3
1	CA	1084	A	2.3
1	CA	2173	A	2.3
35	DB	48	MET	2.3
9	AK	37	THR	2.3
9	AK	74	LEU	2.3
36	BC	95	THR	2.3
46	DM	90	LEU	2.3
23	CZ	57	ILE	2.3
35	BB	214	ILE	2.3
59	BZ	402	ILE	2.3
59	DZ	402	ILE	2.3
10	CL	86	LYS	2.3
46	DM	113	PRO	2.3
47	BN	50	LYS	2.3
52	BS	32	LYS	2.3
1	CA	1074	G	2.3
1	CA	2125	G	2.3
1	CA	2160	G	2.3
11	CN	140	VAL	2.3
34	DA	80	G	2.3
34	DA	1030(A)	G	2.3
58	BY	15	G	2.3
28	C4	64	GLY	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
35	DB	122	PHE	2.3
8	CH	58	GLU	2.3
17	CT	107	ASP	2.3
33	C9	12	ASP	2.3
28	C4	18	CYS	2.3
35	BB	90	MET	2.3
35	BB	215	LEU	2.3
1	AA	155	C	2.3
23	CZ	170	THR	2.3
38	DE	13	ILE	2.3
40	BG	154	TYR	2.3
47	BN	22	THR	2.3
59	BZ	437	THR	2.3
41	BH	116	LYS	2.3
45	DL	13	LYS	2.3
52	DS	6	LYS	2.3
1	CA	1963	U	2.3
3	AC	227	PRO	2.3
3	CC	165	ARG	2.3
58	BY	20	U	2.3
9	CK	129	PRO	2.3
11	AN	9	VAL	2.3
11	CN	9	VAL	2.3
59	DZ	679	VAL	2.3
9	CK	103	GLY	2.3
19	AV	101	GLY	2.3
35	DB	89	GLY	2.3
59	DZ	618	GLY	2.3
42	DI	29	ASN	2.3
36	BC	186	PHE	2.3
34	BA	976	G	2.3
42	DI	15	ALA	2.3
35	DB	166	ASP	2.3
21	CX	95	LEU	2.3
36	BC	37	GLN	2.3
8	CH	136	ILE	2.3
22	CY	44	ILE	2.3
23	AZ	149	SER	2.3
36	DC	157	ILE	2.3
41	DH	56	LYS	2.3
54	BU	14	TRP	2.3
46	DM	103	THR	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
54	BU	8	THR	2.3
59	DZ	238	THR	2.3
13	CP	15	ARG	2.3
35	BB	31	TYR	2.3
37	DD	49	ARG	2.3
47	DN	41	ARG	2.3
23	CZ	108	PRO	2.3
36	DC	138	VAL	2.3
59	DZ	405	PRO	2.3
1	CA	1109	C	2.3
1	CA	1082	U	2.3
1	CA	1847	A	2.3
34	BA	1531	A	2.3
34	DA	994	A	2.3
34	DA	1223	C	2.3
34	DA	1251	A	2.3
34	DA	1321	C	2.3
2	CB	1	U	2.3
3	AC	160	GLY	2.3
3	CC	220	GLY	2.3
21	AX	94	GLY	2.3
23	CZ	115	GLY	2.3
28	C4	54	GLY	2.3
59	DZ	597	GLY	2.3
49	BP	80	PHE	2.3
9	AK	97	ALA	2.3
20	CW	30	GLU	2.3
9	CK	26	LEU	2.3
23	CZ	70	LEU	2.3
35	DB	44	LEU	2.3
42	DI	19	LEU	2.3
43	DJ	89	ASP	2.3
47	DN	44	LEU	2.3
59	DZ	500	GLN	2.3
59	DZ	684	GLN	2.3
43	BJ	7	LYS	2.3
1	AA	2146	G	2.3
28	C4	31	ILE	2.3
34	DA	1001(A)	G	2.3
34	DA	1032	G	2.3
36	DC	124	ILE	2.3
43	DJ	23	ILE	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	AC	165	ARG	2.3
10	CL	132	ARG	2.3
28	A4	52	THR	2.3
41	DH	18	ARG	2.3
52	BS	37	ARG	2.3
53	DT	8	ARG	2.3
10	AL	76	TYR	2.3
42	DI	36	TYR	2.3
22	CY	45	VAL	2.3
23	CZ	96	VAL	2.3
59	DZ	322	VAL	2.3
11	CN	49	GLY	2.3
1	CA	1420	U	2.3
1	AA	218	A	2.2
1	AA	2200	C	2.2
1	CA	229	A	2.2
3	CC	38	PHE	2.2
34	DA	1116	C	2.2
42	DI	18	PHE	2.2
17	AT	1	MET	2.2
3	AC	205	ALA	2.2
3	CC	159	ALA	2.2
10	CL	108	ALA	2.2
42	DI	52	ALA	2.2
43	BJ	32	ALA	2.2
47	DN	30	ALA	2.2
59	DZ	528	ALA	2.2
9	CK	61	LEU	2.2
10	CL	77	LEU	2.2
35	BB	158	LEU	2.2
35	DB	98	LEU	2.2
41	DH	63	LEU	2.2
42	DI	79	LEU	2.2
52	DS	5	LEU	2.2
59	BZ	253	LEU	2.2
24	C0	49	LYS	2.2
37	BD	160	GLN	2.2
40	DG	29	LYS	2.2
42	DI	127	LYS	2.2
35	DB	201	ILE	2.2
17	CT	115	ARG	2.2
42	DI	120	ARG	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
28	C4	27	THR	2.2
36	DC	67	THR	2.2
43	BJ	42	THR	2.2
47	BN	13	THR	2.2
50	DQ	7	THR	2.2
35	BB	230	VAL	2.2
37	BD	170	VAL	2.2
59	BZ	180	VAL	2.2
59	DZ	94	VAL	2.2
59	DZ	561	VAL	2.2
28	C4	67	TYR	2.2
35	DB	92	TYR	2.2
41	BH	58	TYR	2.2
1	CA	2893	G	2.2
34	DA	976	G	2.2
56	DW	6	G	2.2
59	DZ	654	GLY	2.2
45	DL	32	PHE	2.2
22	AY	91	GLU	2.2
24	C0	2	ALA	2.2
37	DD	179	GLU	2.2
43	DJ	64	GLU	2.2
10	AL	86	LYS	2.2
34	BA	1006	C	2.2
34	BA	1030	C	2.2
34	DA	532	A	2.2
34	DA	1286	A	2.2
53	BT	75	ASN	2.2
36	BC	8	ILE	2.2
59	BZ	462	ILE	2.2
8	CH	60	ARG	2.2
43	BJ	73	ASP	2.2
52	BS	78	ARG	2.2
59	DZ	348	ARG	2.2
3	AC	202	PRO	2.2
6	CF	175	THR	2.2
36	BC	7	PRO	2.2
47	DN	14	PRO	2.2
3	CC	61	GLY	2.2
20	AW	112	GLY	2.2
36	BC	25	GLY	2.2
47	DN	37	PHE	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	AA	2163	G	2.2
1	CA	2123	G	2.2
3	AC	29	LEU	2.2
7	CG	164	GLU	2.2
9	CK	119	ALA	2.2
37	BD	24	GLU	2.2
43	DJ	20	ALA	2.2
59	BZ	406	GLU	2.2
16	CS	17	ARG	2.2
16	CS	20	ARG	2.2
23	CZ	120	ILE	2.2
28	A4	62	ARG	2.2
49	DP	81	ARG	2.2
50	DQ	26	GLN	2.2
59	BZ	641	GLN	2.2
1	CA	652(B)	A	2.2
34	DA	1287	A	2.2
43	DJ	13	HIS	2.2
58	DY	56	C	2.2
3	AC	15	VAL	2.2
23	AZ	141	VAL	2.2
42	BI	109	VAL	2.2
42	DI	17	VAL	2.2
43	DJ	77	PRO	2.2
53	DT	98	PRO	2.2
54	DU	17	THR	2.2
47	DN	27	CYS	2.2
3	AC	5	GLY	2.2
9	CK	45	LYS	2.2
35	DB	70	PHE	2.2
36	BC	26	LYS	2.2
36	BC	150	LYS	2.2
7	CG	152	LEU	2.2
24	A0	7	LEU	2.2
40	DG	22	LEU	2.2
59	DZ	567	LEU	2.2
3	AC	34	ALA	2.2
7	AG	48	GLU	2.2
26	A2	11	GLU	2.2
32	C8	65	GLU	2.2
36	DC	149	ALA	2.2
53	DT	97	ALA	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
38	BE	13	ILE	2.2
1	CA	2122	U	2.2
41	BH	91	ARG	2.2
46	DM	80	ARG	2.2
52	DS	3	ARG	2.2
53	BT	22	ARG	2.2
59	DZ	-10	ARG	2.2
3	AC	226	ASN	2.2
10	CL	110	GLN	2.2
28	A4	60	GLN	2.2
46	DM	106	ASN	2.2
59	BZ	426	GLN	2.2
3	CC	67	HIS	2.2
52	DS	69	HIS	2.2
57	DX	70	G	2.2
1	AA	2803	A	2.2
3	AC	56	ASP	2.2
31	A7	46	VAL	2.2
34	BA	383	A	2.2
42	DI	28	VAL	2.2
59	BZ	436	PRO	2.2
59	DZ	172	ASP	2.2
34	BA	1452	C	2.2
43	DJ	100	THR	2.2
59	DZ	84	THR	2.2
24	C0	5	LYS	2.2
35	DB	228	GLY	2.2
46	DM	85	GLY	2.2
48	BO	89	GLY	2.2
59	DZ	471	LYS	2.2
16	CS	29	PHE	2.2
28	A4	49	PHE	2.2
42	DI	62	TYR	2.2
35	DB	115	LEU	2.2
43	DJ	59	SER	2.2
50	BQ	99	SER	2.2
59	BZ	431	LEU	2.2
3	CC	34	ALA	2.2
7	CG	35	GLU	2.2
25	C1	75	GLU	2.2
42	BI	15	ALA	2.2
47	DN	59	ALA	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
9	CK	19	ARG	2.1
22	CY	2	ARG	2.1
28	A4	68	ARG	2.1
35	BB	30	ARG	2.1
35	DB	108	ILE	2.1
41	DH	45	ILE	2.1
47	DN	29	ARG	2.1
59	DZ	644	ARG	2.1
9	CK	95	GLN	2.1
40	DG	13	GLN	2.1
59	BZ	421	GLN	2.1
6	CF	14	PRO	2.1
36	DC	66	VAL	2.1
36	DC	173	VAL	2.1
42	DI	49	PRO	2.1
43	DJ	72	VAL	2.1
37	BD	102	ASP	2.1
44	BK	36	ASP	2.1
45	DL	92	ASP	2.1
59	BZ	393	ASP	2.1
59	BZ	671	MET	2.1
1	AA	2145	G	2.1
1	CA	2110	G	2.1
3	CC	70	GLY	2.1
9	CK	118	THR	2.1
17	AT	37	GLY	2.1
23	CZ	107	THR	2.1
34	DA	975	A	2.1
34	DA	1036	G	2.1
34	DA	1053	G	2.1
34	DA	1101	A	2.1
37	DD	69	GLY	2.1
44	DK	49	GLY	2.1
46	DM	100	GLY	2.1
55	BV	15	A	2.1
56	DW	73	A	2.1
59	DZ	667	GLY	2.1
1	CA	2789	C	2.1
7	CG	34	LEU	2.1
9	CK	71	LEU	2.1
34	BA	1039	C	2.1
34	BA	1317	C	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
34	DA	1149	C	2.1
34	DA	1267	C	2.1
35	BB	10	LEU	2.1
3	AC	46	ALA	2.1
3	AC	54	ARG	2.1
9	AK	84	GLU	2.1
9	CK	50	ARG	2.1
9	CK	123	GLU	2.1
37	DD	76	ARG	2.1
40	BG	79	ARG	2.1
59	DZ	615	GLU	2.1
9	CK	59	ILE	2.1
43	DJ	74	ILE	2.1
3	CC	200	HIS	2.1
59	BZ	302	HIS	2.1
1	AA	1466	U	2.1
10	CL	113	PRO	2.1
41	DH	67	PRO	2.1
52	BS	67	VAL	2.1
35	DB	22	LYS	2.1
46	BM	120	LYS	2.1
51	DR	23	LYS	2.1
3	AC	39	ASP	2.1
3	CC	24	ASP	2.1
4	CD	122	ASP	2.1
9	AK	32	LEU	2.1
43	BJ	54	PHE	2.1
47	BN	16	PHE	2.1
49	BP	48	TRP	2.1
1	CA	2119	A	2.1
1	CA	2602	A	2.1
9	CK	90	ALA	2.1
17	AT	115	ARG	2.1
34	DA	978	A	2.1
34	DA	1503	A	2.1
37	BD	147	ALA	2.1
54	DU	18	TYR	2.1
59	DZ	427	ALA	2.1
1	AA	1105	G	2.1
1	AA	1114	G	2.1
8	CH	86	GLU	2.1
23	AZ	97	GLU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
34	DA	631	G	2.1
34	DA	971	G	2.1
41	DH	29	SER	2.1
42	DI	81	ILE	2.1
46	DM	86	CYS	2.1
48	BO	6	GLU	2.1
59	DZ	451	ILE	2.1
1	CA	1080	C	2.1
56	BW	2	C	2.1
56	BW	72	C	2.1
59	DZ	571	SER	2.1
9	AK	75	GLN	2.1
36	DC	170	GLN	2.1
42	BI	117	HIS	2.1
43	DJ	56	HIS	2.1
8	AH	175	LYS	2.1
23	CZ	139	VAL	2.1
35	BB	22	LYS	2.1
35	BB	81	VAL	2.1
52	BS	11	VAL	2.1
41	DH	72	PRO	2.1
34	BA	202	U	2.1
6	AF	207	GLY	2.1
9	AK	67	GLY	2.1
9	AK	111	LEU	2.1
9	CK	76	GLY	2.1
22	CY	90	LEU	2.1
24	A0	84	LEU	2.1
35	DB	138	LEU	2.1
52	DS	15	LEU	2.1
59	BZ	477	GLY	2.1
43	DJ	67	THR	2.1
59	DZ	91	THR	2.1
8	CH	51	ARG	2.1
41	DH	84	ARG	2.1
23	AZ	171	ILE	2.1
35	BB	29	ALA	2.1
42	DI	43	ALA	2.1
42	DI	45	ALA	2.1
3	CC	198	GLU	2.1
3	CC	203	GLU	2.1
36	DC	48	TYR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
43	DJ	83	GLU	2.1
59	DZ	434	GLU	2.1
1	AA	1134	A	2.1
35	DB	124	SER	2.1
37	BD	113	SER	2.1
23	CZ	50	GLN	2.1
1	AA	2188	G	2.1
1	CA	1062	G	2.1
1	CA	1115	G	2.1
1	CA	2127	G	2.1
1	CA	2181	G	2.1
3	CC	219	MET	2.1
22	CY	46	LYS	2.1
24	A0	5	LYS	2.1
34	BA	79	G	2.1
34	DA	1356	G	2.1
40	DG	75	VAL	2.1
42	DI	116	LYS	2.1
56	BW	15	G	2.1
59	BZ	617	MET	2.1
35	DB	234	PRO	2.1
52	BS	2	PRO	2.1
59	DZ	436	PRO	2.1
23	AZ	157	LEU	2.1
59	DZ	229	LEU	2.1
1	CA	1061	U	2.1
3	AC	181	PHE	2.1
3	CC	207	GLY	2.1
36	DC	96	GLY	2.1
37	BD	110	PHE	2.1
41	DH	128	GLY	2.1
42	DI	8	GLY	2.1
3	CC	28	ARG	2.1
7	CG	136	ARG	2.1
28	C4	44	THR	2.1
43	BJ	81	THR	2.1
53	DT	83	ARG	2.1
54	DU	9	ARG	2.1
7	CG	100	TRP	2.1
23	CZ	133	ILE	2.1
35	BB	185	ILE	2.1
42	DI	77	ILE	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
51	DR	20	ALA	2.1
52	DS	40	ILE	2.1
59	BZ	310	ALA	2.1
59	BZ	650	ALA	2.1
4	AD	28	GLU	2.1
13	AP	98	GLU	2.1
38	DE	50	GLU	2.1
59	DZ	368	GLU	2.1
40	DG	85	TYR	2.1
41	DH	94	TYR	2.1
59	DZ	676	TYR	2.1
3	AC	47	LYS	2.0
37	BD	42	GLN	2.0
39	DF	92	LYS	2.0
52	DS	66	MET	2.0
59	DZ	489	LYS	2.0
1	CA	1057	A	2.0
23	CZ	56	VAL	2.0
38	DE	33	VAL	2.0
38	DE	67	VAL	2.0
56	DW	14	A	2.0
3	AC	182	PRO	2.0
9	AK	69	PRO	2.0
1	AA	2807	C	2.0
1	CA	1049	C	2.0
3	AC	58	ASN	2.0
36	BC	188	LEU	2.0
40	DG	37	ASN	2.0
46	DM	77	ASN	2.0
50	DQ	98	LEU	2.0
52	DS	22	LEU	2.0
1	CA	545	G	2.0
7	CG	118	ARG	2.0
33	C9	37	GLY	2.0
34	BA	306	G	2.0
34	BA	1033	G	2.0
36	BC	10	PHE	2.0
41	DH	71	GLY	2.0
43	DJ	60	ARG	2.0
47	DN	16	PHE	2.0
48	DO	38	ARG	2.0
58	BY	5	G	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
59	BZ	523	PHE	2.0
1	CA	1097	U	2.0
10	AL	118	THR	2.0
34	DA	1257	U	2.0
37	BD	5	ILE	2.0
42	BI	105	ASP	2.0
47	DN	7	ILE	2.0
58	DY	33	U	2.0
18	CU	56	ASP	2.0
45	DL	68	ALA	2.0
59	DZ	67	ALA	2.0
59	DZ	619	ASP	2.0
6	CF	161	GLU	2.0
7	CG	29	TRP	2.0
22	CY	40	GLU	2.0
26	C2	66	GLU	2.0
43	BJ	25	GLU	2.0
50	DQ	24	GLU	2.0
42	DI	92	TYR	2.0
44	BK	25	TYR	2.0
8	CH	52	VAL	2.0
36	DC	151	VAL	2.0
46	DM	7	VAL	2.0
59	BZ	575	VAL	2.0
35	DB	131	PRO	2.0
59	DZ	444	PRO	2.0
1	AA	302	A	2.0
1	AA	1113	A	2.0
1	AA	1157	A	2.0
1	CA	1046	A	2.0
1	CA	1073	A	2.0
36	BC	43	LEU	2.0
37	BD	21	LEU	2.0
59	BZ	157	LEU	2.0
59	BZ	206	LEU	2.0
59	BZ	517	LEU	2.0
14	CQ	6	ARG	2.0
22	AY	92	ASN	2.0
52	BS	3	ARG	2.0
59	BZ	348	ARG	2.0
59	DZ	639	ASN	2.0
23	AZ	115	GLY	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
42	DI	39	GLY	2.0
49	DP	9	PHE	2.0
53	DT	69	GLY	2.0
1	AA	944	C	2.0
1	CA	1102	C	2.0
34	BA	174	C	2.0
59	BZ	688	ILE	2.0
3	AC	217	THR	2.0
35	DB	171	ALA	2.0
42	DI	13	ALA	2.0
43	DJ	48	THR	2.0
59	DZ	645	ALA	2.0
1	CA	11	G	2.0
1	CA	530	G	2.0
1	CA	2318	G	2.0
7	CG	143	GLU	2.0
9	CK	15	GLU	2.0
34	BA	204	U	2.0
35	BB	134	GLU	2.0
36	BC	90	GLU	2.0
37	DD	163	GLU	2.0
50	BQ	87	LYS	2.0
50	DQ	49	GLU	2.0
52	BS	21	GLU	2.0
59	BZ	598	ASP	2.0
44	DK	51	LYS	2.0
42	BI	4	TYR	2.0
8	CH	44	VAL	2.0
28	C4	10	VAL	2.0
36	BC	76	VAL	2.0
40	DG	9	VAL	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	PSU	DY	55	20/21	0.30	0.19	222,222,222,222	0
56	7MG	DW	46	24/25	0.32	0.14	244,244,244,244	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	7MG	BW	46	24/25	0.40	0.14	203,203,203,203	0
56	PSU	DW	55	20/21	0.43	0.16	190,190,190,190	0
56	4SU	DW	8	20/21	0.43	0.13	225,225,225,225	0
58	5MU	BY	54	21/22	0.46	0.16	217,217,217,217	0
58	7MG	BY	46	24/25	0.52	0.12	200,200,200,200	0
56	4SU	BW	8	20/21	0.52	0.12	200,200,200,200	0
58	PSU	BY	55	20/21	0.53	0.13	205,205,205,205	0
58	5MU	DY	54	21/22	0.56	0.17	200,200,200,200	0
58	7MG	DY	46	24/25	0.57	0.13	206,206,206,206	0
58	4SU	BY	8	20/21	0.66	0.11	191,191,191,191	0
58	MIA	DY	37	22/30	0.68	0.18	156,156,156,156	0
58	PSU	DY	39	20/21	0.71	0.14	138,138,138,138	0
58	PSU	DY	32	20/21	0.71	0.13	154,154,154,154	0
58	MIA	BY	37	22/30	0.74	0.14	118,118,118,118	0
58	4SU	DY	8	20/21	0.74	0.11	193,193,193,193	0
56	PSU	BW	55	20/21	0.76	0.13	113,113,113,113	0
58	PSU	BY	32	20/21	0.76	0.12	126,126,126,126	0
56	PSU	DW	32	20/21	0.79	0.15	139,139,139,139	0
56	PSU	BW	39	20/21	0.81	0.13	96,96,96,96	0
56	MIA	DW	37	22/30	0.82	0.12	116,116,116,116	0
58	PSU	BY	39	20/21	0.83	0.12	106,106,106,106	0
56	MIA	BW	37	29/30	0.83	0.17	95,95,95,95	1
56	PSU	DW	39	20/21	0.84	0.10	118,118,118,118	0
56	5MU	BW	54	21/22	0.84	0.13	89,89,89,89	0
56	5MU	DW	54	21/22	0.85	0.11	118,118,118,118	0
57	31H	DX	76	32/33	0.86	0.23	58,58,58,58	4
56	PSU	BW	32	20/21	0.86	0.13	110,110,110,110	0
57	5MU	BX	54	21/22	0.88	0.11	85,85,85,85	0
57	PSU	DX	55	20/21	0.88	0.09	95,95,95,95	0
57	5MU	DX	54	21/22	0.89	0.11	108,108,108,108	0
56	F3N	DW	76	33/34	0.90	0.19	75,75,75,75	1
57	5MC	DX	32	21/22	0.90	0.12	86,86,86,86	0
57	4SU	BX	8	20/21	0.90	0.10	70,70,70,70	1
57	4SU	DX	8	20/21	0.91	0.09	96,96,96,96	0
57	PSU	BX	55	20/21	0.92	0.08	74,74,74,74	0
57	31H	BX	76	32/33	0.93	0.15	58,58,58,58	4
57	5MC	BX	32	21/22	0.93	0.11	65,65,65,65	0
56	F3N	BW	76	33/34	0.96	0.12	54,54,54,54	1

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	DA	1686	1/1	0.15	0.17	102,102,102,102	0
60	MG	CA	3543	1/1	0.25	0.14	114,114,114,114	0
60	MG	AA	3770	1/1	0.36	0.86	57,57,57,57	1
60	MG	AA	3040	1/1	0.40	0.27	93,93,93,93	0
60	MG	CB	3008	1/1	0.44	0.29	87,87,87,87	0
60	MG	AA	3108	1/1	0.45	0.40	88,88,88,88	0
60	MG	CA	3631	1/1	0.45	0.24	88,88,88,88	0
60	MG	AA	3490	1/1	0.46	0.25	87,87,87,87	0
60	MG	BA	1709	1/1	0.49	0.25	96,96,96,96	0
60	MG	CA	3136	1/1	0.49	0.25	112,112,112,112	0
60	MG	CA	3550	1/1	0.51	0.20	88,88,88,88	0
60	MG	CA	3491	1/1	0.51	0.21	99,99,99,99	0
60	MG	CA	3619	1/1	0.55	0.22	78,78,78,78	0
60	MG	CA	3622	1/1	0.56	0.24	106,106,106,106	0
60	MG	CA	3616	1/1	0.56	0.25	62,62,62,62	0
60	MG	AA	3203	1/1	0.57	0.54	125,125,125,125	0
60	MG	CA	3506	1/1	0.57	0.23	120,120,120,120	0
60	MG	CA	3597	1/1	0.57	0.26	108,108,108,108	0
60	MG	BX	112	1/1	0.58	0.21	78,78,78,78	0
60	MG	CA	3575	1/1	0.58	0.20	77,77,77,77	0
60	MG	CA	3079	1/1	0.58	0.27	82,82,82,82	0
60	MG	DA	1739	1/1	0.58	0.25	85,85,85,85	0
60	MG	BA	1712	1/1	0.59	0.36	68,68,68,68	0
60	MG	CA	3664	1/1	0.59	0.24	69,69,69,69	0
60	MG	AA	3225	1/1	0.59	0.38	91,91,91,91	0
60	MG	CA	3482	1/1	0.59	0.15	89,89,89,89	0
60	MG	CA	3042	1/1	0.59	0.48	84,84,84,84	0
60	MG	CA	3073	1/1	0.61	0.19	94,94,94,94	0
60	MG	AA	3773	1/1	0.61	0.21	77,77,77,77	0
60	MG	CA	3592	1/1	0.63	0.21	87,87,87,87	0
60	MG	BK	3101	1/1	0.63	0.27	95,95,95,95	0
60	MG	AA	3438	1/1	0.63	0.20	75,75,75,75	0
60	MG	AA	3613	1/1	0.63	0.26	96,96,96,96	0
60	MG	BA	1779	1/1	0.63	0.20	82,82,82,82	0
60	MG	CA	3101	1/1	0.64	0.20	86,86,86,86	0
60	MG	BA	1691	1/1	0.64	0.27	98,98,98,98	0
60	MG	CA	3177	1/1	0.64	0.32	98,98,98,98	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	CA	3388	1/1	0.64	0.12	97,97,97,97	0
60	MG	DA	1715	1/1	0.64	0.24	87,87,87,87	0
60	MG	BA	1706	1/1	0.64	0.22	82,82,82,82	0
60	MG	BW	101	1/1	0.65	0.25	82,82,82,82	0
60	MG	AD	307	1/1	0.66	0.36	108,108,108,108	0
60	MG	AA	3689	1/1	0.66	0.16	84,84,84,84	0
60	MG	AA	3739	1/1	0.66	0.31	90,90,90,90	0
60	MG	DA	1767	1/1	0.66	0.28	88,88,88,88	0
60	MG	CA	3481	1/1	0.67	0.18	86,86,86,86	0
60	MG	AA	3805	1/1	0.67	0.43	117,117,117,117	0
60	MG	CA	3614	1/1	0.67	0.21	79,79,79,79	0
60	MG	CA	3643	1/1	0.67	0.35	83,83,83,83	0
60	MG	CA	3524	1/1	0.67	0.24	87,87,87,87	0
60	MG	BL	201	1/1	0.68	0.10	104,104,104,104	0
60	MG	DA	1671	1/1	0.68	0.40	77,77,77,77	0
60	MG	DA	1753	1/1	0.68	0.19	85,85,85,85	0
60	MG	CA	3122	1/1	0.68	0.51	95,95,95,95	0
60	MG	AA	3744	1/1	0.69	0.20	79,79,79,79	0
60	MG	CA	3206	1/1	0.69	0.29	109,109,109,109	0
60	MG	CA	3293	1/1	0.69	0.14	82,82,82,82	0
60	MG	AA	3578	1/1	0.69	0.23	71,71,71,71	0
60	MG	BA	1800	1/1	0.70	0.42	116,116,116,116	0
60	MG	AA	3783	1/1	0.70	0.22	68,68,68,68	0
60	MG	AA	3271	1/1	0.70	0.36	81,81,81,81	0
60	MG	DA	1651	1/1	0.70	0.43	86,86,86,86	0
60	MG	CA	3063	1/1	0.70	0.33	74,74,74,74	0
60	MG	BA	1740	1/1	0.71	0.13	89,89,89,89	0
60	MG	BA	1674	1/1	0.71	0.25	78,78,78,78	0
60	MG	AA	3183	1/1	0.71	0.45	89,89,89,89	0
60	MG	AA	3136	1/1	0.71	0.19	74,74,74,74	0
60	MG	AA	3221	1/1	0.71	0.26	72,72,72,72	0
60	MG	AA	3648	1/1	0.71	0.17	80,80,80,80	0
60	MG	CQ	201	1/1	0.71	0.29	85,85,85,85	0
60	MG	DX	3001	1/1	0.71	0.31	75,75,75,75	0
60	MG	AA	3098	1/1	0.72	0.27	65,65,65,65	0
60	MG	BA	1703	1/1	0.72	0.19	65,65,65,65	0
60	MG	BA	1786	1/1	0.72	0.38	79,79,79,79	0
60	MG	AA	3440	1/1	0.72	0.20	63,63,63,63	0
60	MG	AA	3582	1/1	0.72	0.25	78,78,78,78	0
60	MG	CA	3244	1/1	0.72	0.22	70,70,70,70	0
60	MG	AA	3725	1/1	0.72	0.16	42,42,42,42	0
60	MG	CA	3091	1/1	0.73	0.20	60,60,60,60	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	CA	3478	1/1	0.73	0.21	91,91,91,91	0
60	MG	DA	1640	1/1	0.73	0.26	73,73,73,73	0
60	MG	AA	3688	1/1	0.73	0.16	76,76,76,76	0
60	MG	BA	1609	1/1	0.73	0.17	77,77,77,77	0
60	MG	BA	1638	1/1	0.73	0.31	83,83,83,83	0
60	MG	AA	3646	1/1	0.73	0.32	82,82,82,82	0
60	MG	DA	1738	1/1	0.73	0.25	100,100,100,100	0
60	MG	CA	3511	1/1	0.73	0.28	66,66,66,66	0
60	MG	AA	3710	1/1	0.73	0.14	55,55,55,55	0
60	MG	AA	3200	1/1	0.73	0.20	73,73,73,73	0
60	MG	AA	3654	1/1	0.73	0.23	81,81,81,81	0
60	MG	CE	304	1/1	0.74	0.38	74,74,74,74	0
60	MG	CA	3138	1/1	0.74	0.18	67,67,67,67	0
60	MG	DA	1626	1/1	0.74	0.34	63,63,63,63	0
60	MG	BA	1656	1/1	0.74	0.24	83,83,83,83	0
60	MG	BA	1790	1/1	0.74	0.20	87,87,87,87	0
60	MG	CA	3220	1/1	0.74	0.42	89,89,89,89	0
60	MG	CA	3094	1/1	0.74	0.33	92,92,92,92	0
60	MG	DA	1712	1/1	0.74	0.14	67,67,67,67	0
60	MG	BA	1715	1/1	0.74	0.19	90,90,90,90	0
60	MG	CA	3348	1/1	0.74	0.12	78,78,78,78	0
60	MG	AA	3026	1/1	0.74	0.17	69,69,69,69	0
60	MG	CA	3646	1/1	0.74	0.12	90,90,90,90	0
60	MG	A8	5001	1/1	0.74	0.21	66,66,66,66	0
60	MG	CA	3581	1/1	0.74	0.23	100,100,100,100	0
60	MG	AA	3489	1/1	0.75	0.20	39,39,39,39	0
60	MG	CA	3588	1/1	0.75	0.12	78,78,78,78	0
60	MG	AA	3163	1/1	0.75	0.16	73,73,73,73	0
60	MG	A0	104	1/1	0.75	0.31	81,81,81,81	0
60	MG	CA	3068	1/1	0.75	0.25	73,73,73,73	0
60	MG	AA	3329	1/1	0.75	0.23	82,82,82,82	0
60	MG	CA	3209	1/1	0.75	0.39	101,101,101,101	0
60	MG	AA	3204	1/1	0.75	0.36	83,83,83,83	0
60	MG	CA	3234	1/1	0.75	0.21	96,96,96,96	0
60	MG	DA	1719	1/1	0.75	0.20	87,87,87,87	0
60	MG	AA	3246	1/1	0.75	0.19	86,86,86,86	0
60	MG	AA	3625	1/1	0.75	0.32	88,88,88,88	0
60	MG	CA	3573	1/1	0.75	0.13	82,82,82,82	0
60	MG	BA	1722	1/1	0.75	0.17	86,86,86,86	0
60	MG	CB	3013	1/1	0.75	0.18	90,90,90,90	0
60	MG	DA	1704	1/1	0.76	0.21	83,83,83,83	0
60	MG	BX	103	1/1	0.76	0.15	88,88,88,88	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	CA	3067	1/1	0.76	0.27	82,82,82,82	0
60	MG	CA	3542	1/1	0.76	0.18	82,82,82,82	0
60	MG	DA	1632	1/1	0.76	0.23	77,77,77,77	0
60	MG	AA	3201	1/1	0.76	0.24	71,71,71,71	0
60	MG	CA	3485	1/1	0.76	0.22	76,76,76,76	0
60	MG	CA	3376	1/1	0.76	0.21	94,94,94,94	0
60	MG	DE	201	1/1	0.76	0.36	93,93,93,93	0
60	MG	BA	1624	1/1	0.76	0.24	75,75,75,75	0
60	MG	DA	1615	1/1	0.77	0.29	87,87,87,87	0
60	MG	CA	3053	1/1	0.77	0.24	71,71,71,71	0
60	MG	AA	3579	1/1	0.77	0.14	66,66,66,66	0
60	MG	CA	3608	1/1	0.77	0.15	69,69,69,69	0
60	MG	AA	3027	1/1	0.77	0.48	85,85,85,85	0
60	MG	BA	1803	1/1	0.77	0.16	79,79,79,79	0
60	MG	AA	3631	1/1	0.77	0.25	74,74,74,74	0
60	MG	BA	1610	1/1	0.77	0.13	112,112,112,112	0
60	MG	CA	3535	1/1	0.77	0.17	74,74,74,74	0
60	MG	CA	3250	1/1	0.77	0.18	69,69,69,69	0
60	MG	BA	1774	1/1	0.77	0.12	79,79,79,79	0
60	MG	AA	3664	1/1	0.77	0.23	94,94,94,94	0
60	MG	AA	3638	1/1	0.77	0.18	72,72,72,72	0
60	MG	CB	3010	1/1	0.77	0.16	67,67,67,67	0
60	MG	DA	1765	1/1	0.77	0.14	66,66,66,66	0
60	MG	CA	3007	1/1	0.77	0.23	75,75,75,75	0
60	MG	CA	3011	1/1	0.77	0.19	75,75,75,75	0
60	MG	BA	1788	1/1	0.77	0.12	79,79,79,79	0
60	MG	AA	3419	1/1	0.78	0.22	88,88,88,88	0
60	MG	CA	3194	1/1	0.78	0.38	87,87,87,87	0
60	MG	CA	3462	1/1	0.78	0.27	63,63,63,63	0
60	MG	CA	3545	1/1	0.78	0.12	93,93,93,93	0
60	MG	CA	3642	1/1	0.78	0.09	75,75,75,75	0
60	MG	BA	1605	1/1	0.78	0.15	76,76,76,76	0
60	MG	AZ	5001	1/1	0.78	0.12	67,67,67,67	0
60	MG	BA	1804	1/1	0.78	0.31	94,94,94,94	0
60	MG	CA	3484	1/1	0.78	0.21	56,56,56,56	0
60	MG	CA	3584	1/1	0.78	0.14	91,91,91,91	0
60	MG	CA	3022	1/1	0.78	0.38	76,76,76,76	0
60	MG	DA	1751	1/1	0.78	0.17	84,84,84,84	0
60	MG	BA	1670	1/1	0.78	0.19	76,76,76,76	0
60	MG	BA	1671	1/1	0.78	0.26	71,71,71,71	0
60	MG	DA	1604	1/1	0.78	0.14	90,90,90,90	0
60	MG	AA	3728	1/1	0.78	0.21	75,75,75,75	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	DW	3001	1/1	0.78	0.15	90,90,90,90	0
60	MG	BW	102	1/1	0.78	0.16	75,75,75,75	0
60	MG	CA	3312	1/1	0.79	0.16	52,52,52,52	0
60	MG	CA	3532	1/1	0.79	0.16	59,59,59,59	0
60	MG	AA	3763	1/1	0.79	0.20	66,66,66,66	0
60	MG	AA	3765	1/1	0.79	0.11	62,62,62,62	0
60	MG	CA	3635	1/1	0.79	0.27	77,77,77,77	0
60	MG	CA	3387	1/1	0.79	0.25	73,73,73,73	0
60	MG	BY	3002	1/1	0.79	0.11	83,83,83,83	0
60	MG	CA	3183	1/1	0.79	0.28	83,83,83,83	0
60	MG	DA	1718	1/1	0.79	0.12	66,66,66,66	0
60	MG	CA	3653	1/1	0.79	0.35	102,102,102,102	0
60	MG	CA	3070	1/1	0.79	0.16	78,78,78,78	0
60	MG	AB	3022	1/1	0.79	0.14	79,79,79,79	0
60	MG	DA	1749	1/1	0.79	0.24	72,72,72,72	0
60	MG	AA	3766	1/1	0.79	0.17	69,69,69,69	0
60	MG	AA	3245	1/1	0.79	0.34	79,79,79,79	0
60	MG	CA	3031	1/1	0.79	0.42	102,102,102,102	0
60	MG	CA	3095	1/1	0.79	0.19	92,92,92,92	0
60	MG	CA	3505	1/1	0.79	0.15	66,66,66,66	0
60	MG	AA	3736	1/1	0.79	0.19	74,74,74,74	0
60	MG	BX	102	1/1	0.79	0.13	78,78,78,78	0
60	MG	AA	3342	1/1	0.80	0.17	77,77,77,77	0
60	MG	DA	1607	1/1	0.80	0.35	63,63,63,63	0
60	MG	DA	1608	1/1	0.80	0.42	79,79,79,79	0
60	MG	CA	3464	1/1	0.80	0.34	78,78,78,78	0
60	MG	AB	3004	1/1	0.80	0.27	69,69,69,69	0
60	MG	CA	3591	1/1	0.80	0.13	69,69,69,69	0
60	MG	CA	3202	1/1	0.80	0.17	67,67,67,67	0
60	MG	CA	3086	1/1	0.80	0.15	65,65,65,65	0
60	MG	DA	1657	1/1	0.80	0.15	75,75,75,75	0
60	MG	AA	3630	1/1	0.80	0.22	66,66,66,66	0
60	MG	AA	3692	1/1	0.80	0.36	86,86,86,86	0
60	MG	CA	3057	1/1	0.80	0.33	77,77,77,77	0
60	MG	AN	3001	1/1	0.80	0.16	64,64,64,64	0
60	MG	CA	3111	1/1	0.80	0.28	82,82,82,82	0
60	MG	CA	3267	1/1	0.80	0.25	110,110,110,110	0
60	MG	CA	3521	1/1	0.80	0.20	59,59,59,59	0
60	MG	CA	3281	1/1	0.80	0.19	74,74,74,74	0
60	MG	CA	3527	1/1	0.80	0.19	83,83,83,83	0
60	MG	CA	3064	1/1	0.80	0.19	72,72,72,72	0
60	MG	BA	1808	1/1	0.80	0.16	80,80,80,80	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	AA	3263	1/1	0.80	0.20	75,75,75,75	0
60	MG	CA	3361	1/1	0.80	0.12	70,70,70,70	0
60	MG	CA	3139	1/1	0.80	0.27	83,83,83,83	0
60	MG	CA	3386	1/1	0.80	0.15	79,79,79,79	0
60	MG	CA	3142	1/1	0.80	0.12	73,73,73,73	0
60	MG	AA	3621	1/1	0.80	0.10	34,34,34,34	0
60	MG	AA	3320	1/1	0.81	0.18	65,65,65,65	0
60	MG	BA	1767	1/1	0.81	0.16	73,73,73,73	0
60	MG	CA	3265	1/1	0.81	0.23	66,66,66,66	0
60	MG	CA	3497	1/1	0.81	0.21	85,85,85,85	0
60	MG	CA	3598	1/1	0.81	0.15	66,66,66,66	0
60	MG	AA	3777	1/1	0.81	0.11	58,58,58,58	0
60	MG	BA	1776	1/1	0.81	0.10	64,64,64,64	0
60	MG	CA	3507	1/1	0.81	0.22	99,99,99,99	0
60	MG	AA	3157	1/1	0.81	0.35	93,93,93,93	0
60	MG	AA	3487	1/1	0.81	0.17	66,66,66,66	0
60	MG	CA	3152	1/1	0.81	0.11	67,67,67,67	0
60	MG	CA	3155	1/1	0.81	0.28	69,69,69,69	0
60	MG	AA	3753	1/1	0.81	0.15	59,59,59,59	0
60	MG	AA	3604	1/1	0.81	0.14	44,44,44,44	1
60	MG	AA	3210	1/1	0.81	0.40	106,106,106,106	0
60	MG	DA	1730	1/1	0.81	0.18	65,65,65,65	0
60	MG	DA	1734	1/1	0.81	0.26	75,75,75,75	0
60	MG	AA	3615	1/1	0.81	0.10	65,65,65,65	0
60	MG	CA	3658	1/1	0.81	0.24	62,62,62,62	0
60	MG	DA	1741	1/1	0.81	0.18	81,81,81,81	0
60	MG	CA	3661	1/1	0.81	0.15	78,78,78,78	0
60	MG	BA	1717	1/1	0.81	0.14	77,77,77,77	0
60	MG	AA	3291	1/1	0.81	0.18	84,84,84,84	0
60	MG	DA	1764	1/1	0.81	0.13	94,94,94,94	0
60	MG	CA	3572	1/1	0.81	0.15	82,82,82,82	0
60	MG	CA	3475	1/1	0.81	0.13	55,55,55,55	0
60	MG	CA	3212	1/1	0.81	0.24	78,78,78,78	0
60	MG	CA	3097	1/1	0.81	0.23	79,79,79,79	0
60	MG	BA	1737	1/1	0.81	0.09	87,87,87,87	0
60	MG	AA	3265	1/1	0.82	0.33	64,64,64,64	0
60	MG	CA	3081	1/1	0.82	0.25	69,69,69,69	0
60	MG	CA	3235	1/1	0.82	0.31	78,78,78,78	0
60	MG	BA	1657	1/1	0.82	0.32	72,72,72,72	0
60	MG	CA	3467	1/1	0.82	0.29	99,99,99,99	0
60	MG	CA	3529	1/1	0.82	0.23	69,69,69,69	0
60	MG	CA	3055	1/1	0.82	0.22	77,77,77,77	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	AA	3802	1/1	0.82	0.12	55,55,55,55	0
60	MG	AA	3462	1/1	0.82	0.14	73,73,73,73	0
60	MG	AA	3694	1/1	0.82	0.10	49,49,49,49	0
60	MG	DA	1748	1/1	0.82	0.17	78,78,78,78	0
60	MG	DA	1611	1/1	0.82	0.12	80,80,80,80	0
60	MG	CA	3483	1/1	0.82	0.13	67,67,67,67	0
60	MG	BA	1719	1/1	0.82	0.17	75,75,75,75	0
60	MG	CA	3199	1/1	0.82	0.40	92,92,92,92	0
60	MG	BA	1633	1/1	0.82	0.27	65,65,65,65	0
60	MG	CA	3121	1/1	0.82	0.31	78,78,78,78	0
60	MG	CA	3648	1/1	0.82	0.23	78,78,78,78	0
60	MG	CA	3030	1/1	0.82	0.23	52,52,52,52	0
60	MG	AA	3109	1/1	0.82	0.17	75,75,75,75	0
60	MG	BA	1784	1/1	0.83	0.11	59,59,59,59	0
60	MG	CQ	203	1/1	0.83	0.20	62,62,62,62	0
60	MG	AA	3458	1/1	0.83	0.15	79,79,79,79	0
60	MG	AA	3764	1/1	0.83	0.23	48,48,48,48	0
60	MG	AA	3599	1/1	0.83	0.33	113,113,113,113	0
60	MG	CA	3410	1/1	0.83	0.17	72,72,72,72	0
60	MG	AA	3231	1/1	0.83	0.35	87,87,87,87	0
60	MG	BA	1696	1/1	0.83	0.12	84,84,84,84	0
60	MG	AA	3713	1/1	0.83	0.20	48,48,48,48	0
60	MG	A5	102	1/1	0.83	0.29	89,89,89,89	0
60	MG	CA	3195	1/1	0.83	0.10	36,36,36,36	0
60	MG	AA	3337	1/1	0.83	0.16	52,52,52,52	0
60	MG	DA	1658	1/1	0.83	0.18	89,89,89,89	0
60	MG	BA	1603	1/1	0.83	0.27	65,65,65,65	0
60	MG	DA	1673	1/1	0.83	0.21	68,68,68,68	0
60	MG	CA	3611	1/1	0.83	0.18	64,64,64,64	0
60	MG	AA	3268	1/1	0.83	0.14	80,80,80,80	0
60	MG	AA	3655	1/1	0.83	0.12	55,55,55,55	0
60	MG	CA	3618	1/1	0.83	0.16	79,79,79,79	0
60	MG	AA	3789	1/1	0.83	0.18	71,71,71,71	0
60	MG	AA	3793	1/1	0.83	0.29	76,76,76,76	0
60	MG	CA	3225	1/1	0.83	0.26	73,73,73,73	0
60	MG	CA	3092	1/1	0.83	0.26	74,74,74,74	0
60	MG	BX	105	1/1	0.83	0.14	87,87,87,87	0
60	MG	CA	3243	1/1	0.83	0.26	55,55,55,55	0
60	MG	BA	1630	1/1	0.83	0.10	61,61,61,61	0
60	MG	CA	3096	1/1	0.83	0.29	75,75,75,75	0
60	MG	AA	3121	1/1	0.83	0.19	63,63,63,63	0
60	MG	DA	1750	1/1	0.83	0.28	86,86,86,86	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	BA	1755	1/1	0.83	0.11	92,92,92,92	0
60	MG	CA	3103	1/1	0.83	0.19	80,80,80,80	0
60	MG	CA	3283	1/1	0.83	0.15	57,57,57,57	0
60	MG	AA	3067	1/1	0.83	0.38	82,82,82,82	0
60	MG	BA	1646	1/1	0.83	0.37	71,71,71,71	0
60	MG	AA	3105	1/1	0.83	0.21	77,77,77,77	0
60	MG	AB	3021	1/1	0.83	0.14	75,75,75,75	0
60	MG	CF	303	1/1	0.83	0.14	63,63,63,63	0
60	MG	AB	3019	1/1	0.84	0.13	61,61,61,61	0
60	MG	BA	1809	1/1	0.84	0.13	74,74,74,74	0
60	MG	CA	3371	1/1	0.84	0.38	70,70,70,70	0
60	MG	BA	1629	1/1	0.84	0.20	71,71,71,71	0
60	MG	CA	3377	1/1	0.84	0.09	53,53,53,53	0
60	MG	AA	3705	1/1	0.84	0.24	29,29,29,29	1
60	MG	CA	3187	1/1	0.84	0.16	70,70,70,70	0
60	MG	AA	3036	1/1	0.84	0.16	63,63,63,63	0
60	MG	DA	1614	1/1	0.84	0.17	71,71,71,71	0
60	MG	CA	3393	1/1	0.84	0.21	47,47,47,47	0
60	MG	CA	3583	1/1	0.84	0.34	114,114,114,114	0
60	MG	DA	1629	1/1	0.84	0.35	79,79,79,79	0
60	MG	BA	1636	1/1	0.84	0.23	66,66,66,66	0
60	MG	CA	3442	1/1	0.84	0.19	70,70,70,70	0
60	MG	DA	1648	1/1	0.84	0.22	66,66,66,66	0
60	MG	CA	3457	1/1	0.84	0.12	60,60,60,60	0
60	MG	AA	3651	1/1	0.84	0.15	66,66,66,66	0
60	MG	AD	310	1/1	0.84	0.16	58,58,58,58	0
60	MG	CA	3089	1/1	0.84	0.39	78,78,78,78	0
60	MG	BA	1762	1/1	0.84	0.12	57,57,57,57	0
60	MG	DA	1676	1/1	0.84	0.20	69,69,69,69	0
60	MG	AA	3575	1/1	0.84	0.13	63,63,63,63	0
60	MG	CA	3613	1/1	0.84	0.18	42,42,42,42	0
60	MG	AQ	3002	1/1	0.84	0.15	79,79,79,79	0
60	MG	AX	101	1/1	0.84	0.22	78,78,78,78	0
60	MG	CA	3226	1/1	0.84	0.24	56,56,56,56	0
60	MG	AA	3450	1/1	0.84	0.13	71,71,71,71	0
60	MG	DA	1722	1/1	0.84	0.13	69,69,69,69	0
60	MG	CA	3016	1/1	0.84	0.38	69,69,69,69	0
60	MG	CA	3488	1/1	0.84	0.09	58,58,58,58	0
60	MG	AA	3002	1/1	0.84	0.17	53,53,53,53	0
60	MG	AA	3351	1/1	0.84	0.13	80,80,80,80	0
60	MG	BA	1787	1/1	0.84	0.16	64,64,64,64	0
60	MG	DA	1743	1/1	0.84	0.11	83,83,83,83	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	CA	3645	1/1	0.84	0.11	78,78,78,78	0
60	MG	AA	3243	1/1	0.84	0.37	79,79,79,79	0
60	MG	AA	3600	1/1	0.84	0.14	70,70,70,70	0
60	MG	AA	3016	1/1	0.84	0.15	44,44,44,44	0
60	MG	CA	3519	1/1	0.84	0.18	68,68,68,68	0
60	MG	CA	3659	1/1	0.84	0.19	72,72,72,72	0
60	MG	CA	3056	1/1	0.84	0.28	83,83,83,83	0
60	MG	AA	3702	1/1	0.84	0.22	45,45,45,45	1
60	MG	AB	3014	1/1	0.84	0.14	70,70,70,70	0
60	MG	CA	3329	1/1	0.84	0.17	59,59,59,59	0
60	MG	CA	3342	1/1	0.84	0.14	84,84,84,84	0
60	MG	AA	3127	1/1	0.85	0.31	83,83,83,83	0
60	MG	CA	3043	1/1	0.85	0.19	75,75,75,75	0
60	MG	BA	1687	1/1	0.85	0.26	73,73,73,73	0
60	MG	CA	3534	1/1	0.85	0.13	58,58,58,58	0
60	MG	CA	3366	1/1	0.85	0.23	60,60,60,60	0
60	MG	CA	3540	1/1	0.85	0.17	71,71,71,71	0
60	MG	AA	3639	1/1	0.85	0.19	74,74,74,74	0
60	MG	CA	3373	1/1	0.85	0.24	71,71,71,71	0
60	MG	AA	3640	1/1	0.85	0.24	74,74,74,74	0
60	MG	BA	1699	1/1	0.85	0.24	70,70,70,70	0
60	MG	CA	3552	1/1	0.85	0.09	60,60,60,60	0
60	MG	CA	3181	1/1	0.85	0.18	68,68,68,68	0
60	MG	BA	1799	1/1	0.85	0.09	69,69,69,69	0
60	MG	DA	1620	1/1	0.85	0.16	68,68,68,68	0
60	MG	AA	3195	1/1	0.85	0.20	55,55,55,55	0
60	MG	BA	1704	1/1	0.85	0.20	68,68,68,68	0
60	MG	CA	3406	1/1	0.85	0.11	54,54,54,54	0
60	MG	AA	3592	1/1	0.85	0.21	67,67,67,67	0
60	MG	DA	1642	1/1	0.85	0.15	67,67,67,67	0
60	MG	CA	3587	1/1	0.85	0.17	72,72,72,72	0
60	MG	AA	3442	1/1	0.85	0.14	73,73,73,73	0
60	MG	AB	3006	1/1	0.85	0.21	84,84,84,84	0
60	MG	BA	1613	1/1	0.85	0.10	92,92,92,92	0
60	MG	AA	3324	1/1	0.85	0.11	69,69,69,69	0
60	MG	AA	3238	1/1	0.85	0.17	68,68,68,68	0
60	MG	CA	3605	1/1	0.85	0.19	72,72,72,72	0
60	MG	CA	3607	1/1	0.85	0.19	76,76,76,76	0
60	MG	DA	1695	1/1	0.85	0.17	79,79,79,79	0
60	MG	DA	1699	1/1	0.85	0.14	79,79,79,79	0
60	MG	AA	3755	1/1	0.85	0.20	77,77,77,77	0
60	MG	BA	1732	1/1	0.85	0.19	65,65,65,65	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	BA	1736	1/1	0.85	0.15	66,66,66,66	0
60	MG	AA	3612	1/1	0.85	0.15	60,60,60,60	0
60	MG	AA	3070	1/1	0.85	0.19	68,68,68,68	0
60	MG	CA	3238	1/1	0.85	0.13	73,73,73,73	0
60	MG	DA	1729	1/1	0.85	0.15	82,82,82,82	0
60	MG	BX	113	1/1	0.85	0.07	78,78,78,78	0
60	MG	AA	3270	1/1	0.85	0.33	92,92,92,92	0
60	MG	CA	3623	1/1	0.85	0.21	71,71,71,71	0
60	MG	CA	3629	1/1	0.85	0.16	74,74,74,74	0
60	MG	CA	3098	1/1	0.85	0.33	90,90,90,90	0
60	MG	BA	1760	1/1	0.85	0.16	68,68,68,68	0
60	MG	CA	3498	1/1	0.85	0.24	68,68,68,68	0
60	MG	CA	3503	1/1	0.85	0.09	67,67,67,67	0
60	MG	AE	304	1/1	0.85	0.17	70,70,70,70	0
60	MG	CA	3275	1/1	0.85	0.14	73,73,73,73	0
60	MG	AA	3173	1/1	0.85	0.28	74,74,74,74	0
60	MG	AA	3353	1/1	0.85	0.15	68,68,68,68	0
60	MG	CA	3515	1/1	0.85	0.15	72,72,72,72	0
60	MG	AA	3362	1/1	0.85	0.16	69,69,69,69	0
60	MG	CA	3132	1/1	0.85	0.22	67,67,67,67	0
60	MG	AA	3283	1/1	0.85	0.20	48,48,48,48	0
60	MG	CB	3006	1/1	0.85	0.17	82,82,82,82	0
60	MG	BA	1697	1/1	0.86	0.17	80,80,80,80	0
60	MG	CA	3644	1/1	0.86	0.12	60,60,60,60	0
60	MG	CA	3204	1/1	0.86	0.28	88,88,88,88	0
60	MG	A4	502	1/1	0.86	0.07	81,81,81,81	0
60	MG	AA	3559	1/1	0.86	0.12	37,37,37,37	0
60	MG	BA	1806	1/1	0.86	0.12	63,63,63,63	0
60	MG	CA	3077	1/1	0.86	0.12	62,62,62,62	0
60	MG	BA	1807	1/1	0.86	0.20	72,72,72,72	0
60	MG	AA	3671	1/1	0.86	0.23	31,31,31,31	1
60	MG	CA	3083	1/1	0.86	0.29	80,80,80,80	0
60	MG	CA	3085	1/1	0.86	0.29	82,82,82,82	0
60	MG	CA	3237	1/1	0.86	0.24	70,70,70,70	0
60	MG	AB	3005	1/1	0.86	0.18	70,70,70,70	0
60	MG	CB	3012	1/1	0.86	0.14	74,74,74,74	0
60	MG	CA	3516	1/1	0.86	0.17	58,58,58,58	0
60	MG	AA	3247	1/1	0.86	0.22	75,75,75,75	0
60	MG	CA	3090	1/1	0.86	0.28	98,98,98,98	0
60	MG	AA	3248	1/1	0.86	0.25	79,79,79,79	0
60	MG	AB	3017	1/1	0.86	0.12	76,76,76,76	0
60	MG	AA	3460	1/1	0.86	0.26	81,81,81,81	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	BA	1615	1/1	0.86	0.12	65,65,65,65	0
60	MG	BA	1622	1/1	0.86	0.22	64,64,64,64	0
60	MG	DA	1610	1/1	0.86	0.28	59,59,59,59	0
60	MG	BA	1623	1/1	0.86	0.21	67,67,67,67	0
60	MG	CA	3538	1/1	0.86	0.22	58,58,58,58	0
60	MG	CA	3539	1/1	0.86	0.16	72,72,72,72	0
60	MG	AA	3435	1/1	0.86	0.14	54,54,54,54	0
60	MG	CA	3311	1/1	0.86	0.14	54,54,54,54	0
60	MG	AA	3017	1/1	0.86	0.17	71,71,71,71	0
60	MG	AD	306	1/1	0.86	0.20	75,75,75,75	0
60	MG	DA	1636	1/1	0.86	0.30	77,77,77,77	0
60	MG	BA	1748	1/1	0.86	0.17	75,75,75,75	0
60	MG	CA	3113	1/1	0.86	0.41	75,75,75,75	0
60	MG	CA	3553	1/1	0.86	0.17	77,77,77,77	0
60	MG	CA	3560	1/1	0.86	0.15	103,103,103,103	0
60	MG	CA	3355	1/1	0.86	0.11	71,71,71,71	0
60	MG	CA	3114	1/1	0.86	0.15	59,59,59,59	0
60	MG	DA	1659	1/1	0.86	0.25	79,79,79,79	0
60	MG	DA	1668	1/1	0.86	0.14	68,68,68,68	0
60	MG	AA	3352	1/1	0.86	0.18	64,64,64,64	0
60	MG	CA	3576	1/1	0.86	0.22	91,91,91,91	0
60	MG	AD	308	1/1	0.86	0.10	54,54,54,54	0
60	MG	DA	1677	1/1	0.86	0.19	67,67,67,67	0
60	MG	CA	3582	1/1	0.86	0.10	60,60,60,60	0
60	MG	CA	3123	1/1	0.86	0.16	63,63,63,63	0
60	MG	CA	3129	1/1	0.86	0.13	76,76,76,76	0
60	MG	DA	1701	1/1	0.86	0.15	61,61,61,61	0
60	MG	CA	3021	1/1	0.86	0.34	91,91,91,91	0
60	MG	AA	3708	1/1	0.86	0.21	71,71,71,71	0
60	MG	DA	1713	1/1	0.86	0.11	59,59,59,59	0
60	MG	AE	301	1/1	0.86	0.17	65,65,65,65	0
60	MG	BA	1651	1/1	0.86	0.11	69,69,69,69	0
60	MG	CA	3032	1/1	0.86	0.31	67,67,67,67	0
60	MG	CA	3398	1/1	0.86	0.14	57,57,57,57	0
60	MG	CA	3601	1/1	0.86	0.22	61,61,61,61	0
60	MG	AA	3063	1/1	0.86	0.09	46,46,46,46	0
60	MG	CA	3409	1/1	0.86	0.21	63,63,63,63	0
60	MG	AH	201	1/1	0.86	0.29	83,83,83,83	0
60	MG	CA	3428	1/1	0.86	0.20	50,50,50,50	0
60	MG	CA	3162	1/1	0.86	0.26	57,57,57,57	0
60	MG	CA	3169	1/1	0.86	0.21	65,65,65,65	0
60	MG	CA	3173	1/1	0.86	0.26	72,72,72,72	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	AA	3495	1/1	0.86	0.23	58,58,58,58	0
60	MG	AA	3517	1/1	0.86	0.19	44,44,44,44	0
60	MG	CA	3474	1/1	0.86	0.18	72,72,72,72	0
60	MG	AA	3530	1/1	0.86	0.11	60,60,60,60	0
60	MG	DA	1759	1/1	0.86	0.24	64,64,64,64	0
60	MG	CA	3624	1/1	0.86	0.25	76,76,76,76	0
60	MG	CA	3626	1/1	0.86	0.08	52,52,52,52	0
60	MG	AA	3732	1/1	0.86	0.14	63,63,63,63	0
60	MG	A0	101	1/1	0.86	0.15	88,88,88,88	0
60	MG	AA	3541	1/1	0.86	0.14	61,61,61,61	0
60	MG	CA	3066	1/1	0.86	0.36	69,69,69,69	0
60	MG	CA	3282	1/1	0.87	0.26	75,75,75,75	0
60	MG	AA	3066	1/1	0.87	0.17	63,63,63,63	0
60	MG	CA	3291	1/1	0.87	0.09	74,74,74,74	0
60	MG	CA	3523	1/1	0.87	0.10	77,77,77,77	0
60	MG	AA	3164	1/1	0.87	0.28	106,106,106,106	0
60	MG	CA	3308	1/1	0.87	0.11	35,35,35,35	0
60	MG	AA	3046	1/1	0.87	0.19	47,47,47,47	0
60	MG	CA	3531	1/1	0.87	0.10	67,67,67,67	0
60	MG	AA	3605	1/1	0.87	0.09	66,66,66,66	0
60	MG	CD	301	1/1	0.87	0.15	61,61,61,61	0
60	MG	CA	3321	1/1	0.87	0.11	65,65,65,65	0
60	MG	CF	301	1/1	0.87	0.19	61,61,61,61	0
60	MG	BA	1614	1/1	0.87	0.20	70,70,70,70	0
60	MG	CA	3131	1/1	0.87	0.13	61,61,61,61	0
60	MG	AA	3181	1/1	0.87	0.14	55,55,55,55	0
60	MG	BA	1743	1/1	0.87	0.10	60,60,60,60	0
60	MG	AA	3479	1/1	0.87	0.09	66,66,66,66	0
60	MG	CA	3365	1/1	0.87	0.16	69,69,69,69	0
60	MG	CA	3544	1/1	0.87	0.19	74,74,74,74	0
60	MG	AA	3614	1/1	0.87	0.09	66,66,66,66	0
60	MG	BA	1757	1/1	0.87	0.18	63,63,63,63	0
60	MG	AA	3251	1/1	0.87	0.16	50,50,50,50	0
60	MG	AA	3347	1/1	0.87	0.20	63,63,63,63	0
60	MG	DA	1623	1/1	0.87	0.30	70,70,70,70	0
60	MG	BA	1766	1/1	0.87	0.16	81,81,81,81	0
60	MG	AA	3624	1/1	0.87	0.13	56,56,56,56	0
60	MG	AA	3182	1/1	0.87	0.21	73,73,73,73	0
60	MG	AA	3010	1/1	0.87	0.18	68,68,68,68	0
60	MG	AA	3266	1/1	0.87	0.17	55,55,55,55	0
60	MG	CA	3578	1/1	0.87	0.10	96,96,96,96	0
60	MG	BA	1645	1/1	0.87	0.27	58,58,58,58	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	AA	3360	1/1	0.87	0.23	72,72,72,72	0
60	MG	AA	3738	1/1	0.87	0.10	73,73,73,73	0
60	MG	BA	1653	1/1	0.87	0.18	62,62,62,62	0
60	MG	CA	3412	1/1	0.87	0.14	52,52,52,52	0
60	MG	AA	3222	1/1	0.87	0.15	58,58,58,58	0
60	MG	CA	3429	1/1	0.87	0.19	80,80,80,80	0
60	MG	DA	1672	1/1	0.87	0.19	61,61,61,61	0
60	MG	CA	3201	1/1	0.87	0.18	70,70,70,70	0
60	MG	CA	3445	1/1	0.87	0.19	70,70,70,70	0
60	MG	AA	3740	1/1	0.87	0.17	54,54,54,54	0
60	MG	DA	1678	1/1	0.87	0.29	66,66,66,66	0
60	MG	DA	1684	1/1	0.87	0.21	54,54,54,54	0
60	MG	BA	1666	1/1	0.87	0.27	70,70,70,70	0
60	MG	DA	1689	1/1	0.87	0.11	68,68,68,68	0
60	MG	CA	3603	1/1	0.87	0.30	93,93,93,93	0
60	MG	AA	3551	1/1	0.87	0.12	58,58,58,58	0
60	MG	AE	302	1/1	0.87	0.14	62,62,62,62	0
60	MG	AA	3747	1/1	0.87	0.16	65,65,65,65	0
60	MG	AA	3644	1/1	0.87	0.17	74,74,74,74	0
60	MG	AA	3380	1/1	0.87	0.19	75,75,75,75	0
60	MG	AA	3756	1/1	0.87	0.12	57,57,57,57	0
60	MG	DA	1717	1/1	0.87	0.18	70,70,70,70	0
60	MG	AA	3269	1/1	0.87	0.14	78,78,78,78	0
60	MG	CA	3617	1/1	0.87	0.12	41,41,41,41	0
60	MG	AA	3650	1/1	0.87	0.17	62,62,62,62	0
60	MG	DA	1724	1/1	0.87	0.22	74,74,74,74	0
60	MG	CA	3236	1/1	0.87	0.24	80,80,80,80	0
60	MG	AA	3186	1/1	0.87	0.21	53,53,53,53	0
60	MG	AA	3652	1/1	0.87	0.20	87,87,87,87	0
60	MG	DA	1735	1/1	0.87	0.18	75,75,75,75	0
60	MG	DA	1737	1/1	0.87	0.15	73,73,73,73	0
60	MG	CA	3239	1/1	0.87	0.23	76,76,76,76	0
60	MG	CA	3496	1/1	0.87	0.24	58,58,58,58	0
60	MG	BA	1705	1/1	0.87	0.16	61,61,61,61	0
60	MG	AA	3192	1/1	0.87	0.33	69,69,69,69	0
60	MG	CA	3633	1/1	0.87	0.14	85,85,85,85	0
60	MG	CA	3500	1/1	0.87	0.25	56,56,56,56	0
60	MG	CA	3638	1/1	0.87	0.27	68,68,68,68	0
60	MG	CA	3502	1/1	0.87	0.10	66,66,66,66	0
60	MG	DA	1752	1/1	0.87	0.24	73,73,73,73	0
60	MG	AA	3089	1/1	0.87	0.17	58,58,58,58	0
60	MG	AA	3199	1/1	0.87	0.24	61,61,61,61	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	CA	3108	1/1	0.87	0.16	84,84,84,84	0
60	MG	BA	1602	1/1	0.87	0.15	75,75,75,75	0
60	MG	CA	3647	1/1	0.87	0.24	61,61,61,61	0
60	MG	DD	502	1/1	0.87	0.23	64,64,64,64	0
60	MG	CA	3280	1/1	0.87	0.10	43,43,43,43	0
60	MG	DT	3001	1/1	0.87	0.17	59,59,59,59	0
60	MG	AA	3778	1/1	0.87	0.12	68,68,68,68	0
60	MG	CA	3655	1/1	0.87	0.29	69,69,69,69	0
60	MG	CA	3249	1/1	0.88	0.17	67,67,67,67	0
60	MG	BE	3001	1/1	0.88	0.09	83,83,83,83	0
60	MG	CB	3007	1/1	0.88	0.16	57,57,57,57	0
60	MG	CA	3255	1/1	0.88	0.25	61,61,61,61	0
60	MG	CA	3261	1/1	0.88	0.12	50,50,50,50	0
60	MG	AA	3696	1/1	0.88	0.12	62,62,62,62	0
60	MG	AA	3598	1/1	0.88	0.18	57,57,57,57	0
60	MG	CA	3270	1/1	0.88	0.23	69,69,69,69	0
60	MG	BL	202	1/1	0.88	0.10	56,56,56,56	0
60	MG	BV	101	1/1	0.88	0.12	78,78,78,78	0
60	MG	AA	3285	1/1	0.88	0.11	72,72,72,72	0
60	MG	CF	306	1/1	0.88	0.26	85,85,85,85	0
60	MG	BA	1626	1/1	0.88	0.14	72,72,72,72	0
60	MG	BX	101	1/1	0.88	0.16	63,63,63,63	0
60	MG	CR	201	1/1	0.88	0.16	63,63,63,63	0
60	MG	CA	3284	1/1	0.88	0.15	49,49,49,49	0
60	MG	DA	1605	1/1	0.88	0.21	59,59,59,59	0
60	MG	AA	3159	1/1	0.88	0.23	66,66,66,66	0
60	MG	CA	3536	1/1	0.88	0.15	95,95,95,95	0
60	MG	CA	3292	1/1	0.88	0.12	56,56,56,56	0
60	MG	AA	3317	1/1	0.88	0.14	56,56,56,56	0
60	MG	AF	307	1/1	0.88	0.16	69,69,69,69	0
60	MG	BX	106	1/1	0.88	0.14	85,85,85,85	0
60	MG	AA	3511	1/1	0.88	0.21	84,84,84,84	0
60	MG	AA	3715	1/1	0.88	0.11	62,62,62,62	0
60	MG	DA	1624	1/1	0.88	0.14	83,83,83,83	0
60	MG	BX	114	1/1	0.88	0.25	57,57,57,57	0
60	MG	DA	1628	1/1	0.88	0.21	69,69,69,69	0
60	MG	CA	3333	1/1	0.88	0.18	64,64,64,64	0
60	MG	BY	3001	1/1	0.88	0.14	78,78,78,78	0
60	MG	AA	3782	1/1	0.88	0.16	70,70,70,70	0
60	MG	CA	3555	1/1	0.88	0.08	59,59,59,59	0
60	MG	CA	3135	1/1	0.88	0.09	73,73,73,73	0
60	MG	CA	3569	1/1	0.88	0.18	71,71,71,71	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	DA	1649	1/1	0.88	0.18	53,53,53,53	0
60	MG	CA	3001	1/1	0.88	0.13	81,81,81,81	0
60	MG	DA	1656	1/1	0.88	0.10	67,67,67,67	0
60	MG	AA	3724	1/1	0.88	0.14	37,37,37,37	0
60	MG	AA	3611	1/1	0.88	0.23	57,57,57,57	0
60	MG	CA	3015	1/1	0.88	0.23	66,66,66,66	0
60	MG	DA	1664	1/1	0.88	0.24	49,49,49,49	0
60	MG	DA	1667	1/1	0.88	0.37	70,70,70,70	0
60	MG	CA	3150	1/1	0.88	0.11	52,52,52,52	0
60	MG	CA	3374	1/1	0.88	0.10	74,74,74,74	0
60	MG	BA	1754	1/1	0.88	0.09	75,75,75,75	0
60	MG	AA	3137	1/1	0.88	0.23	55,55,55,55	0
60	MG	AA	3447	1/1	0.88	0.12	44,44,44,44	0
60	MG	CA	3163	1/1	0.88	0.17	41,41,41,41	0
60	MG	BA	1758	1/1	0.88	0.13	56,56,56,56	0
60	MG	DA	1679	1/1	0.88	0.17	70,70,70,70	0
60	MG	AA	3249	1/1	0.88	0.16	64,64,64,64	0
60	MG	CA	3394	1/1	0.88	0.10	54,54,54,54	0
60	MG	CA	3595	1/1	0.88	0.20	67,67,67,67	0
60	MG	CA	3397	1/1	0.88	0.12	80,80,80,80	0
60	MG	CA	3176	1/1	0.88	0.24	60,60,60,60	0
60	MG	BA	1659	1/1	0.88	0.31	68,68,68,68	0
60	MG	CA	3407	1/1	0.88	0.14	41,41,41,41	0
60	MG	BA	1763	1/1	0.88	0.10	75,75,75,75	0
60	MG	BA	1660	1/1	0.88	0.26	55,55,55,55	0
60	MG	BA	1661	1/1	0.88	0.21	59,59,59,59	0
60	MG	CA	3610	1/1	0.88	0.32	94,94,94,94	0
60	MG	CA	3190	1/1	0.88	0.16	77,77,77,77	0
60	MG	AA	3093	1/1	0.88	0.38	81,81,81,81	0
60	MG	DA	1721	1/1	0.88	0.15	60,60,60,60	0
60	MG	CA	3440	1/1	0.88	0.24	69,69,69,69	0
60	MG	AA	3656	1/1	0.88	0.13	62,62,62,62	1
60	MG	DA	1727	1/1	0.88	0.15	65,65,65,65	0
60	MG	BA	1777	1/1	0.88	0.12	76,76,76,76	0
60	MG	CA	3200	1/1	0.88	0.11	65,65,65,65	0
60	MG	BA	1601	1/1	0.88	0.09	66,66,66,66	0
60	MG	BA	1781	1/1	0.88	0.11	63,63,63,63	0
60	MG	DA	1736	1/1	0.88	0.14	63,63,63,63	0
60	MG	AA	3657	1/1	0.88	0.15	73,73,73,73	0
60	MG	CA	3205	1/1	0.88	0.17	66,66,66,66	0
60	MG	BA	1681	1/1	0.88	0.23	69,69,69,69	0
60	MG	AA	3365	1/1	0.88	0.18	55,55,55,55	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	BA	1688	1/1	0.88	0.24	71,71,71,71	0
60	MG	CA	3213	1/1	0.88	0.12	62,62,62,62	0
60	MG	BA	1604	1/1	0.88	0.26	85,85,85,85	0
60	MG	AA	3158	1/1	0.88	0.26	50,50,50,50	0
60	MG	BA	1606	1/1	0.88	0.14	74,74,74,74	0
60	MG	AA	3474	1/1	0.88	0.13	74,74,74,74	0
60	MG	CA	3489	1/1	0.88	0.11	64,64,64,64	0
60	MG	BA	1702	1/1	0.88	0.26	56,56,56,56	0
60	MG	BA	1805	1/1	0.88	0.09	55,55,55,55	0
60	MG	AA	3412	1/1	0.88	0.08	58,58,58,58	0
60	MG	AA	3486	1/1	0.88	0.11	34,34,34,34	0
60	MG	AA	3759	1/1	0.88	0.08	29,29,29,29	0
60	MG	CA	3240	1/1	0.88	0.09	49,49,49,49	0
60	MG	AA	3175	1/1	0.88	0.19	50,50,50,50	1
60	MG	BA	1813	1/1	0.88	0.10	66,66,66,66	0
60	MG	CA	3246	1/1	0.88	0.17	79,79,79,79	0
60	MG	CO	201	1/1	0.89	0.19	72,72,72,72	0
60	MG	AA	3449	1/1	0.89	0.13	46,46,46,46	0
60	MG	CA	3050	1/1	0.89	0.18	55,55,55,55	0
60	MG	AA	3589	1/1	0.89	0.23	31,31,31,31	1
60	MG	C5	101	1/1	0.89	0.20	64,64,64,64	0
60	MG	CA	3548	1/1	0.89	0.11	53,53,53,53	0
60	MG	AP	203	1/1	0.89	0.14	70,70,70,70	0
60	MG	AA	3336	1/1	0.89	0.14	52,52,52,52	0
60	MG	BA	1667	1/1	0.89	0.10	69,69,69,69	0
60	MG	BA	1669	1/1	0.89	0.21	70,70,70,70	0
60	MG	AA	3207	1/1	0.89	0.22	67,67,67,67	0
60	MG	AA	3208	1/1	0.89	0.13	55,55,55,55	0
60	MG	CA	3570	1/1	0.89	0.11	61,61,61,61	0
60	MG	BA	1673	1/1	0.89	0.32	63,63,63,63	0
60	MG	AA	3209	1/1	0.89	0.14	64,64,64,64	0
60	MG	AA	3772	1/1	0.89	0.25	37,37,37,37	0
60	MG	BA	1684	1/1	0.89	0.18	64,64,64,64	0
60	MG	AA	3051	1/1	0.89	0.39	84,84,84,84	0
60	MG	AA	3088	1/1	0.89	0.18	42,42,42,42	0
60	MG	BA	1690	1/1	0.89	0.19	59,59,59,59	0
60	MG	DA	1634	1/1	0.89	0.21	66,66,66,66	0
60	MG	AA	3609	1/1	0.89	0.14	57,57,57,57	0
60	MG	BA	1693	1/1	0.89	0.12	69,69,69,69	0
60	MG	CA	3411	1/1	0.89	0.11	49,49,49,49	0
60	MG	AA	3130	1/1	0.89	0.15	59,59,59,59	0
60	MG	CA	3589	1/1	0.89	0.14	67,67,67,67	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	CA	3590	1/1	0.89	0.26	78,78,78,78	0
60	MG	AA	3161	1/1	0.89	0.38	89,89,89,89	0
60	MG	CA	3218	1/1	0.89	0.31	63,63,63,63	0
60	MG	CA	3593	1/1	0.89	0.13	62,62,62,62	0
60	MG	CA	3431	1/1	0.89	0.16	80,80,80,80	0
60	MG	DA	1661	1/1	0.89	0.21	74,74,74,74	0
60	MG	AA	3788	1/1	0.89	0.24	64,64,64,64	0
60	MG	BA	1700	1/1	0.89	0.20	62,62,62,62	0
60	MG	AA	3230	1/1	0.89	0.29	55,55,55,55	0
60	MG	CA	3228	1/1	0.89	0.32	68,68,68,68	0
60	MG	CA	3232	1/1	0.89	0.15	69,69,69,69	0
60	MG	CA	3093	1/1	0.89	0.21	77,77,77,77	0
60	MG	AA	3193	1/1	0.89	0.19	63,63,63,63	0
60	MG	AA	3795	1/1	0.89	0.15	26,26,26,26	1
60	MG	AA	3800	1/1	0.89	0.16	59,59,59,59	0
60	MG	AA	3494	1/1	0.89	0.08	66,66,66,66	0
60	MG	DA	1682	1/1	0.89	0.24	60,60,60,60	0
60	MG	AA	3369	1/1	0.89	0.13	59,59,59,59	0
60	MG	AA	3816	1/1	0.89	0.18	49,49,49,49	0
60	MG	CA	3102	1/1	0.89	0.15	50,50,50,50	0
60	MG	AA	3056	1/1	0.89	0.27	72,72,72,72	0
60	MG	BA	1620	1/1	0.89	0.13	60,60,60,60	0
60	MG	CA	3487	1/1	0.89	0.12	64,64,64,64	0
60	MG	BA	1621	1/1	0.89	0.30	78,78,78,78	0
60	MG	DA	1710	1/1	0.89	0.12	56,56,56,56	0
60	MG	CA	3112	1/1	0.89	0.33	76,76,76,76	0
60	MG	AA	3516	1/1	0.89	0.16	38,38,38,38	0
60	MG	BA	1730	1/1	0.89	0.20	68,68,68,68	0
60	MG	CA	3118	1/1	0.89	0.12	67,67,67,67	0
60	MG	CA	3632	1/1	0.89	0.10	55,55,55,55	0
60	MG	CA	3119	1/1	0.89	0.22	63,63,63,63	0
60	MG	DA	1720	1/1	0.89	0.09	61,61,61,61	0
60	MG	AA	3242	1/1	0.89	0.15	69,69,69,69	0
60	MG	CA	3271	1/1	0.89	0.12	59,59,59,59	0
60	MG	AA	3525	1/1	0.89	0.15	45,45,45,45	0
60	MG	AA	3061	1/1	0.89	0.35	64,64,64,64	0
60	MG	CA	3124	1/1	0.89	0.29	68,68,68,68	0
60	MG	CA	3126	1/1	0.89	0.29	71,71,71,71	0
60	MG	AA	3537	1/1	0.89	0.10	90,90,90,90	0
60	MG	CA	3512	1/1	0.89	0.09	58,58,58,58	0
60	MG	AA	3165	1/1	0.89	0.23	64,64,64,64	0
60	MG	AA	3146	1/1	0.89	0.14	53,53,53,53	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	CA	3517	1/1	0.89	0.16	75,75,75,75	0
60	MG	AA	3147	1/1	0.89	0.22	52,52,52,52	0
60	MG	AA	3743	1/1	0.89	0.11	66,66,66,66	0
60	MG	CA	3301	1/1	0.89	0.20	56,56,56,56	0
60	MG	DA	1747	1/1	0.89	0.10	67,67,67,67	0
60	MG	CA	3663	1/1	0.89	0.20	74,74,74,74	0
60	MG	CA	3302	1/1	0.89	0.09	67,67,67,67	0
60	MG	CB	3004	1/1	0.89	0.12	70,70,70,70	0
60	MG	AA	3568	1/1	0.89	0.10	23,23,23,23	0
60	MG	AA	3573	1/1	0.89	0.08	47,47,47,47	0
60	MG	BA	1647	1/1	0.89	0.10	57,57,57,57	0
60	MG	CA	3144	1/1	0.89	0.22	84,84,84,84	0
60	MG	DA	1762	1/1	0.89	0.10	86,86,86,86	0
60	MG	CA	3146	1/1	0.89	0.32	79,79,79,79	0
60	MG	CA	3029	1/1	0.89	0.19	68,68,68,68	0
60	MG	CA	3338	1/1	0.89	0.12	58,58,58,58	0
60	MG	CD	302	1/1	0.89	0.17	51,51,51,51	0
60	MG	AA	3752	1/1	0.89	0.18	75,75,75,75	0
60	MG	DJ	5001	1/1	0.89	0.11	94,94,94,94	0
60	MG	AA	3156	1/1	0.89	0.13	46,46,46,46	0
60	MG	AA	3444	1/1	0.89	0.09	52,52,52,52	0
60	MG	AA	3331	1/1	0.89	0.18	61,61,61,61	0
60	MG	CA	3033	1/1	0.90	0.08	47,47,47,47	0
60	MG	CA	3127	1/1	0.90	0.17	68,68,68,68	0
60	MG	CA	3039	1/1	0.90	0.27	76,76,76,76	0
60	MG	DA	1621	1/1	0.90	0.08	69,69,69,69	0
60	MG	AF	305	1/1	0.90	0.17	42,42,42,42	0
60	MG	BA	1789	1/1	0.90	0.08	68,68,68,68	0
60	MG	CA	3134	1/1	0.90	0.22	64,64,64,64	0
60	MG	CA	3049	1/1	0.90	0.18	63,63,63,63	0
60	MG	AA	3095	1/1	0.90	0.11	58,58,58,58	0
60	MG	DA	1631	1/1	0.90	0.16	55,55,55,55	0
60	MG	CA	3052	1/1	0.90	0.13	46,46,46,46	0
60	MG	BA	1793	1/1	0.90	0.08	68,68,68,68	0
60	MG	CA	3141	1/1	0.90	0.22	51,51,51,51	0
60	MG	CA	3486	1/1	0.90	0.08	48,48,48,48	0
60	MG	BA	1798	1/1	0.90	0.17	62,62,62,62	0
60	MG	DA	1646	1/1	0.90	0.20	51,51,51,51	0
60	MG	AA	3779	1/1	0.90	0.14	41,41,41,41	0
60	MG	CA	3145	1/1	0.90	0.22	65,65,65,65	0
60	MG	AA	3150	1/1	0.90	0.24	63,63,63,63	0
60	MG	CA	3492	1/1	0.90	0.18	60,60,60,60	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	CA	3287	1/1	0.90	0.18	43,43,43,43	0
60	MG	CA	3059	1/1	0.90	0.27	66,66,66,66	0
60	MG	CA	3151	1/1	0.90	0.23	66,66,66,66	0
60	MG	AA	3073	1/1	0.90	0.20	61,61,61,61	0
60	MG	DA	1662	1/1	0.90	0.12	51,51,51,51	0
60	MG	CA	3501	1/1	0.90	0.14	78,78,78,78	0
60	MG	CA	3300	1/1	0.90	0.13	56,56,56,56	0
60	MG	AA	3279	1/1	0.90	0.28	62,62,62,62	0
60	MG	DA	1670	1/1	0.90	0.22	74,74,74,74	0
60	MG	AV	203	1/1	0.90	0.12	39,39,39,39	0
60	MG	BA	1710	1/1	0.90	0.21	83,83,83,83	0
60	MG	AA	3282	1/1	0.90	0.31	65,65,65,65	0
60	MG	CA	3630	1/1	0.90	0.15	91,91,91,91	0
60	MG	BA	1713	1/1	0.90	0.18	61,61,61,61	0
60	MG	AA	3214	1/1	0.90	0.09	47,47,47,47	0
60	MG	CA	3514	1/1	0.90	0.10	68,68,68,68	0
60	MG	CA	3634	1/1	0.90	0.16	82,82,82,82	0
60	MG	CA	3074	1/1	0.90	0.17	64,64,64,64	0
60	MG	CA	3178	1/1	0.90	0.23	54,54,54,54	0
60	MG	CA	3639	1/1	0.90	0.18	54,54,54,54	0
60	MG	CA	3640	1/1	0.90	0.10	47,47,47,47	0
60	MG	DA	1696	1/1	0.90	0.19	65,65,65,65	0
60	MG	CA	3075	1/1	0.90	0.14	51,51,51,51	0
60	MG	DA	1700	1/1	0.90	0.19	66,66,66,66	0
60	MG	AA	3059	1/1	0.90	0.30	62,62,62,62	0
60	MG	AA	3055	1/1	0.90	0.16	61,61,61,61	0
60	MG	A2	3001	1/1	0.90	0.11	62,62,62,62	0
60	MG	BA	1723	1/1	0.90	0.13	61,61,61,61	0
60	MG	AA	3298	1/1	0.90	0.09	28,28,28,28	0
60	MG	AA	3372	1/1	0.90	0.17	59,59,59,59	0
60	MG	CA	3652	1/1	0.90	0.21	79,79,79,79	0
60	MG	AA	3300	1/1	0.90	0.11	43,43,43,43	0
60	MG	AA	3745	1/1	0.90	0.17	42,42,42,42	0
60	MG	AA	3403	1/1	0.90	0.09	55,55,55,55	0
60	MG	AA	3310	1/1	0.90	0.14	37,37,37,37	0
60	MG	CA	3660	1/1	0.90	0.13	65,65,65,65	0
60	MG	AA	3028	1/1	0.90	0.17	40,40,40,40	1
60	MG	CA	3662	1/1	0.90	0.20	60,60,60,60	0
60	MG	CA	3383	1/1	0.90	0.24	66,66,66,66	0
60	MG	AA	3672	1/1	0.90	0.18	71,71,71,71	0
60	MG	DA	1733	1/1	0.90	0.09	73,73,73,73	0
60	MG	CB	3001	1/1	0.90	0.16	68,68,68,68	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	AA	3318	1/1	0.90	0.14	64,64,64,64	0
60	MG	BA	1672	1/1	0.90	0.19	61,61,61,61	0
60	MG	AA	3160	1/1	0.90	0.26	96,96,96,96	0
60	MG	AA	3254	1/1	0.90	0.16	47,47,47,47	0
60	MG	CA	3219	1/1	0.90	0.15	57,57,57,57	0
60	MG	BA	1675	1/1	0.90	0.15	50,50,50,50	0
60	MG	DA	1742	1/1	0.90	0.14	52,52,52,52	0
60	MG	AA	3618	1/1	0.90	0.09	39,39,39,39	0
60	MG	DA	1746	1/1	0.90	0.20	67,67,67,67	0
60	MG	BA	1765	1/1	0.90	0.24	67,67,67,67	0
60	MG	BA	1682	1/1	0.90	0.20	71,71,71,71	0
60	MG	AA	3110	1/1	0.90	0.23	57,57,57,57	0
60	MG	AA	3233	1/1	0.90	0.28	85,85,85,85	0
60	MG	BA	1618	1/1	0.90	0.28	54,54,54,54	0
60	MG	CA	3419	1/1	0.90	0.17	55,55,55,55	0
60	MG	CA	3420	1/1	0.90	0.15	50,50,50,50	0
60	MG	DA	1754	1/1	0.90	0.10	77,77,77,77	0
60	MG	AA	3445	1/1	0.90	0.11	59,59,59,59	0
60	MG	DA	1761	1/1	0.90	0.07	68,68,68,68	0
60	MG	AA	3234	1/1	0.90	0.11	58,58,58,58	0
60	MG	CA	3023	1/1	0.90	0.11	56,56,56,56	0
60	MG	CA	3577	1/1	0.90	0.12	52,52,52,52	0
60	MG	CA	3433	1/1	0.90	0.09	45,45,45,45	0
60	MG	AA	3448	1/1	0.90	0.16	74,74,74,74	0
60	MG	DA	1606	1/1	0.90	0.08	66,66,66,66	0
60	MG	DF	3001	1/1	0.90	0.10	53,53,53,53	0
60	MG	AA	3162	1/1	0.90	0.13	35,35,35,35	0
60	MG	AE	305	1/1	0.90	0.23	44,44,44,44	0
60	MG	CA	3451	1/1	0.90	0.15	78,78,78,78	0
60	MG	BA	1625	1/1	0.90	0.19	53,53,53,53	0
60	MG	AA	3751	1/1	0.91	0.10	76,76,76,76	0
60	MG	BA	1664	1/1	0.91	0.29	64,64,64,64	0
60	MG	BA	1665	1/1	0.91	0.26	68,68,68,68	0
60	MG	AA	3094	1/1	0.91	0.35	82,82,82,82	0
60	MG	CA	3495	1/1	0.91	0.12	64,64,64,64	0
60	MG	AA	3117	1/1	0.91	0.12	64,64,64,64	0
60	MG	AA	3586	1/1	0.91	0.17	75,75,75,75	0
60	MG	AA	3358	1/1	0.91	0.09	72,72,72,72	0
60	MG	CA	3084	1/1	0.91	0.37	73,73,73,73	0
60	MG	AA	3757	1/1	0.91	0.22	67,67,67,67	0
60	MG	CA	3242	1/1	0.91	0.22	48,48,48,48	0
60	MG	BA	1796	1/1	0.91	0.11	75,75,75,75	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	CA	3504	1/1	0.91	0.16	77,77,77,77	0
60	MG	CF	302	1/1	0.91	0.22	64,64,64,64	0
60	MG	CA	3088	1/1	0.91	0.45	85,85,85,85	0
60	MG	AA	3758	1/1	0.91	0.15	70,70,70,70	0
60	MG	CG	3001	1/1	0.91	0.21	66,66,66,66	0
60	MG	AA	3252	1/1	0.91	0.22	76,76,76,76	0
60	MG	AA	3760	1/1	0.91	0.12	50,50,50,50	0
60	MG	CA	3251	1/1	0.91	0.16	62,62,62,62	0
60	MG	CA	3513	1/1	0.91	0.19	109,109,109,109	0
60	MG	CV	201	1/1	0.91	0.12	84,84,84,84	0
60	MG	C0	102	1/1	0.91	0.07	56,56,56,56	0
60	MG	AA	3060	1/1	0.91	0.12	23,23,23,23	0
60	MG	BA	1677	1/1	0.91	0.25	57,57,57,57	0
60	MG	AA	3660	1/1	0.91	0.28	58,58,58,58	0
60	MG	CA	3266	1/1	0.91	0.24	67,67,67,67	0
60	MG	AA	3151	1/1	0.91	0.18	63,63,63,63	0
60	MG	AA	3670	1/1	0.91	0.16	66,66,66,66	0
60	MG	A0	105	1/1	0.91	0.09	52,52,52,52	0
60	MG	AA	3769	1/1	0.91	0.37	48,48,48,48	1
60	MG	CA	3526	1/1	0.91	0.08	69,69,69,69	0
60	MG	BA	1689	1/1	0.91	0.21	65,65,65,65	0
60	MG	AA	3309	1/1	0.91	0.15	72,72,72,72	0
60	MG	AA	3484	1/1	0.91	0.18	48,48,48,48	0
60	MG	CA	3106	1/1	0.91	0.09	45,45,45,45	0
60	MG	AA	3680	1/1	0.91	0.10	70,70,70,70	0
60	MG	CA	3285	1/1	0.91	0.07	41,41,41,41	0
60	MG	BA	1694	1/1	0.91	0.22	78,78,78,78	0
60	MG	CA	3290	1/1	0.91	0.15	61,61,61,61	0
60	MG	BN	502	1/1	0.91	0.18	64,64,64,64	0
60	MG	BN	503	1/1	0.91	0.11	61,61,61,61	0
60	MG	DA	1633	1/1	0.91	0.31	67,67,67,67	0
60	MG	AA	3001	1/1	0.91	0.15	39,39,39,39	0
60	MG	CA	3295	1/1	0.91	0.13	55,55,55,55	0
60	MG	AA	3240	1/1	0.91	0.30	39,39,39,39	0
60	MG	DA	1641	1/1	0.91	0.07	55,55,55,55	0
60	MG	AA	3691	1/1	0.91	0.10	51,51,51,51	0
60	MG	AA	3780	1/1	0.91	0.17	51,51,51,51	1
60	MG	CA	3305	1/1	0.91	0.19	64,64,64,64	0
60	MG	AA	3381	1/1	0.91	0.09	34,34,34,34	0
60	MG	AA	3015	1/1	0.91	0.30	74,74,74,74	0
60	MG	DA	1655	1/1	0.91	0.19	72,72,72,72	0
60	MG	BX	104	1/1	0.91	0.20	67,67,67,67	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	BA	1608	1/1	0.91	0.09	52,52,52,52	0
60	MG	CA	3564	1/1	0.91	0.11	33,33,33,33	0
60	MG	AA	3695	1/1	0.91	0.12	50,50,50,50	0
60	MG	BX	110	1/1	0.91	0.22	67,67,67,67	0
60	MG	CA	3334	1/1	0.91	0.07	56,56,56,56	0
60	MG	BX	111	1/1	0.91	0.07	67,67,67,67	0
60	MG	DA	1665	1/1	0.91	0.12	57,57,57,57	0
60	MG	CA	3339	1/1	0.91	0.20	75,75,75,75	0
60	MG	AA	3408	1/1	0.91	0.09	41,41,41,41	0
60	MG	AA	3698	1/1	0.91	0.17	51,51,51,51	1
60	MG	AA	3701	1/1	0.91	0.26	62,62,62,62	0
60	MG	AA	3797	1/1	0.91	0.18	60,60,60,60	0
60	MG	CA	3363	1/1	0.91	0.10	55,55,55,55	0
60	MG	DA	1674	1/1	0.91	0.15	60,60,60,60	0
60	MG	AA	3041	1/1	0.91	0.19	41,41,41,41	0
60	MG	AA	3414	1/1	0.91	0.10	43,43,43,43	0
60	MG	BA	1716	1/1	0.91	0.18	71,71,71,71	0
60	MG	AA	3021	1/1	0.91	0.15	49,49,49,49	0
60	MG	AA	3811	1/1	0.91	0.26	65,65,65,65	0
60	MG	DA	1683	1/1	0.91	0.26	60,60,60,60	0
60	MG	AA	3812	1/1	0.91	0.16	78,78,78,78	0
60	MG	AA	3177	1/1	0.91	0.09	43,43,43,43	0
60	MG	CA	3382	1/1	0.91	0.15	70,70,70,70	0
60	MG	DA	1694	1/1	0.91	0.18	60,60,60,60	0
60	MG	AA	3817	1/1	0.91	0.22	72,72,72,72	0
60	MG	AB	3001	1/1	0.91	0.13	80,80,80,80	0
60	MG	DA	1698	1/1	0.91	0.15	75,75,75,75	0
60	MG	CA	3596	1/1	0.91	0.08	75,75,75,75	0
60	MG	CA	3026	1/1	0.91	0.23	55,55,55,55	0
60	MG	BA	1628	1/1	0.91	0.22	59,59,59,59	0
60	MG	CA	3156	1/1	0.91	0.27	92,92,92,92	0
60	MG	DA	1706	1/1	0.91	0.15	70,70,70,70	0
60	MG	DA	1707	1/1	0.91	0.09	79,79,79,79	0
60	MG	DA	1709	1/1	0.91	0.14	57,57,57,57	0
60	MG	CA	3158	1/1	0.91	0.17	54,54,54,54	0
60	MG	AA	3436	1/1	0.91	0.09	31,31,31,31	0
60	MG	AA	3275	1/1	0.91	0.17	56,56,56,56	0
60	MG	CA	3399	1/1	0.91	0.13	45,45,45,45	0
60	MG	CA	3168	1/1	0.91	0.16	65,65,65,65	0
60	MG	AA	3439	1/1	0.91	0.14	43,43,43,43	0
60	MG	CA	3612	1/1	0.91	0.10	59,59,59,59	0
60	MG	CA	3170	1/1	0.91	0.34	68,68,68,68	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	AA	3277	1/1	0.91	0.22	48,48,48,48	0
60	MG	CA	3175	1/1	0.91	0.13	59,59,59,59	0
60	MG	CA	3036	1/1	0.91	0.23	65,65,65,65	0
60	MG	DA	1725	1/1	0.91	0.13	78,78,78,78	0
60	MG	CA	3037	1/1	0.91	0.22	65,65,65,65	0
60	MG	AA	3632	1/1	0.91	0.15	97,97,97,97	0
60	MG	CA	3423	1/1	0.91	0.12	57,57,57,57	0
60	MG	CA	3427	1/1	0.91	0.15	69,69,69,69	0
60	MG	CA	3041	1/1	0.91	0.30	67,67,67,67	0
60	MG	BA	1642	1/1	0.91	0.18	59,59,59,59	0
60	MG	CA	3628	1/1	0.91	0.12	76,76,76,76	0
60	MG	BA	1756	1/1	0.91	0.17	43,43,43,43	0
60	MG	CA	3045	1/1	0.91	0.14	68,68,68,68	0
60	MG	CA	3048	1/1	0.91	0.19	48,48,48,48	0
60	MG	BA	1643	1/1	0.91	0.13	56,56,56,56	0
60	MG	AA	3633	1/1	0.91	0.13	51,51,51,51	0
60	MG	AA	3441	1/1	0.91	0.07	62,62,62,62	0
60	MG	AA	3558	1/1	0.91	0.15	72,72,72,72	0
60	MG	AA	3278	1/1	0.91	0.32	58,58,58,58	0
60	MG	CA	3463	1/1	0.91	0.27	75,75,75,75	0
60	MG	BA	1652	1/1	0.91	0.14	65,65,65,65	0
60	MG	CA	3641	1/1	0.91	0.36	59,59,59,59	0
60	MG	CA	3466	1/1	0.91	0.12	56,56,56,56	0
60	MG	AA	3642	1/1	0.91	0.17	60,60,60,60	0
60	MG	CA	3469	1/1	0.91	0.32	76,76,76,76	0
60	MG	CA	3470	1/1	0.91	0.12	55,55,55,55	0
60	MG	CA	3472	1/1	0.91	0.20	49,49,49,49	0
60	MG	AA	3180	1/1	0.91	0.11	53,53,53,53	0
60	MG	BA	1772	1/1	0.91	0.17	51,51,51,51	0
60	MG	BA	1773	1/1	0.91	0.16	69,69,69,69	0
60	MG	CA	3480	1/1	0.91	0.09	61,61,61,61	0
60	MG	CA	3654	1/1	0.91	0.30	76,76,76,76	0
60	MG	AA	3344	1/1	0.91	0.14	65,65,65,65	0
60	MG	BA	1658	1/1	0.91	0.29	68,68,68,68	0
60	MG	AA	3281	1/1	0.91	0.28	38,38,38,38	0
60	MG	AA	3228	1/1	0.91	0.20	63,63,63,63	0
60	MG	CA	3222	1/1	0.91	0.42	81,81,81,81	0
60	MG	CA	3071	1/1	0.91	0.17	53,53,53,53	0
60	MG	CA	3072	1/1	0.91	0.17	54,54,54,54	0
60	MG	AA	3809	1/1	0.92	0.09	46,46,46,46	0
60	MG	CA	3210	1/1	0.92	0.18	44,44,44,44	0
60	MG	DA	1619	1/1	0.92	0.18	50,50,50,50	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	AA	3092	1/1	0.92	0.22	41,41,41,41	0
60	MG	AA	3637	1/1	0.92	0.12	54,54,54,54	0
60	MG	CA	3214	1/1	0.92	0.16	50,50,50,50	0
60	MG	CA	3418	1/1	0.92	0.15	53,53,53,53	0
60	MG	CA	3215	1/1	0.92	0.33	50,50,50,50	0
60	MG	AA	3813	1/1	0.92	0.21	68,68,68,68	0
60	MG	AA	3731	1/1	0.92	0.09	34,34,34,34	0
60	MG	AA	3032	1/1	0.92	0.23	62,62,62,62	0
60	MG	AA	3437	1/1	0.92	0.08	25,25,25,25	0
60	MG	AA	3276	1/1	0.92	0.20	64,64,64,64	0
60	MG	BA	1708	1/1	0.92	0.18	55,55,55,55	0
60	MG	AA	3034	1/1	0.92	0.22	84,84,84,84	0
60	MG	DA	1639	1/1	0.92	0.14	59,59,59,59	0
60	MG	AA	3341	1/1	0.92	0.17	74,74,74,74	0
60	MG	AB	3010	1/1	0.92	0.06	56,56,56,56	1
60	MG	BA	1627	1/1	0.92	0.11	63,63,63,63	0
60	MG	DA	1644	1/1	0.92	0.17	49,49,49,49	0
60	MG	DA	1645	1/1	0.92	0.28	58,58,58,58	0
60	MG	AB	3013	1/1	0.92	0.09	55,55,55,55	0
60	MG	AA	3194	1/1	0.92	0.20	58,58,58,58	0
60	MG	CA	3602	1/1	0.92	0.07	49,49,49,49	0
60	MG	AA	3571	1/1	0.92	0.09	53,53,53,53	0
60	MG	DA	1654	1/1	0.92	0.24	48,48,48,48	0
60	MG	BA	1632	1/1	0.92	0.26	60,60,60,60	0
60	MG	CA	3606	1/1	0.92	0.11	58,58,58,58	0
60	MG	AB	3018	1/1	0.92	0.07	76,76,76,76	0
60	MG	BX	107	1/1	0.92	0.20	69,69,69,69	0
60	MG	CA	3609	1/1	0.92	0.10	62,62,62,62	0
60	MG	DA	1660	1/1	0.92	0.19	81,81,81,81	0
60	MG	BX	109	1/1	0.92	0.23	55,55,55,55	0
60	MG	AA	3215	1/1	0.92	0.09	48,48,48,48	0
60	MG	BA	1725	1/1	0.92	0.20	52,52,52,52	0
60	MG	BA	1726	1/1	0.92	0.14	59,59,59,59	0
60	MG	BA	1727	1/1	0.92	0.24	53,53,53,53	0
60	MG	AA	3280	1/1	0.92	0.21	63,63,63,63	0
60	MG	CA	3477	1/1	0.92	0.17	65,65,65,65	0
60	MG	AA	3220	1/1	0.92	0.14	65,65,65,65	0
60	MG	CA	3260	1/1	0.92	0.10	59,59,59,59	0
60	MG	BA	1735	1/1	0.92	0.11	58,58,58,58	0
60	MG	CA	3120	1/1	0.92	0.12	47,47,47,47	0
60	MG	AA	3029	1/1	0.92	0.11	50,50,50,50	0
60	MG	CA	3003	1/1	0.92	0.20	49,49,49,49	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	AA	3581	1/1	0.92	0.13	48,48,48,48	0
60	MG	AA	3196	1/1	0.92	0.19	48,48,48,48	0
60	MG	AA	3197	1/1	0.92	0.22	42,42,42,42	0
60	MG	AA	3080	1/1	0.92	0.26	54,54,54,54	0
60	MG	CA	3018	1/1	0.92	0.08	59,59,59,59	0
60	MG	CA	3490	1/1	0.92	0.18	81,81,81,81	0
60	MG	BA	1751	1/1	0.92	0.16	49,49,49,49	0
60	MG	DA	1690	1/1	0.92	0.08	74,74,74,74	0
60	MG	DA	1691	1/1	0.92	0.17	66,66,66,66	0
60	MG	AA	3293	1/1	0.92	0.13	68,68,68,68	0
60	MG	AA	3459	1/1	0.92	0.12	65,65,65,65	0
60	MG	BA	1655	1/1	0.92	0.17	65,65,65,65	0
60	MG	CA	3286	1/1	0.92	0.11	62,62,62,62	0
60	MG	AA	3297	1/1	0.92	0.08	56,56,56,56	0
60	MG	AA	3260	1/1	0.92	0.28	67,67,67,67	0
60	MG	AF	306	1/1	0.92	0.17	54,54,54,54	0
60	MG	CA	3140	1/1	0.92	0.33	54,54,54,54	0
60	MG	AA	3675	1/1	0.92	0.10	67,67,67,67	0
60	MG	AA	3262	1/1	0.92	0.46	70,70,70,70	0
60	MG	DA	1708	1/1	0.92	0.15	67,67,67,67	0
60	MG	AA	3687	1/1	0.92	0.07	48,48,48,48	0
60	MG	BA	1662	1/1	0.92	0.13	45,45,45,45	0
60	MG	BA	1663	1/1	0.92	0.12	66,66,66,66	0
60	MG	BA	1770	1/1	0.92	0.11	62,62,62,62	0
60	MG	AA	3768	1/1	0.92	0.19	67,67,67,67	0
60	MG	AA	3100	1/1	0.92	0.12	34,34,34,34	0
60	MG	CA	3154	1/1	0.92	0.12	68,68,68,68	0
60	MG	AU	203	1/1	0.92	0.15	55,55,55,55	0
60	MG	CA	3322	1/1	0.92	0.16	41,41,41,41	0
60	MG	CA	3046	1/1	0.92	0.12	72,72,72,72	0
60	MG	CA	3331	1/1	0.92	0.24	62,62,62,62	0
60	MG	AA	3135	1/1	0.92	0.17	53,53,53,53	0
60	MG	AA	3388	1/1	0.92	0.09	55,55,55,55	0
60	MG	AA	3399	1/1	0.92	0.13	51,51,51,51	0
60	MG	CB	3002	1/1	0.92	0.12	78,78,78,78	0
60	MG	CA	3051	1/1	0.92	0.15	52,52,52,52	0
60	MG	DA	1731	1/1	0.92	0.10	51,51,51,51	0
60	MG	AA	3315	1/1	0.92	0.17	56,56,56,56	0
60	MG	AA	3101	1/1	0.92	0.34	68,68,68,68	0
60	MG	AA	3491	1/1	0.92	0.15	40,40,40,40	0
60	MG	AA	3065	1/1	0.92	0.23	51,51,51,51	0
60	MG	AA	3700	1/1	0.92	0.10	48,48,48,48	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	CA	3058	1/1	0.92	0.39	74,74,74,74	0
60	MG	AA	3620	1/1	0.92	0.09	49,49,49,49	0
60	MG	A6	102	1/1	0.92	0.18	69,69,69,69	0
60	MG	CD	303	1/1	0.92	0.07	70,70,70,70	0
60	MG	CE	303	1/1	0.92	0.19	55,55,55,55	0
60	MG	DA	1745	1/1	0.92	0.13	54,54,54,54	0
60	MG	AA	3206	1/1	0.92	0.15	55,55,55,55	0
60	MG	BA	1794	1/1	0.92	0.17	63,63,63,63	0
60	MG	CA	3188	1/1	0.92	0.25	55,55,55,55	0
60	MG	AA	3622	1/1	0.92	0.07	52,52,52,52	0
60	MG	CA	3379	1/1	0.92	0.10	62,62,62,62	0
60	MG	AA	3498	1/1	0.92	0.08	56,56,56,56	0
60	MG	AA	3049	1/1	0.92	0.07	35,35,35,35	0
60	MG	CA	3196	1/1	0.92	0.13	57,57,57,57	0
60	MG	CA	3551	1/1	0.92	0.12	76,76,76,76	0
60	MG	DA	1755	1/1	0.92	0.12	69,69,69,69	0
60	MG	CA	3197	1/1	0.92	0.17	48,48,48,48	0
60	MG	AA	3421	1/1	0.92	0.13	73,73,73,73	0
60	MG	CA	3554	1/1	0.92	0.10	60,60,60,60	0
60	MG	C3	101	1/1	0.92	0.19	91,91,91,91	0
60	MG	CA	3390	1/1	0.92	0.10	42,42,42,42	0
60	MG	BA	1802	1/1	0.92	0.11	58,58,58,58	0
60	MG	DA	1768	1/1	0.92	0.09	57,57,57,57	0
60	MG	AA	3433	1/1	0.92	0.16	50,50,50,50	0
60	MG	CA	3396	1/1	0.92	0.14	59,59,59,59	0
60	MG	AA	3718	1/1	0.92	0.12	40,40,40,40	0
60	MG	AA	3803	1/1	0.92	0.15	37,37,37,37	0
60	MG	DK	202	1/1	0.92	0.09	80,80,80,80	0
60	MG	DA	1609	1/1	0.92	0.11	49,49,49,49	0
60	MG	AA	3434	1/1	0.92	0.13	58,58,58,58	0
60	MG	AA	3807	1/1	0.92	0.13	62,62,62,62	0
60	MG	BA	1801	1/1	0.93	0.10	55,55,55,55	0
60	MG	BA	1668	1/1	0.93	0.15	72,72,72,72	0
60	MG	CA	3253	1/1	0.93	0.22	61,61,61,61	0
60	MG	CA	3499	1/1	0.93	0.13	68,68,68,68	0
60	MG	AA	3492	1/1	0.93	0.09	41,41,41,41	0
60	MG	AA	3176	1/1	0.93	0.22	70,70,70,70	0
60	MG	AA	3626	1/1	0.93	0.22	59,59,59,59	0
60	MG	CA	3262	1/1	0.93	0.18	59,59,59,59	0
60	MG	AA	3628	1/1	0.93	0.15	62,62,62,62	0
60	MG	CQ	202	1/1	0.93	0.17	56,56,56,56	0
60	MG	AA	3316	1/1	0.93	0.17	64,64,64,64	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	CQ	204	1/1	0.93	0.12	74,74,74,74	0
60	MG	AA	3140	1/1	0.93	0.09	66,66,66,66	0
60	MG	CU	201	1/1	0.93	0.16	62,62,62,62	0
60	MG	CA	3269	1/1	0.93	0.25	64,64,64,64	0
60	MG	CV	202	1/1	0.93	0.19	82,82,82,82	0
60	MG	CA	3509	1/1	0.93	0.09	52,52,52,52	0
60	MG	CA	3510	1/1	0.93	0.15	71,71,71,71	0
60	MG	AG	201	1/1	0.93	0.12	59,59,59,59	0
60	MG	DA	1602	1/1	0.93	0.09	65,65,65,65	0
60	MG	CA	3104	1/1	0.93	0.15	64,64,64,64	0
60	MG	BA	1676	1/1	0.93	0.15	39,39,39,39	0
60	MG	CA	3107	1/1	0.93	0.10	64,64,64,64	0
60	MG	BB	3001	1/1	0.93	0.19	67,67,67,67	0
60	MG	CA	3109	1/1	0.93	0.10	65,65,65,65	0
60	MG	BD	502	1/1	0.93	0.19	56,56,56,56	0
60	MG	AG	203	1/1	0.93	0.09	69,69,69,69	0
60	MG	AA	3503	1/1	0.93	0.10	41,41,41,41	0
60	MG	AA	3748	1/1	0.93	0.17	62,62,62,62	0
60	MG	CA	3115	1/1	0.93	0.12	71,71,71,71	0
60	MG	CA	3116	1/1	0.93	0.30	57,57,57,57	0
60	MG	BA	1683	1/1	0.93	0.13	50,50,50,50	0
60	MG	AN	3002	1/1	0.93	0.15	76,76,76,76	0
60	MG	AA	3749	1/1	0.93	0.09	30,30,30,30	0
60	MG	AQ	3001	1/1	0.93	0.19	56,56,56,56	0
60	MG	CA	3296	1/1	0.93	0.10	61,61,61,61	0
60	MG	CA	3298	1/1	0.93	0.09	68,68,68,68	0
60	MG	AA	3509	1/1	0.93	0.19	51,51,51,51	0
60	MG	AA	3634	1/1	0.93	0.15	63,63,63,63	0
60	MG	AA	3179	1/1	0.93	0.11	62,62,62,62	0
60	MG	CA	3303	1/1	0.93	0.14	52,52,52,52	0
60	MG	CA	3125	1/1	0.93	0.23	58,58,58,58	0
60	MG	BA	1692	1/1	0.93	0.26	69,69,69,69	0
60	MG	DA	1638	1/1	0.93	0.12	60,60,60,60	0
60	MG	AA	3420	1/1	0.93	0.07	26,26,26,26	0
60	MG	AA	3143	1/1	0.93	0.05	37,37,37,37	0
60	MG	CA	3320	1/1	0.93	0.16	47,47,47,47	0
60	MG	BA	1695	1/1	0.93	0.05	64,64,64,64	0
60	MG	AA	3428	1/1	0.93	0.16	36,36,36,36	0
60	MG	AA	3018	1/1	0.93	0.33	55,55,55,55	0
60	MG	AA	3531	1/1	0.93	0.14	61,61,61,61	0
60	MG	CA	3332	1/1	0.93	0.15	47,47,47,47	0
60	MG	AA	3106	1/1	0.93	0.16	43,43,43,43	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	DA	1650	1/1	0.93	0.24	48,48,48,48	0
60	MG	CA	3556	1/1	0.93	0.07	77,77,77,77	0
60	MG	CA	3557	1/1	0.93	0.19	76,76,76,76	0
60	MG	AA	3047	1/1	0.93	0.15	40,40,40,40	0
60	MG	AA	3332	1/1	0.93	0.09	55,55,55,55	0
60	MG	AA	3333	1/1	0.93	0.05	33,33,33,33	0
60	MG	CA	3341	1/1	0.93	0.11	35,35,35,35	0
60	MG	AA	3334	1/1	0.93	0.12	62,62,62,62	0
60	MG	AA	3767	1/1	0.93	0.21	75,75,75,75	0
60	MG	CA	3351	1/1	0.93	0.08	50,50,50,50	0
60	MG	AA	3561	1/1	0.93	0.13	64,64,64,64	0
60	MG	CA	3360	1/1	0.93	0.10	52,52,52,52	0
60	MG	AA	3563	1/1	0.93	0.10	37,37,37,37	1
60	MG	CA	3579	1/1	0.93	0.09	58,58,58,58	0
60	MG	AA	3033	1/1	0.93	0.23	48,48,48,48	0
60	MG	AA	3152	1/1	0.93	0.20	80,80,80,80	0
60	MG	CA	3010	1/1	0.93	0.07	49,49,49,49	0
60	MG	AA	3659	1/1	0.93	0.08	56,56,56,56	0
60	MG	AA	3050	1/1	0.93	0.14	29,29,29,29	0
60	MG	AA	3663	1/1	0.93	0.17	61,61,61,61	0
60	MG	DA	1675	1/1	0.93	0.12	61,61,61,61	0
60	MG	AA	3113	1/1	0.93	0.10	41,41,41,41	0
60	MG	BA	1612	1/1	0.93	0.11	79,79,79,79	0
60	MG	AA	3669	1/1	0.93	0.14	36,36,36,36	0
60	MG	AA	3443	1/1	0.93	0.09	58,58,58,58	0
60	MG	BA	1724	1/1	0.93	0.13	60,60,60,60	0
60	MG	AA	3024	1/1	0.93	0.21	60,60,60,60	0
60	MG	AA	3787	1/1	0.93	0.13	55,55,55,55	0
60	MG	BA	1619	1/1	0.93	0.07	54,54,54,54	0
60	MG	DA	1688	1/1	0.93	0.14	46,46,46,46	0
60	MG	AA	3346	1/1	0.93	0.09	32,32,32,32	0
60	MG	CA	3392	1/1	0.93	0.12	66,66,66,66	0
60	MG	AA	3673	1/1	0.93	0.14	58,58,58,58	0
60	MG	AA	3119	1/1	0.93	0.12	41,41,41,41	0
60	MG	AA	3096	1/1	0.93	0.20	54,54,54,54	0
60	MG	AA	3681	1/1	0.93	0.15	52,52,52,52	0
60	MG	AA	3799	1/1	0.93	0.07	45,45,45,45	0
60	MG	AA	3198	1/1	0.93	0.10	47,47,47,47	0
60	MG	CA	3403	1/1	0.93	0.13	70,70,70,70	0
60	MG	BA	1746	1/1	0.93	0.10	70,70,70,70	0
60	MG	DA	1702	1/1	0.93	0.10	58,58,58,58	0
60	MG	AA	3591	1/1	0.93	0.16	61,61,61,61	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	CA	3191	1/1	0.93	0.17	61,61,61,61	0
60	MG	CA	3193	1/1	0.93	0.20	47,47,47,47	0
60	MG	AA	3062	1/1	0.93	0.24	60,60,60,60	0
60	MG	AA	3690	1/1	0.93	0.12	58,58,58,58	0
60	MG	AA	3595	1/1	0.93	0.10	60,60,60,60	0
60	MG	BA	1631	1/1	0.93	0.06	44,44,44,44	0
60	MG	AA	3597	1/1	0.93	0.15	58,58,58,58	0
60	MG	AA	3693	1/1	0.93	0.10	47,47,47,47	0
60	MG	CA	3426	1/1	0.93	0.12	46,46,46,46	0
60	MG	AA	3356	1/1	0.93	0.09	51,51,51,51	0
60	MG	CA	3054	1/1	0.93	0.09	50,50,50,50	0
60	MG	CA	3203	1/1	0.93	0.17	45,45,45,45	0
60	MG	CA	3430	1/1	0.93	0.14	38,38,38,38	0
60	MG	BA	1761	1/1	0.93	0.15	74,74,74,74	0
60	MG	BA	1637	1/1	0.93	0.08	64,64,64,64	0
60	MG	CA	3434	1/1	0.93	0.17	67,67,67,67	0
60	MG	AA	3099	1/1	0.93	0.10	48,48,48,48	0
60	MG	BA	1639	1/1	0.93	0.17	42,42,42,42	0
60	MG	BA	1641	1/1	0.93	0.20	56,56,56,56	0
60	MG	CA	3636	1/1	0.93	0.20	60,60,60,60	0
60	MG	AA	3134	1/1	0.93	0.23	49,49,49,49	0
60	MG	CA	3452	1/1	0.93	0.10	37,37,37,37	0
60	MG	AA	3290	1/1	0.93	0.15	78,78,78,78	0
60	MG	CA	3458	1/1	0.93	0.09	28,28,28,28	0
60	MG	CA	3460	1/1	0.93	0.14	57,57,57,57	0
60	MG	AA	3464	1/1	0.93	0.11	69,69,69,69	0
60	MG	AA	3607	1/1	0.93	0.10	39,39,39,39	0
60	MG	AA	3083	1/1	0.93	0.27	48,48,48,48	1
60	MG	CA	3069	1/1	0.93	0.17	66,66,66,66	0
60	MG	AA	3475	1/1	0.93	0.14	73,73,73,73	0
60	MG	AA	3476	1/1	0.93	0.06	50,50,50,50	0
60	MG	AA	3054	1/1	0.93	0.15	26,26,26,26	0
60	MG	CA	3471	1/1	0.93	0.18	59,59,59,59	0
60	MG	AA	3711	1/1	0.93	0.18	41,41,41,41	0
60	MG	BA	1782	1/1	0.93	0.11	72,72,72,72	0
60	MG	CA	3230	1/1	0.93	0.15	64,64,64,64	0
60	MG	CA	3476	1/1	0.93	0.12	60,60,60,60	0
60	MG	AA	3294	1/1	0.93	0.20	56,56,56,56	0
60	MG	CA	3233	1/1	0.93	0.22	52,52,52,52	0
60	MG	AA	3205	1/1	0.93	0.20	45,45,45,45	0
60	MG	AA	3616	1/1	0.93	0.06	33,33,33,33	0
60	MG	DA	1756	1/1	0.93	0.16	60,60,60,60	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	DA	1757	1/1	0.93	0.14	77,77,77,77	0
60	MG	DA	1758	1/1	0.93	0.19	80,80,80,80	0
60	MG	AA	3721	1/1	0.93	0.09	21,21,21,21	0
60	MG	AA	3167	1/1	0.93	0.16	69,69,69,69	0
60	MG	AB	3023	1/1	0.93	0.16	63,63,63,63	0
60	MG	DA	1763	1/1	0.93	0.10	61,61,61,61	0
60	MG	AD	301	1/1	0.93	0.17	64,64,64,64	0
60	MG	AA	3619	1/1	0.93	0.09	39,39,39,39	0
60	MG	BA	1795	1/1	0.93	0.19	64,64,64,64	0
60	MG	AA	3170	1/1	0.93	0.28	44,44,44,44	1
60	MG	AA	3102	1/1	0.93	0.19	38,38,38,38	0
60	MG	CB	3011	1/1	0.93	0.19	51,51,51,51	0
60	MG	CA	3245	1/1	0.93	0.08	53,53,53,53	0
60	MG	AA	3138	1/1	0.93	0.06	58,58,58,58	0
60	MG	CA	3247	1/1	0.93	0.07	45,45,45,45	0
60	MG	CA	3494	1/1	0.93	0.11	58,58,58,58	0
60	MG	AA	3623	1/1	0.93	0.07	58,58,58,58	0
60	MG	CE	301	1/1	0.93	0.19	54,54,54,54	0
60	MG	CA	3207	1/1	0.94	0.27	62,62,62,62	0
60	MG	AA	3653	1/1	0.94	0.07	47,47,47,47	0
60	MG	CA	3044	1/1	0.94	0.25	64,64,64,64	0
60	MG	AA	3426	1/1	0.94	0.12	47,47,47,47	0
60	MG	AA	3111	1/1	0.94	0.14	47,47,47,47	0
60	MG	CA	3047	1/1	0.94	0.07	54,54,54,54	0
60	MG	AA	3325	1/1	0.94	0.09	78,78,78,78	0
60	MG	CA	3216	1/1	0.94	0.14	32,32,32,32	0
60	MG	BA	1607	1/1	0.94	0.07	64,64,64,64	0
60	MG	BA	1731	1/1	0.94	0.07	65,65,65,65	0
60	MG	AA	3327	1/1	0.94	0.06	36,36,36,36	0
60	MG	CA	3221	1/1	0.94	0.29	60,60,60,60	0
60	MG	AA	3141	1/1	0.94	0.10	46,46,46,46	0
60	MG	AA	3569	1/1	0.94	0.08	17,17,17,17	0
60	MG	AA	3661	1/1	0.94	0.26	78,78,78,78	0
60	MG	CE	302	1/1	0.94	0.08	31,31,31,31	0
60	MG	CA	3227	1/1	0.94	0.17	30,30,30,30	0
60	MG	BA	1738	1/1	0.94	0.14	55,55,55,55	0
60	MG	CE	305	1/1	0.94	0.12	37,37,37,37	0
60	MG	CE	306	1/1	0.94	0.07	69,69,69,69	0
60	MG	CA	3479	1/1	0.94	0.16	67,67,67,67	0
60	MG	CA	3229	1/1	0.94	0.21	48,48,48,48	0
60	MG	AA	3662	1/1	0.94	0.22	60,60,60,60	0
60	MG	CA	3231	1/1	0.94	0.25	56,56,56,56	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	BA	1741	1/1	0.94	0.09	49,49,49,49	0
60	MG	AA	3142	1/1	0.94	0.16	50,50,50,50	0
60	MG	AA	3272	1/1	0.94	0.15	74,74,74,74	0
60	MG	CA	3060	1/1	0.94	0.13	50,50,50,50	0
60	MG	BA	1747	1/1	0.94	0.06	53,53,53,53	0
60	MG	BA	1617	1/1	0.94	0.06	64,64,64,64	0
60	MG	BA	1750	1/1	0.94	0.10	54,54,54,54	0
60	MG	AA	3667	1/1	0.94	0.09	45,45,45,45	0
60	MG	AA	3784	1/1	0.94	0.11	69,69,69,69	0
60	MG	AA	3273	1/1	0.94	0.12	57,57,57,57	0
60	MG	AA	3576	1/1	0.94	0.17	49,49,49,49	0
60	MG	AA	3078	1/1	0.94	0.19	54,54,54,54	0
60	MG	AA	3791	1/1	0.94	0.13	48,48,48,48	0
60	MG	AA	3235	1/1	0.94	0.17	42,42,42,42	0
60	MG	AA	3580	1/1	0.94	0.07	26,26,26,26	0
60	MG	AA	3796	1/1	0.94	0.18	45,45,45,45	0
60	MG	AA	3005	1/1	0.94	0.13	63,63,63,63	0
60	MG	AA	3679	1/1	0.94	0.07	64,64,64,64	0
60	MG	AA	3339	1/1	0.94	0.10	18,18,18,18	0
60	MG	AA	3202	1/1	0.94	0.11	46,46,46,46	0
60	MG	CA	3257	1/1	0.94	0.08	45,45,45,45	0
60	MG	AA	3682	1/1	0.94	0.11	58,58,58,58	0
60	MG	AA	3804	1/1	0.94	0.13	70,70,70,70	0
60	MG	AA	3064	1/1	0.94	0.09	31,31,31,31	0
60	MG	DA	1617	1/1	0.94	0.10	47,47,47,47	0
60	MG	DA	1618	1/1	0.94	0.08	51,51,51,51	0
60	MG	BA	1635	1/1	0.94	0.26	62,62,62,62	0
60	MG	AA	3590	1/1	0.94	0.10	71,71,71,71	0
60	MG	AA	3808	1/1	0.94	0.08	47,47,47,47	0
60	MG	AA	3120	1/1	0.94	0.13	54,54,54,54	0
60	MG	BA	1780	1/1	0.94	0.08	44,44,44,44	0
60	MG	AA	3810	1/1	0.94	0.15	49,49,49,49	0
60	MG	CA	3273	1/1	0.94	0.08	42,42,42,42	0
60	MG	BA	1640	1/1	0.94	0.12	56,56,56,56	0
60	MG	DA	1630	1/1	0.94	0.15	51,51,51,51	0
60	MG	CA	3278	1/1	0.94	0.09	38,38,38,38	0
60	MG	CA	3518	1/1	0.94	0.11	72,72,72,72	0
60	MG	AA	3057	1/1	0.94	0.11	56,56,56,56	0
60	MG	BA	1785	1/1	0.94	0.14	69,69,69,69	0
60	MG	AA	3123	1/1	0.94	0.18	55,55,55,55	0
60	MG	AA	3596	1/1	0.94	0.10	39,39,39,39	0
60	MG	CA	3100	1/1	0.94	0.15	75,75,75,75	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	AA	3815	1/1	0.94	0.14	72,72,72,72	0
60	MG	AA	3126	1/1	0.94	0.14	68,68,68,68	0
60	MG	CA	3530	1/1	0.94	0.10	68,68,68,68	0
60	MG	AA	3284	1/1	0.94	0.11	45,45,45,45	0
60	MG	CA	3288	1/1	0.94	0.17	39,39,39,39	0
60	MG	BA	1791	1/1	0.94	0.10	58,58,58,58	0
60	MG	AA	3455	1/1	0.94	0.14	80,80,80,80	0
60	MG	AA	3044	1/1	0.94	0.18	62,62,62,62	0
60	MG	CA	3537	1/1	0.94	0.10	64,64,64,64	0
60	MG	AA	3601	1/1	0.94	0.14	44,44,44,44	0
60	MG	AA	3602	1/1	0.94	0.11	39,39,39,39	0
60	MG	AA	3354	1/1	0.94	0.15	56,56,56,56	0
60	MG	CA	3541	1/1	0.94	0.13	58,58,58,58	0
60	MG	AA	3289	1/1	0.94	0.13	47,47,47,47	0
60	MG	AA	3704	1/1	0.94	0.08	57,57,57,57	0
60	MG	AA	3461	1/1	0.94	0.11	57,57,57,57	0
60	MG	AA	3357	1/1	0.94	0.10	52,52,52,52	0
60	MG	CA	3546	1/1	0.94	0.08	59,59,59,59	0
60	MG	AA	3129	1/1	0.94	0.15	52,52,52,52	0
60	MG	DA	1663	1/1	0.94	0.11	53,53,53,53	0
60	MG	CA	3549	1/1	0.94	0.09	29,29,29,29	0
60	MG	AB	3020	1/1	0.94	0.10	66,66,66,66	0
60	MG	AA	3466	1/1	0.94	0.09	48,48,48,48	0
60	MG	AA	3250	1/1	0.94	0.20	46,46,46,46	1
60	MG	AA	3104	1/1	0.94	0.14	55,55,55,55	0
60	MG	AA	3716	1/1	0.94	0.12	63,63,63,63	0
60	MG	AA	3364	1/1	0.94	0.16	57,57,57,57	0
60	MG	BA	1811	1/1	0.94	0.14	52,52,52,52	0
60	MG	CA	3325	1/1	0.94	0.14	42,42,42,42	0
60	MG	CA	3558	1/1	0.94	0.10	49,49,49,49	1
60	MG	AA	3720	1/1	0.94	0.18	78,78,78,78	0
60	MG	CA	3561	1/1	0.94	0.10	62,62,62,62	0
60	MG	CA	3330	1/1	0.94	0.12	37,37,37,37	0
60	MG	CA	3566	1/1	0.94	0.13	47,47,47,47	0
60	MG	CA	3568	1/1	0.94	0.15	71,71,71,71	0
60	MG	AA	3213	1/1	0.94	0.22	49,49,49,49	0
60	MG	AA	3368	1/1	0.94	0.13	54,54,54,54	0
60	MG	AA	3295	1/1	0.94	0.07	24,24,24,24	0
60	MG	AA	3370	1/1	0.94	0.09	43,43,43,43	0
60	MG	AA	3190	1/1	0.94	0.21	51,51,51,51	0
60	MG	AA	3378	1/1	0.94	0.10	24,24,24,24	0
60	MG	AF	302	1/1	0.94	0.20	46,46,46,46	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	DA	1692	1/1	0.94	0.18	49,49,49,49	0
60	MG	AF	303	1/1	0.94	0.12	46,46,46,46	0
60	MG	CA	3343	1/1	0.94	0.06	37,37,37,37	0
60	MG	AA	3379	1/1	0.94	0.08	40,40,40,40	1
60	MG	CA	3349	1/1	0.94	0.07	36,36,36,36	0
60	MG	CA	3350	1/1	0.94	0.12	74,74,74,74	0
60	MG	BA	1678	1/1	0.94	0.18	52,52,52,52	0
60	MG	AA	3258	1/1	0.94	0.12	32,32,32,32	0
60	MG	CA	3357	1/1	0.94	0.07	34,34,34,34	0
60	MG	AA	3191	1/1	0.94	0.11	57,57,57,57	0
60	MG	AA	3383	1/1	0.94	0.11	31,31,31,31	0
60	MG	CA	3143	1/1	0.94	0.15	62,62,62,62	0
60	MG	AA	3741	1/1	0.94	0.12	47,47,47,47	0
60	MG	BA	1685	1/1	0.94	0.12	41,41,41,41	0
60	MG	CA	3369	1/1	0.94	0.09	65,65,65,65	0
60	MG	BA	1686	1/1	0.94	0.24	58,58,58,58	0
60	MG	CA	3372	1/1	0.94	0.12	63,63,63,63	0
60	MG	DA	1714	1/1	0.94	0.19	82,82,82,82	0
60	MG	CA	3147	1/1	0.94	0.07	51,51,51,51	0
60	MG	CA	3599	1/1	0.94	0.06	75,75,75,75	0
60	MG	AA	3308	1/1	0.94	0.11	45,45,45,45	0
60	MG	AA	3019	1/1	0.94	0.10	53,53,53,53	0
60	MG	BX	108	1/1	0.94	0.14	78,78,78,78	0
60	MG	AA	3402	1/1	0.94	0.14	53,53,53,53	0
60	MG	AN	3003	1/1	0.94	0.07	52,52,52,52	0
60	MG	DA	1723	1/1	0.94	0.13	53,53,53,53	0
60	MG	AA	3068	1/1	0.94	0.23	52,52,52,52	0
60	MG	CA	3384	1/1	0.94	0.12	52,52,52,52	0
60	MG	AA	3264	1/1	0.94	0.14	54,54,54,54	0
60	MG	AA	3409	1/1	0.94	0.09	51,51,51,51	0
60	MG	AA	3025	1/1	0.94	0.13	60,60,60,60	0
60	MG	CA	3389	1/1	0.94	0.07	55,55,55,55	0
60	MG	CA	3167	1/1	0.94	0.28	68,68,68,68	0
60	MG	CA	3391	1/1	0.94	0.08	67,67,67,67	0
60	MG	BX	115	1/1	0.94	0.11	44,44,44,44	0
60	MG	AA	3526	1/1	0.94	0.07	26,26,26,26	0
60	MG	AW	3001	1/1	0.94	0.15	46,46,46,46	0
60	MG	BZ	701	1/1	0.94	0.13	58,58,58,58	0
60	MG	AA	3071	1/1	0.94	0.24	55,55,55,55	0
60	MG	DA	1740	1/1	0.94	0.14	56,56,56,56	0
60	MG	BA	1698	1/1	0.94	0.20	57,57,57,57	0
60	MG	AY	502	1/1	0.94	0.15	54,54,54,54	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	AA	3267	1/1	0.94	0.16	43,43,43,43	0
60	MG	CA	3179	1/1	0.94	0.15	27,27,27,27	0
60	MG	CA	3180	1/1	0.94	0.13	46,46,46,46	0
60	MG	BA	1701	1/1	0.94	0.17	47,47,47,47	0
60	MG	CA	3182	1/1	0.94	0.27	45,45,45,45	0
60	MG	AA	3641	1/1	0.94	0.11	45,45,45,45	0
60	MG	CA	3184	1/1	0.94	0.11	43,43,43,43	0
60	MG	CA	3414	1/1	0.94	0.10	50,50,50,50	0
60	MG	CA	3415	1/1	0.94	0.07	43,43,43,43	0
60	MG	CA	3417	1/1	0.94	0.09	58,58,58,58	0
60	MG	AA	3533	1/1	0.94	0.07	20,20,20,20	0
60	MG	AA	3048	1/1	0.94	0.07	39,39,39,39	0
60	MG	AA	3645	1/1	0.94	0.11	57,57,57,57	0
60	MG	AA	3323	1/1	0.94	0.09	42,42,42,42	0
60	MG	CA	3424	1/1	0.94	0.12	40,40,40,40	0
60	MG	A5	101	1/1	0.94	0.22	68,68,68,68	0
60	MG	AA	3761	1/1	0.94	0.16	72,72,72,72	0
60	MG	A6	101	1/1	0.94	0.11	75,75,75,75	0
60	MG	AA	3549	1/1	0.94	0.07	53,53,53,53	0
60	MG	A7	102	1/1	0.94	0.10	52,52,52,52	0
60	MG	A7	105	1/1	0.94	0.11	34,34,34,34	1
60	MG	AA	3424	1/1	0.94	0.08	48,48,48,48	0
60	MG	CA	3035	1/1	0.94	0.21	47,47,47,47	0
60	MG	CA	3438	1/1	0.94	0.14	45,45,45,45	0
60	MG	CA	3439	1/1	0.94	0.16	47,47,47,47	0
60	MG	DE	202	1/1	0.94	0.06	92,92,92,92	0
60	MG	A8	5002	1/1	0.94	0.11	45,45,45,45	0
60	MG	A9	502	1/1	0.94	0.21	52,52,52,52	0
60	MG	BA	1721	1/1	0.94	0.16	60,60,60,60	0
60	MG	AA	3553	1/1	0.94	0.10	47,47,47,47	0
60	MG	AA	3555	1/1	0.94	0.12	57,57,57,57	0
60	MG	CA	3455	1/1	0.94	0.12	37,37,37,37	0
61	K	AA	3814	1/1	0.94	0.17	87,87,87,87	0
60	MG	DA	1603	1/1	0.95	0.05	52,52,52,52	0
60	MG	AA	3149	1/1	0.95	0.12	15,15,15,15	0
60	MG	AA	3058	1/1	0.95	0.06	38,38,38,38	0
60	MG	AB	3008	1/1	0.95	0.22	46,46,46,46	0
60	MG	CA	3385	1/1	0.95	0.08	48,48,48,48	0
60	MG	AB	3009	1/1	0.95	0.10	62,62,62,62	0
60	MG	AA	3227	1/1	0.95	0.15	75,75,75,75	0
60	MG	BA	1812	1/1	0.95	0.07	47,47,47,47	0
60	MG	AA	3610	1/1	0.95	0.09	66,66,66,66	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	DA	1613	1/1	0.95	0.23	50,50,50,50	0
60	MG	AA	3538	1/1	0.95	0.08	62,62,62,62	0
60	MG	AB	3016	1/1	0.95	0.08	47,47,47,47	0
60	MG	DA	1616	1/1	0.95	0.15	44,44,44,44	0
60	MG	AA	3539	1/1	0.95	0.09	42,42,42,42	0
60	MG	AA	3349	1/1	0.95	0.07	34,34,34,34	0
60	MG	AA	3544	1/1	0.95	0.05	16,16,16,16	0
60	MG	AA	3547	1/1	0.95	0.10	50,50,50,50	0
60	MG	AA	3311	1/1	0.95	0.12	46,46,46,46	0
60	MG	DA	1622	1/1	0.95	0.13	43,43,43,43	0
60	MG	AA	3411	1/1	0.95	0.07	21,21,21,21	0
60	MG	BT	3001	1/1	0.95	0.15	47,47,47,47	0
60	MG	CA	3400	1/1	0.95	0.08	48,48,48,48	0
60	MG	AA	3125	1/1	0.95	0.14	74,74,74,74	0
60	MG	AA	3188	1/1	0.95	0.05	15,15,15,15	0
60	MG	AD	302	1/1	0.95	0.19	46,46,46,46	0
60	MG	BA	1718	1/1	0.95	0.07	48,48,48,48	0
60	MG	AD	303	1/1	0.95	0.11	31,31,31,31	0
60	MG	AA	3081	1/1	0.95	0.06	38,38,38,38	0
60	MG	AA	3683	1/1	0.95	0.10	40,40,40,40	0
60	MG	CA	3413	1/1	0.95	0.08	38,38,38,38	0
60	MG	DA	1637	1/1	0.95	0.14	61,61,61,61	0
60	MG	AA	3468	1/1	0.95	0.06	34,34,34,34	0
60	MG	AA	3762	1/1	0.95	0.12	63,63,63,63	0
60	MG	CA	3416	1/1	0.95	0.15	33,33,33,33	0
60	MG	BA	1634	1/1	0.95	0.24	71,71,71,71	0
60	MG	AD	311	1/1	0.95	0.22	63,63,63,63	0
60	MG	DA	1643	1/1	0.95	0.12	51,51,51,51	0
60	MG	AA	3168	1/1	0.95	0.12	60,60,60,60	0
60	MG	AA	3562	1/1	0.95	0.05	45,45,45,45	0
60	MG	CA	3241	1/1	0.95	0.10	69,69,69,69	0
60	MG	DA	1647	1/1	0.95	0.09	39,39,39,39	0
60	MG	AA	3261	1/1	0.95	0.17	53,53,53,53	0
60	MG	AA	3566	1/1	0.95	0.12	26,26,26,26	0
60	MG	BA	1733	1/1	0.95	0.05	57,57,57,57	0
60	MG	CA	3117	1/1	0.95	0.12	46,46,46,46	0
60	MG	AA	3627	1/1	0.95	0.13	53,53,53,53	0
60	MG	AA	3567	1/1	0.95	0.09	69,69,69,69	0
60	MG	AA	3629	1/1	0.95	0.12	51,51,51,51	0
60	MG	AA	3154	1/1	0.95	0.08	64,64,64,64	0
60	MG	BA	1739	1/1	0.95	0.07	52,52,52,52	0
60	MG	BA	1644	1/1	0.95	0.21	72,72,72,72	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	CA	3600	1/1	0.95	0.07	60,60,60,60	0
60	MG	CA	3002	1/1	0.95	0.16	32,32,32,32	0
60	MG	AA	3425	1/1	0.95	0.12	40,40,40,40	0
60	MG	CA	3004	1/1	0.95	0.16	43,43,43,43	0
60	MG	CA	3604	1/1	0.95	0.10	54,54,54,54	0
60	MG	CA	3443	1/1	0.95	0.17	40,40,40,40	0
60	MG	CA	3005	1/1	0.95	0.17	69,69,69,69	0
60	MG	CA	3446	1/1	0.95	0.12	37,37,37,37	0
60	MG	BA	1742	1/1	0.95	0.04	45,45,45,45	0
60	MG	AA	3570	1/1	0.95	0.07	22,22,22,22	0
60	MG	AA	3699	1/1	0.95	0.12	61,61,61,61	0
60	MG	CA	3133	1/1	0.95	0.12	72,72,72,72	0
60	MG	BA	1649	1/1	0.95	0.28	56,56,56,56	0
60	MG	CA	3459	1/1	0.95	0.07	46,46,46,46	0
60	MG	BA	1650	1/1	0.95	0.18	49,49,49,49	0
60	MG	AA	3171	1/1	0.95	0.26	71,71,71,71	0
60	MG	CA	3137	1/1	0.95	0.22	64,64,64,64	0
60	MG	CA	3274	1/1	0.95	0.21	64,64,64,64	0
60	MG	DA	1681	1/1	0.95	0.10	44,44,44,44	0
60	MG	CA	3465	1/1	0.95	0.07	64,64,64,64	0
60	MG	AA	3236	1/1	0.95	0.12	61,61,61,61	0
60	MG	CA	3276	1/1	0.95	0.07	32,32,32,32	0
60	MG	DA	1685	1/1	0.95	0.13	49,49,49,49	0
60	MG	CA	3468	1/1	0.95	0.10	37,37,37,37	0
60	MG	DA	1687	1/1	0.95	0.11	60,60,60,60	0
60	MG	BA	1753	1/1	0.95	0.10	48,48,48,48	0
60	MG	AA	3636	1/1	0.95	0.14	71,71,71,71	0
60	MG	AA	3703	1/1	0.95	0.07	76,76,76,76	0
60	MG	CA	3028	1/1	0.95	0.21	60,60,60,60	0
60	MG	CA	3473	1/1	0.95	0.09	48,48,48,48	0
60	MG	AP	201	1/1	0.95	0.20	67,67,67,67	0
60	MG	AA	3363	1/1	0.95	0.18	47,47,47,47	0
60	MG	AA	3038	1/1	0.95	0.13	42,42,42,42	0
60	MG	AA	3786	1/1	0.95	0.15	57,57,57,57	0
60	MG	AQ	3003	1/1	0.95	0.13	37,37,37,37	0
60	MG	CA	3149	1/1	0.95	0.11	58,58,58,58	0
60	MG	AU	201	1/1	0.95	0.14	53,53,53,53	0
60	MG	AU	202	1/1	0.95	0.14	65,65,65,65	0
60	MG	DA	1703	1/1	0.95	0.06	59,59,59,59	0
60	MG	AA	3707	1/1	0.95	0.21	59,59,59,59	0
60	MG	CA	3153	1/1	0.95	0.16	54,54,54,54	0
60	MG	CA	3294	1/1	0.95	0.12	40,40,40,40	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	AA	3085	1/1	0.95	0.17	80,80,80,80	0
60	MG	AA	3241	1/1	0.95	0.13	29,29,29,29	0
60	MG	AW	3004	1/1	0.95	0.09	45,45,45,45	0
60	MG	DA	1711	1/1	0.95	0.06	64,64,64,64	0
60	MG	CA	3299	1/1	0.95	0.06	42,42,42,42	0
60	MG	CA	3157	1/1	0.95	0.12	56,56,56,56	0
60	MG	CA	3651	1/1	0.95	0.15	41,41,41,41	0
60	MG	AA	3077	1/1	0.95	0.19	44,44,44,44	0
60	MG	CA	3159	1/1	0.95	0.23	42,42,42,42	0
60	MG	CA	3161	1/1	0.95	0.26	45,45,45,45	0
60	MG	AA	3712	1/1	0.95	0.11	50,50,50,50	0
60	MG	CA	3657	1/1	0.95	0.10	34,34,34,34	0
60	MG	AA	3131	1/1	0.95	0.12	39,39,39,39	0
60	MG	CA	3164	1/1	0.95	0.11	38,38,38,38	0
60	MG	CA	3165	1/1	0.95	0.31	58,58,58,58	0
60	MG	CA	3314	1/1	0.95	0.07	41,41,41,41	0
60	MG	CA	3317	1/1	0.95	0.08	61,61,61,61	0
60	MG	AA	3145	1/1	0.95	0.15	41,41,41,41	1
60	MG	DA	1728	1/1	0.95	0.10	53,53,53,53	0
60	MG	A0	103	1/1	0.95	0.08	67,67,67,67	0
60	MG	AA	3376	1/1	0.95	0.12	39,39,39,39	0
60	MG	AA	3717	1/1	0.95	0.13	47,47,47,47	0
60	MG	CB	3003	1/1	0.95	0.11	61,61,61,61	0
60	MG	CA	3328	1/1	0.95	0.07	40,40,40,40	0
60	MG	CB	3005	1/1	0.95	0.18	65,65,65,65	0
60	MG	A1	101	1/1	0.95	0.10	58,58,58,58	0
60	MG	AA	3296	1/1	0.95	0.10	40,40,40,40	0
60	MG	AA	3719	1/1	0.95	0.07	62,62,62,62	0
60	MG	CB	3009	1/1	0.95	0.12	66,66,66,66	0
60	MG	AA	3504	1/1	0.95	0.08	44,44,44,44	0
60	MG	AA	3507	1/1	0.95	0.12	53,53,53,53	0
60	MG	AA	3219	1/1	0.95	0.11	38,38,38,38	0
60	MG	AA	3806	1/1	0.95	0.18	56,56,56,56	0
60	MG	A7	101	1/1	0.95	0.14	41,41,41,41	0
60	MG	AA	3035	1/1	0.95	0.12	69,69,69,69	0
60	MG	AA	3512	1/1	0.95	0.08	32,32,32,32	0
60	MG	BA	1792	1/1	0.95	0.07	61,61,61,61	0
60	MG	CA	3346	1/1	0.95	0.19	48,48,48,48	0
60	MG	CA	3347	1/1	0.95	0.07	37,37,37,37	0
60	MG	CA	3062	1/1	0.95	0.06	41,41,41,41	0
60	MG	AA	3729	1/1	0.95	0.05	40,40,40,40	0
60	MG	AA	3515	1/1	0.95	0.08	27,27,27,27	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	CA	3065	1/1	0.95	0.13	56,56,56,56	0
60	MG	CA	3192	1/1	0.95	0.22	47,47,47,47	0
60	MG	AA	3299	1/1	0.95	0.15	64,64,64,64	0
60	MG	AA	3733	1/1	0.95	0.06	40,40,40,40	0
60	MG	BA	1797	1/1	0.95	0.13	75,75,75,75	0
60	MG	AA	3079	1/1	0.95	0.05	27,27,27,27	0
60	MG	CO	202	1/1	0.95	0.10	53,53,53,53	0
60	MG	CP	201	1/1	0.95	0.07	57,57,57,57	0
60	MG	CA	3364	1/1	0.95	0.23	64,64,64,64	0
60	MG	CA	3533	1/1	0.95	0.07	63,63,63,63	0
60	MG	AA	3343	1/1	0.95	0.05	60,60,60,60	0
60	MG	CA	3198	1/1	0.95	0.23	49,49,49,49	0
60	MG	AA	3392	1/1	0.95	0.09	31,31,31,31	0
60	MG	CR	202	1/1	0.95	0.18	61,61,61,61	0
60	MG	AA	3529	1/1	0.95	0.08	12,12,12,12	1
60	MG	AA	3397	1/1	0.95	0.10	41,41,41,41	0
60	MG	AB	3002	1/1	0.95	0.16	55,55,55,55	0
60	MG	CY	502	1/1	0.95	0.12	53,53,53,53	0
60	MG	DK	201	1/1	0.95	0.12	55,55,55,55	0
60	MG	C0	101	1/1	0.95	0.06	50,50,50,50	0
60	MG	AB	3003	1/1	0.95	0.07	40,40,40,40	0
60	MG	CA	3076	1/1	0.95	0.14	48,48,48,48	0
60	MG	AA	3742	1/1	0.95	0.11	68,68,68,68	0
60	MG	DZ	701	1/1	0.95	0.13	47,47,47,47	0
60	MG	CA	3078	1/1	0.95	0.07	49,49,49,49	0
62	ZN	C4	501	1/1	0.95	0.06	163,163,163,163	0
64	GDP	BZ	702	28/28	0.95	0.08	57,57,57,57	1
64	GDP	DZ	702	28/28	0.95	0.07	69,69,69,69	0
60	MG	CA	3315	1/1	0.96	0.09	44,44,44,44	0
60	MG	BA	1648	1/1	0.96	0.10	28,28,28,28	0
60	MG	AA	3429	1/1	0.96	0.09	58,58,58,58	0
60	MG	AA	3042	1/1	0.96	0.09	43,43,43,43	0
60	MG	AA	3371	1/1	0.96	0.06	21,21,21,21	0
60	MG	AA	3635	1/1	0.96	0.06	33,33,33,33	0
60	MG	CA	3326	1/1	0.96	0.09	54,54,54,54	0
60	MG	AA	3043	1/1	0.96	0.13	39,39,39,39	0
60	MG	AU	204	1/1	0.96	0.15	55,55,55,55	0
60	MG	AA	3493	1/1	0.96	0.13	56,56,56,56	0
60	MG	AV	204	1/1	0.96	0.14	46,46,46,46	0
60	MG	AA	3374	1/1	0.96	0.05	22,22,22,22	0
60	MG	CA	3621	1/1	0.96	0.10	55,55,55,55	0
60	MG	AA	3072	1/1	0.96	0.03	20,20,20,20	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	AA	3801	1/1	0.96	0.06	39,39,39,39	0
60	MG	CA	3335	1/1	0.96	0.07	38,38,38,38	0
60	MG	DA	1652	1/1	0.96	0.10	68,68,68,68	0
60	MG	CA	3336	1/1	0.96	0.09	64,64,64,64	0
60	MG	AA	3714	1/1	0.96	0.12	44,44,44,44	0
60	MG	AA	3122	1/1	0.96	0.12	39,39,39,39	0
60	MG	BA	1752	1/1	0.96	0.05	48,48,48,48	0
60	MG	CA	3105	1/1	0.96	0.05	47,47,47,47	0
60	MG	CA	3211	1/1	0.96	0.08	19,19,19,19	0
60	MG	CA	3345	1/1	0.96	0.09	41,41,41,41	0
60	MG	AA	3153	1/1	0.96	0.12	47,47,47,47	0
60	MG	CA	3493	1/1	0.96	0.18	66,66,66,66	0
60	MG	AA	3345	1/1	0.96	0.05	34,34,34,34	0
60	MG	CA	3637	1/1	0.96	0.14	78,78,78,78	0
60	MG	AA	3107	1/1	0.96	0.07	51,51,51,51	0
60	MG	DA	1666	1/1	0.96	0.14	45,45,45,45	0
60	MG	AA	3584	1/1	0.96	0.10	63,63,63,63	0
60	MG	AA	3585	1/1	0.96	0.08	60,60,60,60	0
60	MG	CA	3217	1/1	0.96	0.09	52,52,52,52	0
60	MG	A1	102	1/1	0.96	0.05	46,46,46,46	0
60	MG	AA	3226	1/1	0.96	0.08	51,51,51,51	0
60	MG	CA	3358	1/1	0.96	0.08	41,41,41,41	0
60	MG	AA	3587	1/1	0.96	0.07	44,44,44,44	0
60	MG	AA	3348	1/1	0.96	0.11	39,39,39,39	0
60	MG	CA	3013	1/1	0.96	0.11	52,52,52,52	0
60	MG	CA	3224	1/1	0.96	0.12	32,32,32,32	0
60	MG	CA	3650	1/1	0.96	0.08	42,42,42,42	0
60	MG	AA	3287	1/1	0.96	0.06	25,25,25,25	0
60	MG	DA	1680	1/1	0.96	0.10	40,40,40,40	0
60	MG	BA	1764	1/1	0.96	0.10	55,55,55,55	0
60	MG	CA	3508	1/1	0.96	0.09	74,74,74,74	0
60	MG	AA	3288	1/1	0.96	0.08	39,39,39,39	0
60	MG	AA	3446	1/1	0.96	0.05	25,25,25,25	0
60	MG	CA	3656	1/1	0.96	0.20	75,75,75,75	0
60	MG	AA	3321	1/1	0.96	0.09	45,45,45,45	0
60	MG	AA	3518	1/1	0.96	0.09	28,28,28,28	0
60	MG	CA	3024	1/1	0.96	0.35	67,67,67,67	0
60	MG	AA	3524	1/1	0.96	0.19	41,41,41,41	0
60	MG	AA	3084	1/1	0.96	0.08	27,27,27,27	0
60	MG	CA	3378	1/1	0.96	0.16	63,63,63,63	0
60	MG	BA	1679	1/1	0.96	0.10	51,51,51,51	0
60	MG	BA	1775	1/1	0.96	0.10	47,47,47,47	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	CA	3128	1/1	0.96	0.08	31,31,31,31	0
60	MG	AA	3172	1/1	0.96	0.07	50,50,50,50	0
60	MG	DA	1697	1/1	0.96	0.14	67,67,67,67	0
60	MG	CA	3522	1/1	0.96	0.07	25,25,25,25	0
60	MG	CA	3130	1/1	0.96	0.09	57,57,57,57	0
60	MG	AA	3006	1/1	0.96	0.11	56,56,56,56	0
60	MG	AA	3451	1/1	0.96	0.13	43,43,43,43	0
60	MG	CA	3034	1/1	0.96	0.10	51,51,51,51	0
60	MG	AA	3326	1/1	0.96	0.05	22,22,22,22	0
60	MG	AA	3603	1/1	0.96	0.08	68,68,68,68	0
60	MG	DA	1705	1/1	0.96	0.10	61,61,61,61	0
60	MG	AA	3665	1/1	0.96	0.06	63,63,63,63	0
60	MG	BA	1783	1/1	0.96	0.07	61,61,61,61	0
60	MG	AA	3666	1/1	0.96	0.15	28,28,28,28	0
60	MG	AA	3746	1/1	0.96	0.14	62,62,62,62	0
60	MG	AA	3532	1/1	0.96	0.09	20,20,20,20	0
60	MG	AB	3015	1/1	0.96	0.11	51,51,51,51	0
60	MG	AA	3008	1/1	0.96	0.07	28,28,28,28	0
60	MG	AA	3606	1/1	0.96	0.19	62,62,62,62	0
60	MG	CA	3254	1/1	0.96	0.08	35,35,35,35	0
60	MG	CA	3402	1/1	0.96	0.09	46,46,46,46	0
60	MG	DA	1716	1/1	0.96	0.15	56,56,56,56	0
60	MG	AA	3004	1/1	0.96	0.05	30,30,30,30	0
60	MG	CA	3256	1/1	0.96	0.14	73,73,73,73	0
60	MG	AA	3608	1/1	0.96	0.07	66,66,66,66	0
60	MG	AA	3413	1/1	0.96	0.06	34,34,34,34	0
60	MG	AA	3091	1/1	0.96	0.12	62,62,62,62	0
60	MG	AA	3676	1/1	0.96	0.05	46,46,46,46	0
60	MG	CF	304	1/1	0.96	0.05	46,46,46,46	0
60	MG	CF	305	1/1	0.96	0.06	45,45,45,45	0
60	MG	CA	3263	1/1	0.96	0.09	50,50,50,50	0
60	MG	AA	3678	1/1	0.96	0.08	62,62,62,62	0
60	MG	CN	5001	1/1	0.96	0.05	64,64,64,64	0
60	MG	AA	3416	1/1	0.96	0.09	31,31,31,31	0
60	MG	AA	3542	1/1	0.96	0.05	47,47,47,47	0
60	MG	AA	3543	1/1	0.96	0.17	84,84,84,84	0
60	MG	AD	304	1/1	0.96	0.10	46,46,46,46	0
60	MG	AA	3417	1/1	0.96	0.07	16,16,16,16	0
60	MG	CA	3272	1/1	0.96	0.09	56,56,56,56	0
60	MG	AA	3274	1/1	0.96	0.20	48,48,48,48	1
60	MG	CA	3421	1/1	0.96	0.09	39,39,39,39	0
60	MG	AA	3684	1/1	0.96	0.06	47,47,47,47	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	AD	309	1/1	0.96	0.09	49,49,49,49	0
60	MG	CA	3061	1/1	0.96	0.11	36,36,36,36	0
60	MG	CA	3562	1/1	0.96	0.11	69,69,69,69	0
60	MG	AA	3685	1/1	0.96	0.12	58,58,58,58	0
60	MG	AA	3686	1/1	0.96	0.10	62,62,62,62	0
60	MG	DA	1744	1/1	0.96	0.11	57,57,57,57	0
60	MG	AA	3548	1/1	0.96	0.08	69,69,69,69	0
60	MG	BA	1711	1/1	0.96	0.26	63,63,63,63	0
60	MG	AA	3617	1/1	0.96	0.08	32,32,32,32	0
60	MG	C7	101	1/1	0.96	0.12	47,47,47,47	0
60	MG	DA	1601	1/1	0.96	0.09	59,59,59,59	0
60	MG	CA	3432	1/1	0.96	0.06	29,29,29,29	0
60	MG	AA	3467	1/1	0.96	0.09	54,54,54,54	0
60	MG	AA	3014	1/1	0.96	0.18	45,45,45,45	0
60	MG	CA	3435	1/1	0.96	0.10	55,55,55,55	0
60	MG	AA	3552	1/1	0.96	0.14	73,73,73,73	0
60	MG	AA	3472	1/1	0.96	0.11	37,37,37,37	0
60	MG	AF	304	1/1	0.96	0.11	31,31,31,31	0
60	MG	CA	3289	1/1	0.96	0.08	23,23,23,23	0
60	MG	AA	3473	1/1	0.96	0.06	57,57,57,57	0
60	MG	AA	3774	1/1	0.96	0.08	44,44,44,44	0
60	MG	DA	1760	1/1	0.96	0.09	53,53,53,53	0
60	MG	BF	3001	1/1	0.96	0.08	49,49,49,49	0
60	MG	CA	3448	1/1	0.96	0.08	64,64,64,64	0
60	MG	CA	3449	1/1	0.96	0.14	52,52,52,52	0
60	MG	AA	3556	1/1	0.96	0.09	54,54,54,54	0
60	MG	AA	3132	1/1	0.96	0.21	43,43,43,43	0
60	MG	AA	3423	1/1	0.96	0.12	53,53,53,53	0
60	MG	CA	3456	1/1	0.96	0.07	37,37,37,37	0
60	MG	AA	3697	1/1	0.96	0.09	71,71,71,71	0
60	MG	AA	3366	1/1	0.96	0.10	35,35,35,35	0
60	MG	CA	3080	1/1	0.96	0.17	78,78,78,78	0
60	MG	AA	3367	1/1	0.96	0.15	52,52,52,52	0
60	MG	CA	3461	1/1	0.96	0.05	46,46,46,46	0
60	MG	CA	3185	1/1	0.96	0.14	47,47,47,47	0
60	MG	DA	1627	1/1	0.96	0.19	48,48,48,48	0
60	MG	BA	1728	1/1	0.96	0.09	53,53,53,53	0
60	MG	AA	3480	1/1	0.96	0.14	78,78,78,78	0
60	MG	CA	3189	1/1	0.96	0.05	40,40,40,40	0
60	MG	AA	3259	1/1	0.96	0.27	27,27,27,27	0
60	MG	AA	3427	1/1	0.96	0.10	34,34,34,34	0
60	MG	CA	3087	1/1	0.96	0.21	107,107,107,107	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	AA	3237	1/1	0.96	0.06	51,51,51,51	0
60	MG	DA	1635	1/1	0.96	0.22	61,61,61,61	0
60	MG	CA	3082	1/1	0.97	0.14	31,31,31,31	0
60	MG	AA	3482	1/1	0.97	0.11	46,46,46,46	0
60	MG	CA	3313	1/1	0.97	0.12	54,54,54,54	0
60	MG	AA	3483	1/1	0.97	0.05	21,21,21,21	0
60	MG	AA	3022	1/1	0.97	0.03	19,19,19,19	0
60	MG	CA	3316	1/1	0.97	0.06	34,34,34,34	0
60	MG	AA	3485	1/1	0.97	0.06	34,34,34,34	0
60	MG	AA	3229	1/1	0.97	0.05	33,33,33,33	0
60	MG	BA	1734	1/1	0.97	0.08	35,35,35,35	0
60	MG	AA	3792	1/1	0.97	0.16	35,35,35,35	0
60	MG	CA	3323	1/1	0.97	0.08	32,32,32,32	0
60	MG	CA	3324	1/1	0.97	0.10	31,31,31,31	0
60	MG	CA	3620	1/1	0.97	0.07	41,41,41,41	0
60	MG	AR	201	1/1	0.97	0.13	51,51,51,51	0
60	MG	AA	3286	1/1	0.97	0.10	48,48,48,48	0
60	MG	DA	1653	1/1	0.97	0.07	29,29,29,29	0
60	MG	AA	3794	1/1	0.97	0.09	47,47,47,47	0
60	MG	AA	3118	1/1	0.97	0.10	59,59,59,59	0
60	MG	CA	3625	1/1	0.97	0.11	46,46,46,46	0
60	MG	AA	3023	1/1	0.97	0.17	40,40,40,40	1
60	MG	AV	202	1/1	0.97	0.12	56,56,56,56	0
60	MG	AA	3572	1/1	0.97	0.07	51,51,51,51	0
60	MG	AA	3232	1/1	0.97	0.19	58,58,58,58	0
60	MG	BA	1744	1/1	0.97	0.04	48,48,48,48	0
60	MG	CA	3099	1/1	0.97	0.18	55,55,55,55	0
60	MG	AA	3184	1/1	0.97	0.14	39,39,39,39	0
60	MG	AW	3002	1/1	0.97	0.11	59,59,59,59	0
60	MG	AA	3133	1/1	0.97	0.20	92,92,92,92	1
60	MG	AA	3187	1/1	0.97	0.07	29,29,29,29	0
60	MG	AA	3373	1/1	0.97	0.08	23,23,23,23	0
60	MG	AA	3647	1/1	0.97	0.05	35,35,35,35	0
60	MG	CA	3344	1/1	0.97	0.07	27,27,27,27	0
60	MG	AA	3496	1/1	0.97	0.04	43,43,43,43	0
60	MG	AA	3649	1/1	0.97	0.05	78,78,78,78	0
60	MG	AA	3722	1/1	0.97	0.08	31,31,31,31	0
60	MG	AA	3087	1/1	0.97	0.12	62,62,62,62	0
60	MG	CA	3110	1/1	0.97	0.14	35,35,35,35	0
60	MG	AA	3501	1/1	0.97	0.07	45,45,45,45	0
60	MG	AA	3726	1/1	0.97	0.07	74,74,74,74	0
60	MG	CA	3353	1/1	0.97	0.09	48,48,48,48	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	CA	3354	1/1	0.97	0.07	40,40,40,40	0
60	MG	CA	3008	1/1	0.97	0.15	52,52,52,52	0
60	MG	CA	3356	1/1	0.97	0.07	28,28,28,28	0
60	MG	CA	3223	1/1	0.97	0.11	46,46,46,46	0
60	MG	BA	1759	1/1	0.97	0.07	60,60,60,60	0
60	MG	CA	3359	1/1	0.97	0.10	44,44,44,44	0
60	MG	AA	3727	1/1	0.97	0.09	64,64,64,64	0
60	MG	CA	3012	1/1	0.97	0.05	41,41,41,41	0
60	MG	AA	3097	1/1	0.97	0.13	29,29,29,29	0
60	MG	AA	3377	1/1	0.97	0.05	19,19,19,19	0
60	MG	AA	3505	1/1	0.97	0.06	29,29,29,29	0
60	MG	A5	104	1/1	0.97	0.05	46,46,46,46	0
60	MG	CA	3019	1/1	0.97	0.06	23,23,23,23	0
60	MG	CA	3020	1/1	0.97	0.09	38,38,38,38	0
60	MG	DA	1693	1/1	0.97	0.08	50,50,50,50	0
60	MG	AA	3338	1/1	0.97	0.09	49,49,49,49	0
60	MG	AA	3030	1/1	0.97	0.11	44,44,44,44	1
60	MG	AA	3735	1/1	0.97	0.09	30,30,30,30	0
60	MG	CA	3375	1/1	0.97	0.04	65,65,65,65	0
60	MG	BA	1769	1/1	0.97	0.12	80,80,80,80	0
60	MG	CA	3025	1/1	0.97	0.20	32,32,32,32	1
60	MG	AA	3510	1/1	0.97	0.06	13,13,13,13	0
60	MG	BA	1771	1/1	0.97	0.08	48,48,48,48	0
60	MG	CA	3520	1/1	0.97	0.05	27,27,27,27	0
60	MG	AA	3239	1/1	0.97	0.13	63,63,63,63	0
60	MG	BA	1680	1/1	0.97	0.05	50,50,50,50	0
60	MG	AA	3211	1/1	0.97	0.19	53,53,53,53	0
60	MG	AA	3593	1/1	0.97	0.06	49,49,49,49	0
60	MG	AA	3594	1/1	0.97	0.15	48,48,48,48	0
60	MG	AA	3069	1/1	0.97	0.06	32,32,32,32	0
60	MG	BA	1778	1/1	0.97	0.10	52,52,52,52	0
60	MG	AA	3384	1/1	0.97	0.05	26,26,26,26	0
60	MG	AA	3124	1/1	0.97	0.10	39,39,39,39	1
60	MG	CA	3038	1/1	0.97	0.10	26,26,26,26	0
60	MG	AB	3011	1/1	0.97	0.10	47,47,47,47	0
60	MG	CA	3040	1/1	0.97	0.09	63,63,63,63	0
60	MG	AA	3303	1/1	0.97	0.08	30,30,30,30	0
60	MG	CA	3395	1/1	0.97	0.07	60,60,60,60	0
60	MG	AA	3521	1/1	0.97	0.12	30,30,30,30	0
60	MG	AA	3394	1/1	0.97	0.08	22,22,22,22	0
60	MG	AA	3304	1/1	0.97	0.10	44,44,44,44	0
60	MG	AA	3139	1/1	0.97	0.13	64,64,64,64	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	AA	3527	1/1	0.97	0.08	20,20,20,20	0
60	MG	CA	3148	1/1	0.97	0.05	41,41,41,41	0
60	MG	AA	3528	1/1	0.97	0.09	26,26,26,26	0
60	MG	CA	3404	1/1	0.97	0.06	46,46,46,46	0
60	MG	CA	3405	1/1	0.97	0.06	50,50,50,50	0
60	MG	DA	1726	1/1	0.97	0.12	58,58,58,58	0
60	MG	CA	3264	1/1	0.97	0.10	54,54,54,54	0
60	MG	AA	3452	1/1	0.97	0.07	53,53,53,53	0
60	MG	CA	3408	1/1	0.97	0.11	35,35,35,35	0
60	MG	AA	3453	1/1	0.97	0.08	51,51,51,51	0
60	MG	AA	3401	1/1	0.97	0.08	26,26,26,26	0
60	MG	CA	3268	1/1	0.97	0.11	46,46,46,46	0
60	MG	BA	1616	1/1	0.97	0.05	69,69,69,69	0
60	MG	AA	3456	1/1	0.97	0.09	64,64,64,64	0
60	MG	AA	3216	1/1	0.97	0.07	68,68,68,68	0
60	MG	AA	3535	1/1	0.97	0.05	37,37,37,37	0
60	MG	AA	3217	1/1	0.97	0.05	50,50,50,50	0
60	MG	AA	3406	1/1	0.97	0.06	52,52,52,52	0
60	MG	AA	3350	1/1	0.97	0.11	54,54,54,54	0
60	MG	AA	3540	1/1	0.97	0.06	28,28,28,28	0
60	MG	AA	3174	1/1	0.97	0.10	39,39,39,39	0
60	MG	CA	3563	1/1	0.97	0.17	30,30,30,30	0
60	MG	CA	3279	1/1	0.97	0.11	46,46,46,46	0
60	MG	BA	1707	1/1	0.97	0.12	57,57,57,57	0
60	MG	C8	5001	1/1	0.97	0.11	43,43,43,43	0
60	MG	CA	3567	1/1	0.97	0.06	42,42,42,42	0
60	MG	AA	3312	1/1	0.97	0.08	25,25,25,25	0
60	MG	CA	3425	1/1	0.97	0.11	45,45,45,45	0
60	MG	AA	3465	1/1	0.97	0.06	49,49,49,49	0
60	MG	AA	3031	1/1	0.97	0.17	29,29,29,29	1
60	MG	AA	3012	1/1	0.97	0.07	38,38,38,38	0
60	MG	AA	3045	1/1	0.97	0.12	58,58,58,58	0
60	MG	AA	3178	1/1	0.97	0.18	50,50,50,50	0
60	MG	CA	3172	1/1	0.97	0.11	41,41,41,41	0
60	MG	BA	1714	1/1	0.97	0.11	44,44,44,44	0
60	MG	CA	3174	1/1	0.97	0.06	31,31,31,31	0
60	MG	AA	3771	1/1	0.97	0.13	40,40,40,40	0
60	MG	BA	1810	1/1	0.97	0.08	39,39,39,39	0
60	MG	CA	3437	1/1	0.97	0.09	41,41,41,41	0
60	MG	AA	3115	1/1	0.97	0.25	44,44,44,44	0
60	MG	AA	3359	1/1	0.97	0.10	31,31,31,31	0
60	MG	AA	3144	1/1	0.97	0.12	48,48,48,48	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	CA	3441	1/1	0.97	0.06	37,37,37,37	0
60	MG	AA	3361	1/1	0.97	0.06	33,33,33,33	0
60	MG	BA	1720	1/1	0.97	0.07	51,51,51,51	0
60	MG	CA	3297	1/1	0.97	0.06	55,55,55,55	0
60	MG	AA	3477	1/1	0.97	0.05	47,47,47,47	0
60	MG	CA	3594	1/1	0.97	0.08	62,62,62,62	0
60	MG	DA	1625	1/1	0.97	0.04	38,38,38,38	0
60	MG	AA	3557	1/1	0.97	0.05	21,21,21,21	0
60	MG	AA	3478	1/1	0.97	0.06	70,70,70,70	0
60	MG	CA	3450	1/1	0.97	0.09	38,38,38,38	0
60	MG	AA	3322	1/1	0.97	0.07	37,37,37,37	0
60	MG	CA	3186	1/1	0.97	0.09	49,49,49,49	0
60	MG	CA	3453	1/1	0.97	0.06	43,43,43,43	0
60	MG	AA	3560	1/1	0.97	0.07	49,49,49,49	0
60	MG	CA	3304	1/1	0.97	0.08	48,48,48,48	0
60	MG	AA	3256	1/1	0.97	0.14	24,24,24,24	0
60	MG	CA	3307	1/1	0.97	0.09	31,31,31,31	0
62	ZN	DN	501	1/1	0.97	0.04	120,120,120,120	0
60	MG	AA	3785	1/1	0.97	0.12	54,54,54,54	0
60	MG	CA	3310	1/1	0.97	0.11	45,45,45,45	0
60	MG	AA	3224	1/1	0.98	0.04	26,26,26,26	0
60	MG	AA	3112	1/1	0.98	0.12	44,44,44,44	0
60	MG	AA	3643	1/1	0.98	0.06	56,56,56,56	0
60	MG	DA	1669	1/1	0.98	0.12	63,63,63,63	0
60	MG	AA	3709	1/1	0.98	0.24	39,39,39,39	0
60	MG	AA	3128	1/1	0.98	0.14	53,53,53,53	1
60	MG	AA	3519	1/1	0.98	0.06	39,39,39,39	0
60	MG	CA	3436	1/1	0.98	0.05	34,34,34,34	0
60	MG	AA	3039	1/1	0.98	0.15	34,34,34,34	0
60	MG	CA	3327	1/1	0.98	0.08	37,37,37,37	0
60	MG	AA	3522	1/1	0.98	0.06	31,31,31,31	0
60	MG	AA	3523	1/1	0.98	0.08	35,35,35,35	0
60	MG	AG	202	1/1	0.98	0.04	41,41,41,41	0
60	MG	AA	3114	1/1	0.98	0.15	55,55,55,55	0
60	MG	AA	3463	1/1	0.98	0.07	41,41,41,41	0
60	MG	CA	3444	1/1	0.98	0.10	70,70,70,70	0
60	MG	AA	3020	1/1	0.98	0.04	25,25,25,25	0
60	MG	AA	3335	1/1	0.98	0.04	14,14,14,14	0
60	MG	CA	3447	1/1	0.98	0.03	44,44,44,44	0
60	MG	AA	3301	1/1	0.98	0.11	59,59,59,59	0
60	MG	AO	5001	1/1	0.98	0.05	43,43,43,43	0
60	MG	AA	3302	1/1	0.98	0.19	58,58,58,58	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	AP	202	1/1	0.98	0.22	35,35,35,35	0
60	MG	AA	3422	1/1	0.98	0.07	22,22,22,22	0
60	MG	AA	3469	1/1	0.98	0.07	37,37,37,37	0
60	MG	AA	3185	1/1	0.98	0.14	35,35,35,35	0
60	MG	AA	3658	1/1	0.98	0.06	25,25,25,25	0
60	MG	AA	3166	1/1	0.98	0.07	52,52,52,52	0
60	MG	AR	202	1/1	0.98	0.04	34,34,34,34	0
60	MG	CA	3574	1/1	0.98	0.05	31,31,31,31	0
60	MG	AA	3534	1/1	0.98	0.12	34,34,34,34	0
60	MG	AA	3305	1/1	0.98	0.07	38,38,38,38	0
60	MG	BA	1729	1/1	0.98	0.08	38,38,38,38	0
60	MG	AA	3306	1/1	0.98	0.05	3,3,3,3	0
60	MG	AA	3730	1/1	0.98	0.11	34,34,34,34	0
60	MG	CA	3580	1/1	0.98	0.05	37,37,37,37	0
60	MG	CA	3352	1/1	0.98	0.09	40,40,40,40	0
60	MG	AV	201	1/1	0.98	0.07	45,45,45,45	0
60	MG	AA	3375	1/1	0.98	0.04	16,16,16,16	0
60	MG	AA	3255	1/1	0.98	0.08	64,64,64,64	0
60	MG	CA	3586	1/1	0.98	0.14	75,75,75,75	0
60	MG	BM	201	1/1	0.98	0.05	60,60,60,60	0
60	MG	CA	3252	1/1	0.98	0.11	30,30,30,30	0
60	MG	AA	3116	1/1	0.98	0.21	36,36,36,36	0
60	MG	AA	3430	1/1	0.98	0.04	23,23,23,23	0
60	MG	BA	1654	1/1	0.98	0.04	45,45,45,45	0
60	MG	CA	3160	1/1	0.98	0.14	33,33,33,33	0
60	MG	CA	3362	1/1	0.98	0.04	20,20,20,20	0
60	MG	AA	3431	1/1	0.98	0.06	25,25,25,25	0
60	MG	CA	3258	1/1	0.98	0.08	54,54,54,54	0
60	MG	CA	3259	1/1	0.98	0.08	19,19,19,19	0
60	MG	AW	3003	1/1	0.98	0.13	38,38,38,38	0
60	MG	CA	3367	1/1	0.98	0.10	39,39,39,39	0
60	MG	CA	3368	1/1	0.98	0.07	45,45,45,45	0
60	MG	AA	3668	1/1	0.98	0.06	25,25,25,25	0
60	MG	AA	3481	1/1	0.98	0.04	53,53,53,53	0
60	MG	AA	3432	1/1	0.98	0.09	24,24,24,24	0
60	MG	CA	3166	1/1	0.98	0.10	31,31,31,31	0
60	MG	AA	3545	1/1	0.98	0.04	64,64,64,64	0
60	MG	AA	3546	1/1	0.98	0.05	36,36,36,36	0
60	MG	AA	3007	1/1	0.98	0.03	18,18,18,18	0
60	MG	AA	3674	1/1	0.98	0.03	56,56,56,56	0
60	MG	CA	3171	1/1	0.98	0.27	48,48,48,48	0
60	MG	DA	1612	1/1	0.98	0.04	46,46,46,46	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	AA	3169	1/1	0.98	0.09	36,36,36,36	0
60	MG	CA	3380	1/1	0.98	0.07	37,37,37,37	0
60	MG	DA	1732	1/1	0.98	0.07	54,54,54,54	0
60	MG	BA	1749	1/1	0.98	0.13	52,52,52,52	0
60	MG	AA	3103	1/1	0.98	0.09	11,11,11,11	0
60	MG	AA	3677	1/1	0.98	0.11	26,26,26,26	0
60	MG	AA	3550	1/1	0.98	0.09	47,47,47,47	0
60	MG	CA	3615	1/1	0.98	0.08	33,33,33,33	0
60	MG	AA	3313	1/1	0.98	0.11	31,31,31,31	0
60	MG	AB	3007	1/1	0.98	0.03	37,37,37,37	0
60	MG	CA	3277	1/1	0.98	0.05	43,43,43,43	0
60	MG	AA	3750	1/1	0.98	0.04	26,26,26,26	0
60	MG	AA	3382	1/1	0.98	0.05	29,29,29,29	0
60	MG	AA	3488	1/1	0.98	0.08	56,56,56,56	0
60	MG	AA	3554	1/1	0.98	0.04	48,48,48,48	0
60	MG	AB	3012	1/1	0.98	0.07	24,24,24,24	1
60	MG	AA	3314	1/1	0.98	0.11	43,43,43,43	0
60	MG	A7	103	1/1	0.98	0.06	39,39,39,39	0
60	MG	A7	104	1/1	0.98	0.07	49,49,49,49	0
60	MG	CA	3627	1/1	0.98	0.09	59,59,59,59	0
60	MG	AA	3052	1/1	0.98	0.11	15,15,15,15	0
60	MG	A7	106	1/1	0.98	0.06	57,57,57,57	0
60	MG	CA	3006	1/1	0.98	0.03	24,24,24,24	0
60	MG	AA	3385	1/1	0.98	0.06	24,24,24,24	0
60	MG	CA	3401	1/1	0.98	0.05	75,75,75,75	0
60	MG	AA	3037	1/1	0.98	0.04	12,12,12,12	0
60	MG	CA	3009	1/1	0.98	0.03	24,24,24,24	0
60	MG	AA	3389	1/1	0.98	0.08	46,46,46,46	0
60	MG	AA	3082	1/1	0.98	0.32	57,57,57,57	1
60	MG	AA	3155	1/1	0.98	0.15	31,31,31,31	0
60	MG	AA	3395	1/1	0.98	0.05	21,21,21,21	0
60	MG	CA	3014	1/1	0.98	0.09	58,58,58,58	0
60	MG	AA	3497	1/1	0.98	0.04	36,36,36,36	0
60	MG	AA	3009	1/1	0.98	0.04	26,26,26,26	0
60	MG	CA	3017	1/1	0.98	0.04	28,28,28,28	0
60	MG	AA	3355	1/1	0.98	0.04	19,19,19,19	0
60	MG	DA	1766	1/1	0.98	0.04	41,41,41,41	0
60	MG	AA	3074	1/1	0.98	0.14	26,26,26,26	0
60	MG	AA	3075	1/1	0.98	0.07	47,47,47,47	0
60	MG	CA	3525	1/1	0.98	0.04	30,30,30,30	0
60	MG	AA	3086	1/1	0.98	0.14	43,43,43,43	1
60	MG	AA	3404	1/1	0.98	0.07	50,50,50,50	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	BA	1611	1/1	0.98	0.08	31,31,31,31	0
60	MG	AD	305	1/1	0.98	0.17	49,49,49,49	0
60	MG	AA	3405	1/1	0.98	0.06	27,27,27,27	0
60	MG	AA	3292	1/1	0.98	0.10	31,31,31,31	0
60	MG	CA	3027	1/1	0.98	0.02	29,29,29,29	0
60	MG	CA	3422	1/1	0.98	0.08	43,43,43,43	0
60	MG	AA	3454	1/1	0.98	0.07	27,27,27,27	0
60	MG	AA	3244	1/1	0.98	0.15	42,42,42,42	0
60	MG	AA	3577	1/1	0.98	0.06	65,65,65,65	0
62	ZN	A4	501	1/1	0.98	0.04	120,120,120,120	0
60	MG	AA	3776	1/1	0.98	0.05	21,21,21,21	0
60	MG	AA	3514	1/1	0.98	0.09	32,32,32,32	0
63	SF4	DD	501	8/8	0.98	0.04	71,71,71,71	0
60	MG	AA	3076	1/1	0.98	0.04	6,6,6,6	0
60	MG	CA	3318	1/1	0.98	0.07	31,31,31,31	0
60	MG	BA	1745	1/1	0.99	0.04	46,46,46,46	0
60	MG	AA	3754	1/1	0.99	0.03	25,25,25,25	0
60	MG	AA	3393	1/1	0.99	0.04	18,18,18,18	0
60	MG	AA	3513	1/1	0.99	0.08	37,37,37,37	0
60	MG	CA	3547	1/1	0.99	0.02	57,57,57,57	1
60	MG	AE	303	1/1	0.99	0.08	23,23,23,23	0
60	MG	AA	3011	1/1	0.99	0.04	27,27,27,27	0
60	MG	AA	3218	1/1	0.99	0.07	10,10,10,10	0
60	MG	AF	301	1/1	0.99	0.18	40,40,40,40	0
60	MG	AA	3340	1/1	0.99	0.03	3,3,3,3	0
60	MG	AA	3398	1/1	0.99	0.09	29,29,29,29	0
60	MG	AA	3189	1/1	0.99	0.07	31,31,31,31	0
60	MG	AA	3400	1/1	0.99	0.03	19,19,19,19	0
60	MG	AA	3520	1/1	0.99	0.07	34,34,34,34	0
60	MG	AA	3003	1/1	0.99	0.03	14,14,14,14	0
60	MG	AF	308	1/1	0.99	0.03	48,48,48,48	0
60	MG	CA	3559	1/1	0.99	0.03	30,30,30,30	0
60	MG	AA	3457	1/1	0.99	0.04	18,18,18,18	0
60	MG	AA	3212	1/1	0.99	0.16	43,43,43,43	0
60	MG	CA	3248	1/1	0.99	0.03	58,58,58,58	0
60	MG	CA	3306	1/1	0.99	0.04	39,39,39,39	0
60	MG	AA	3148	1/1	0.99	0.08	48,48,48,48	0
60	MG	CA	3565	1/1	0.99	0.06	36,36,36,36	0
60	MG	AA	3328	1/1	0.99	0.06	21,21,21,21	0
60	MG	CA	3309	1/1	0.99	0.06	50,50,50,50	0
60	MG	AA	3818	1/1	0.99	0.06	37,37,37,37	0
60	MG	AA	3253	1/1	0.99	0.08	42,42,42,42	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	AA	3330	1/1	0.99	0.08	33,33,33,33	0
60	MG	CA	3571	1/1	0.99	0.06	52,52,52,52	0
60	MG	AA	3564	1/1	0.99	0.09	17,17,17,17	0
60	MG	BA	1768	1/1	0.99	0.09	64,64,64,64	0
60	MG	AA	3565	1/1	0.99	0.06	26,26,26,26	0
60	MG	AA	3407	1/1	0.99	0.07	22,22,22,22	0
60	MG	AA	3223	1/1	0.99	0.03	21,21,21,21	0
60	MG	CA	3381	1/1	0.99	0.08	37,37,37,37	0
60	MG	AA	3775	1/1	0.99	0.07	52,52,52,52	0
60	MG	CA	3649	1/1	0.99	0.06	15,15,15,15	0
60	MG	CA	3319	1/1	0.99	0.03	32,32,32,32	0
60	MG	AA	3013	1/1	0.99	0.06	38,38,38,38	0
60	MG	AA	3053	1/1	0.99	0.08	21,21,21,21	0
60	MG	AA	3257	1/1	0.99	0.12	18,18,18,18	0
60	MG	AA	3734	1/1	0.99	0.03	23,23,23,23	0
60	MG	AA	3386	1/1	0.99	0.09	19,19,19,19	0
60	MG	CA	3585	1/1	0.99	0.04	44,44,44,44	0
60	MG	CA	3208	1/1	0.99	0.09	24,24,24,24	0
60	MG	AA	3781	1/1	0.99	0.04	49,49,49,49	0
60	MG	CA	3454	1/1	0.99	0.09	43,43,43,43	0
60	MG	AA	3499	1/1	0.99	0.05	46,46,46,46	0
60	MG	AA	3737	1/1	0.99	0.04	25,25,25,25	0
60	MG	AA	3500	1/1	0.99	0.03	27,27,27,27	0
60	MG	AA	3574	1/1	0.99	0.06	26,26,26,26	0
60	MG	AA	3536	1/1	0.99	0.04	36,36,36,36	0
60	MG	AA	3387	1/1	0.99	0.09	34,34,34,34	0
60	MG	AA	3502	1/1	0.99	0.04	41,41,41,41	0
60	MG	AA	3415	1/1	0.99	0.08	29,29,29,29	0
60	MG	AA	3790	1/1	0.99	0.07	11,11,11,11	0
60	MG	CA	3528	1/1	0.99	0.06	51,51,51,51	1
60	MG	AA	3319	1/1	0.99	0.06	28,28,28,28	0
60	MG	CA	3337	1/1	0.99	0.04	27,27,27,27	0
60	MG	AA	3090	1/1	0.99	0.06	52,52,52,52	0
60	MG	AA	3506	1/1	0.99	0.06	19,19,19,19	0
60	MG	CA	3340	1/1	0.99	0.06	38,38,38,38	0
60	MG	AA	3418	1/1	0.99	0.08	22,22,22,22	0
60	MG	AA	3583	1/1	0.99	0.07	18,18,18,18	0
60	MG	A0	102	1/1	0.99	0.03	41,41,41,41	0
60	MG	AA	3508	1/1	0.99	0.06	42,42,42,42	0
60	MG	AA	3706	1/1	0.99	0.21	26,26,26,26	1
62	ZN	BN	501	1/1	0.99	0.03	83,83,83,83	0
62	ZN	CY	501	1/1	0.99	0.03	92,92,92,92	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	AA	3798	1/1	0.99	0.05	34,34,34,34	0
60	MG	CD	304	1/1	0.99	0.08	32,32,32,32	0
63	SF4	BD	501	8/8	0.99	0.04	67,67,67,67	0
60	MG	AA	3390	1/1	0.99	0.05	23,23,23,23	0
60	MG	AA	3391	1/1	0.99	0.06	27,27,27,27	0
60	MG	AA	3307	1/1	0.99	0.03	35,35,35,35	0
62	ZN	A5	103	1/1	1.00	0.02	40,40,40,40	0
62	ZN	A6	103	1/1	1.00	0.02	47,47,47,47	0
62	ZN	A9	501	1/1	1.00	0.03	45,45,45,45	0
60	MG	AA	3723	1/1	1.00	0.04	30,30,30,30	0
60	MG	AA	3588	1/1	1.00	0.06	33,33,33,33	0
60	MG	AA	3410	1/1	1.00	0.03	19,19,19,19	0
62	ZN	C5	102	1/1	1.00	0.02	66,66,66,66	0
62	ZN	C6	501	1/1	1.00	0.02	66,66,66,66	0
62	ZN	C9	501	1/1	1.00	0.01	70,70,70,70	0
60	MG	AA	3396	1/1	1.00	0.06	22,22,22,22	0
60	MG	AA	3470	1/1	1.00	0.01	24,24,24,24	0
60	MG	AA	3471	1/1	1.00	0.06	24,24,24,24	0
62	ZN	AY	501	1/1	1.00	0.01	68,68,68,68	0
60	MG	CA	3370	1/1	1.00	0.02	31,31,31,31	0

6.5 Other polymers (i)

There are no such residues in this entry.