



Full wwPDB EM Validation Report ⓘ

Jun 27, 2026 – 11:26 AM EDT

PDB ID : 9E7F / pdb_00009e7f
EMDB ID : EMD-47668
Title : Cryo-EM structure of the Pyrobaculum calidifontis 70S ribosome in complex with Dri
Authors : Nissley, A.J.; Cate, J.H.D.
Deposited on : 2024-11-01
Resolution : 2.53 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

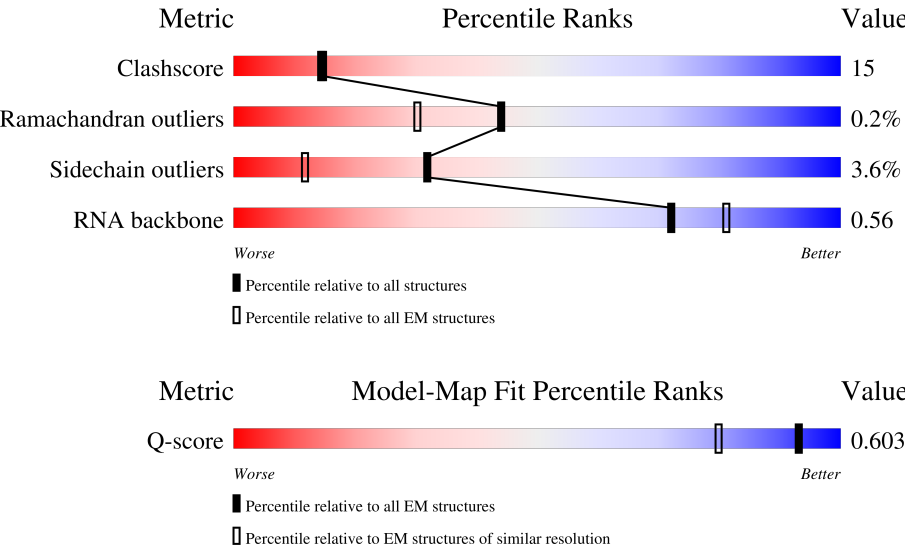
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
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

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.53 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.



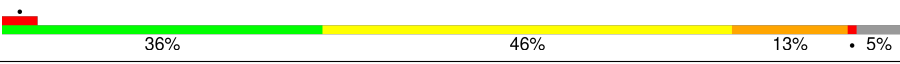
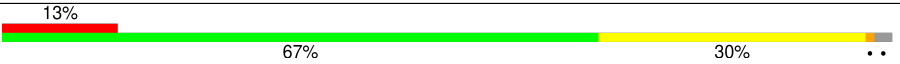
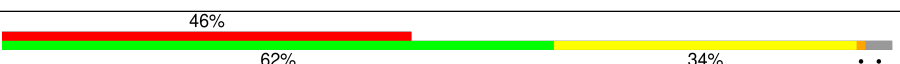
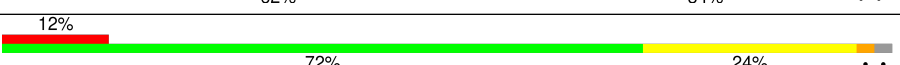
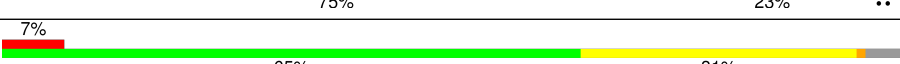
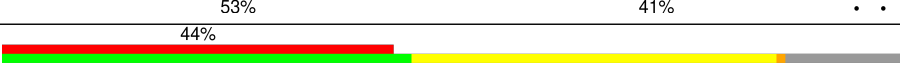
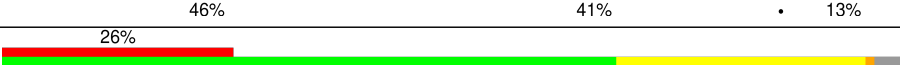
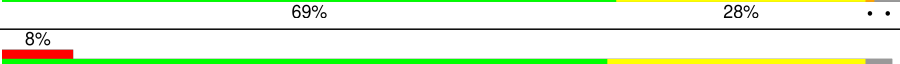
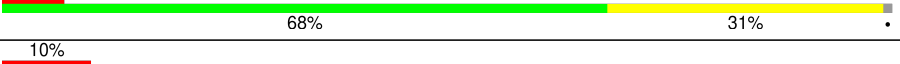
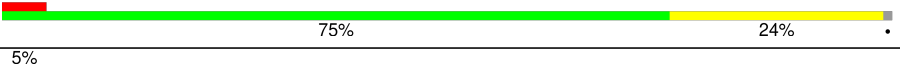
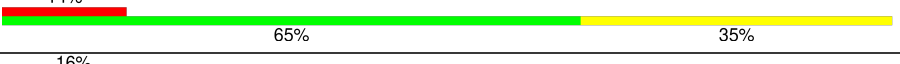
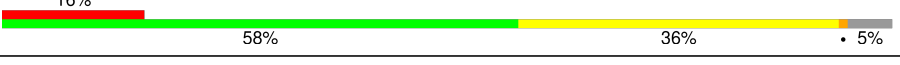
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	7309 (2.03 - 3.03)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	2	129	
2	3	655	
3	1	3024	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	4	1498	
5	AA	244	
6	AB	338	
7	AC	285	
8	AD	178	
9	AE	196	
10	AF	149	
11	AG	186	
12	AH	157	
13	AI	144	
14	AJ	103	
14	AK	103	
15	AL	156	
16	AM	189	
17	AN	178	
18	AO	205	
19	AP	122	
20	AQ	147	
21	AR	78	
22	AS	99	
23	AT	184	
24	AU	81	
25	AV	128	
26	AW	62	
27	AX	79	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
28	AY	179	
29	AZ	101	
30	Aa	91	
31	Ab	153	
32	Ac	84	
33	Ad	52	
34	Ae	67	
35	Af	51	
36	Ag	53	
37	Ah	91	
38	Ai	102	
39	Aj	184	
40	Ak	93	
41	BA	222	
42	BB	208	
43	BC	216	
44	BD	159	
45	BE	237	
46	BF	202	
47	BG	151	
48	BH	223	
49	BI	130	
50	BJ	131	
51	BK	142	
52	BL	106	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
53	BM	141	
54	BN	147	
55	BO	153	
56	BP	54	
57	BQ	151	
58	BR	147	
59	BS	71	
60	BT	158	
61	BU	158	
62	BV	128	
63	BW	110	
64	BX	100	
65	BY	67	
66	BZ	77	
67	Ba	54	
68	Bb	68	
69	Bc	65	

2 Entry composition [i](#)

There are 73 unique types of molecules in this entry. The entry contains 172182 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	129	Total	C	N	O	P	0	0
			2769	1231	512	897	129		

- Molecule 2 is a protein called Putative signal-transduction protein with CBS domains.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3	295	Total	C	N	O	S	0	0
			2251	1421	393	428	9		

- Molecule 3 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	1	2849	Total	C	N	O	P	0	0
			61386	27335	11453	19749	2849		

- Molecule 4 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	1430	Total	C	N	O	P	0	0
			30817	13730	5745	9912	1430		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	5	4AC	C	conflict	GB 343200235
4	1318	4AC	C	conflict	GB 343200235

- Molecule 5 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AA	239	Total	C	N	O	S	0	0
			1803	1136	354	308	5		

- Molecule 6 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AB	336	Total	C	N	O	S	0	0
			2611	1681	476	450	4		

- Molecule 7 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AC	278	Total	C	N	O	S	0	0
			2178	1406	395	371	6		

- Molecule 8 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AD	178	Total	C	N	O	S	0	0
			1412	894	273	238	7		

- Molecule 9 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AE	195	Total	C	N	O	S	0	0
			1520	990	254	272	4		

- Molecule 10 is a protein called Large ribosomal subunit protein eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AF	145	Total	C	N	O	S	0	0
			1095	705	187	202	1		

- Molecule 11 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AG	183	Total	C	N	O	S	0	0
			1510	979	278	246	7		

- Molecule 12 is a protein called Large ribosomal subunit protein eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AH	155	Total	C	N	O	S	0	0
			1244	785	249	209	1		

- Molecule 13 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AI	138	Total	C	N	O	S	0	0
			1068	682	202	181	3		

- Molecule 14 is a protein called Large ribosomal subunit protein eL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AJ	101	Total	C	N	O	S	0	0
			788	500	143	144	1		
14	AK	90	Total	C	N	O	S	0	0
			700	441	130	128	1		

- Molecule 15 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AL	152	Total	C	N	O	S	0	0
			1198	761	232	202	3		

- Molecule 16 is a protein called 50S ribosomal protein L15e.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AM	184	Total	C	N	O	S	0	0
			1558	992	315	245	6		

- Molecule 17 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AN	169	Total	C	N	O	S	0	0
			1336	847	254	227	8		

- Molecule 18 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	AO	200	Total	C	N	O	S	0	0
			1615	1027	309	278	1		

- Molecule 19 is a protein called Large ribosomal subunit protein eL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AP	121	Total	C	N	O	S	0	0
			920	583	181	155	1		

- Molecule 20 is a protein called Large ribosomal subunit protein eL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AQ	146	Total	C	N	O	S	0	0
			1214	759	244	208	3		

- Molecule 21 is a protein called Large ribosomal subunit protein eL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	AR	76	Total	C	N	O	S	0	0
			603	382	109	109	3		

- Molecule 22 is a protein called Large ribosomal subunit protein eL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	AS	98	Total	C	N	O	S	0	0
			788	503	150	134	1		

- Molecule 23 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	AT	183	Total	C	N	O	S	0	0
			1496	978	268	247	3		

- Molecule 24 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	AU	81	Total	C	N	O	S	0	0
			651	417	115	117	2		

- Molecule 25 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	AV	121	Total	C	N	O	S	0	0
			976	619	194	161	2		

- Molecule 26 is a protein called Large ribosomal subunit protein eL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	AW	56	Total	C	N	O	S	0	0
			449	287	86	70	6		

- Molecule 27 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	AX	67	Total	C	N	O	S	0	0
			554	343	117	92	2		

- Molecule 28 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	AY	172	Total	C	N	O	S	0	0
			1374	888	245	235	6		

- Molecule 29 is a protein called Large ribosomal subunit protein eL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	AZ	98	Total	C	N	O	S	0	0
			742	481	128	132	1		

- Molecule 30 is a protein called Large ribosomal subunit protein eL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Aa	88	Total	C	N	O	S	0	0
			726	460	146	120			

- Molecule 31 is a protein called Large ribosomal subunit protein eL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Ab	140	Total	C	N	O	S	0	0
			1183	757	239	186	1		

- Molecule 32 is a protein called Large ribosomal subunit protein eL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Ac	83	Total	C	N	O	S	0	0
			649	407	138	102	2		

- Molecule 33 is a protein called Large ribosomal subunit protein eL37.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Ad	52	Total	C	N	O	S	0	0
			429	265	93	65	6		

- Molecule 34 is a protein called LSU ribosomal protein L38E.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	Ae	66	Total	C	N	O	0	0
			552	363	93	96		

- Molecule 35 is a protein called Large ribosomal subunit protein eL39.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	Af	50	Total	C	N	O	0	0
			415	260	96	59		

- Molecule 36 is a protein called Large ribosomal subunit protein eL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Ag	50	Total	C	N	O	S	0	0
			417	259	88	66	4		

- Molecule 37 is a protein called eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Ah	91	Total	C	N	O	S	0	0
			739	467	142	123	7		

- Molecule 38 is a protein called Large ribosomal subunit protein eL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Ai	99	Total	C	N	O	S	0	0
			769	489	148	127	5		

- Molecule 39 is a protein called DJ-1/PfpI domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Aj	183	Total	C	N	O	S	0	0
			1469	954	248	265	2		

- Molecule 40 is a protein called PaREP1 domain containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Ak	90	Total	C	N	O	S	0	0
			743	478	127	136	2		

- Molecule 41 is a protein called Small ribosomal subunit protein eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	BA	187	Total	C	N	O	S	0	0
			1487	965	263	256	3		

- Molecule 42 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	BB	198	Total	C	N	O	S	0	0
			1600	1037	277	279	7		

- Molecule 43 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	BC	77	Total	C	N	O	S	0	0
			611	393	110	107	1		

- Molecule 44 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	BD	157	Total	C	N	O	S	0	0
			1284	831	240	209	4		

- Molecule 45 is a protein called Small ribosomal subunit protein eS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	BE	236	Total	C	N	O	S	0	0
			1883	1223	336	322	2		

- Molecule 46 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	BF	194	Total	C	N	O	S	0	0
			1498	951	272	271	4		

- Molecule 47 is a protein called Small ribosomal subunit protein eS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	BG	140	Total	C	N	O	S	0	0
			1065	685	190	188	2		

- Molecule 48 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	BH	220	Total	C	N	O	S	0	0
			1773	1128	325	313	7		

- Molecule 49 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	BI	129	Total	C	N	O	S	0	0
			1036	676	177	180	3		

- Molecule 50 is a protein called Small ribosomal subunit protein eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	BJ	130	Total	C	N	O	S	0	0
			1007	636	198	172	1		

- Molecule 51 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	BK	134	Total	C	N	O	S	0	0
			1058	680	191	182	5		

- Molecule 52 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	BL	38	Total	C	N	O	S	0	0
			315	201	64	49	1		

- Molecule 53 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	BM	127	Total	C	N	O	S	0	0
			941	592	182	164	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BM	128	IAS	ASP	conflict	UNP A3MX63

- Molecule 54 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	BN	144	Total	C	N	O	S	0	0
			1133	730	211	189	3		

- Molecule 55 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	BO	143	Total	C	N	O	S	0	0
			1108	700	211	195	2		

- Molecule 56 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	BP	29	Total	C	N	O	S	0	0
			241	150	51	36	4		

- Molecule 57 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	BQ	149	Total	C	N	O	S	0	0
			1224	782	233	208	1		

- Molecule 58 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	BR	144	Total	C	N	O	S	0	0
			1171	756	216	194	5		

- Molecule 59 is a protein called Small ribosomal subunit protein eS17.

Mol	Chain	Residues	Atoms				AltConf	Trace
59	BS	64	Total	C	N	O	0	0
			517	332	94	91		

- Molecule 60 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	BT	135	Total	C	N	O	S	0	0
			1111	720	203	182	6		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BT	6	ALA	GLN	conflict	UNP A0A831L0N9
BT	19	THR	ALA	conflict	UNP A0A831L0N9
BT	28	SER	THR	conflict	UNP A0A831L0N9
BT	43	PRO	SER	conflict	UNP A0A831L0N9
BT	81	MET	ALA	conflict	UNP A0A831L0N9
BT	93	CYS	SER	conflict	UNP A0A831L0N9
BT	137	ARG	LYS	conflict	UNP A0A831L0N9

- Molecule 61 is a protein called Small ribosomal subunit protein eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	BU	155	Total	C	N	O	S	0	0
			1225	789	225	209	2		

- Molecule 62 is a protein called Small ribosomal subunit protein eS24.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	BV	115	Total	C	N	O		0	0
			950	597	185	168			

- Molecule 63 is a protein called SSU ribosomal protein S25E.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	BW	68	Total	C	N	O	S	0	0
			544	351	96	96	1		

- Molecule 64 is a protein called SSU ribosomal protein S26E.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	BX	95	Total	C	N	O	S	0	0
			772	490	150	128	4		

- Molecule 65 is a protein called Small ribosomal subunit protein eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	BY	65	Total	C	N	O	S	0	0
			501	317	100	79	5		

- Molecule 66 is a protein called Small ribosomal subunit protein eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	BZ	71	Total	C	N	O	S	0	0
			552	344	108	99	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BZ	37	ARG	LYS	conflict	UNP B1Y9V2

- Molecule 67 is a protein called SSU ribosomal protein S30E.

Mol	Chain	Residues	Atoms				AltConf	Trace
67	Ba	43	Total	C	N	O	0	0
			357	222	80	55		

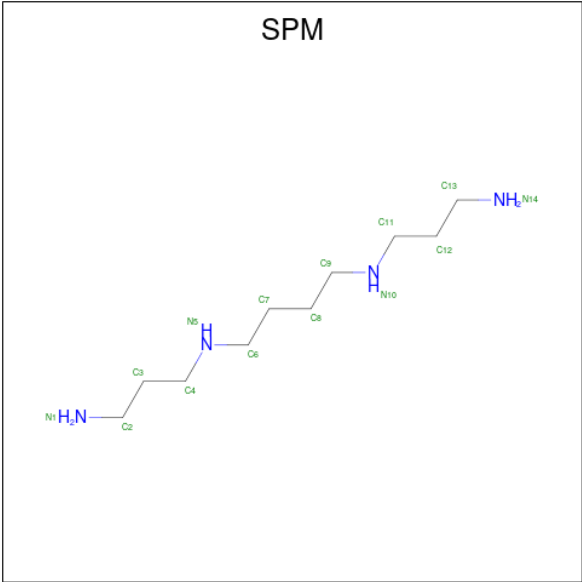
- Molecule 68 is a protein called aS35.

Mol	Chain	Residues	Atoms				AltConf	Trace
68	Bb	60	Total	C	N	O	0	0
			479	301	95	83		

- Molecule 69 is a protein called Small zinc finger protein HVO-2753-like zinc-binding pocket domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	Bc	64	Total	C	N	O	S	0	0
			477	301	90	82	4		

- Molecule 70 is SPERMINE (CCD ID: SPM) (formula: C₁₀H₂₆N₄).



Mol	Chain	Residues	Atoms			AltConf
70	1	1	Total	C	N	0
			14	10	4	
70	1	1	Total	C	N	0
			14	10	4	
70	1	1	Total	C	N	0
			14	10	4	
70	1	1	Total	C	N	0
			14	10	4	
70	1	1	Total	C	N	0
			14	10	4	
70	1	1	Total	C	N	0
			14	10	4	
70	1	1	Total	C	N	0
			14	10	4	
70	1	1	Total	C	N	0
			14	10	4	
70	1	1	Total	C	N	0
			14	10	4	
70	1	1	Total	C	N	0
			14	10	4	
70	1	1	Total	C	N	0
			14	10	4	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
70	1	1	Total	C	N	0
			14	10	4	
70	1	1	Total	C	N	0
			14	10	4	
70	1	1	Total	C	N	0
			14	10	4	
70	1	1	Total	C	N	0
			14	10	4	
70	1	1	Total	C	N	0
			14	10	4	
70	1	1	Total	C	N	0
			14	10	4	
70	1	1	Total	C	N	0
			14	10	4	
70	1	1	Total	C	N	0
			14	10	4	
70	1	1	Total	C	N	0
			14	10	4	
70	1	1	Total	C	N	0
			14	10	4	
70	1	1	Total	C	N	0
			14	10	4	
70	1	1	Total	C	N	0
			14	10	4	
70	1	1	Total	C	N	0
			14	10	4	
70	1	1	Total	C	N	0
			14	10	4	
70	1	1	Total	C	N	0
			14	10	4	
70	1	1	Total	C	N	0
			14	10	4	
70	1	1	Total	C	N	0
			14	10	4	
70	1	1	Total	C	N	0
			14	10	4	
70	1	1	Total	C	N	0
			14	10	4	
70	1	1	Total	C	N	0
			14	10	4	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
70	1	1	Total	C	N	0
			14	10	4	
70	1	1	Total	C	N	0
			14	10	4	
70	1	1	Total	C	N	0
			14	10	4	
70	1	1	Total	C	N	0
			14	10	4	
70	1	1	Total	C	N	0
			14	10	4	
70	1	1	Total	C	N	0
			14	10	4	
70	1	1	Total	C	N	0
			14	10	4	
70	4	1	Total	C	N	0
			14	10	4	
70	4	1	Total	C	N	0
			14	10	4	
70	4	1	Total	C	N	0
			14	10	4	
70	4	1	Total	C	N	0
			14	10	4	
70	4	1	Total	C	N	0
			14	10	4	
70	4	1	Total	C	N	0
			14	10	4	
70	4	1	Total	C	N	0
			14	10	4	
70	4	1	Total	C	N	0
			14	10	4	
70	4	1	Total	C	N	0
			14	10	4	
70	4	1	Total	C	N	0
			14	10	4	
70	4	1	Total	C	N	0
			14	10	4	
70	4	1	Total	C	N	0
			14	10	4	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
70	4	1	Total	C	N	0
			14	10	4	
70	4	1	Total	C	N	0
			14	10	4	
70	4	1	Total	C	N	0
			14	10	4	
70	4	1	Total	C	N	0
			14	10	4	
70	4	1	Total	C	N	0
			14	10	4	
70	AL	1	Total	C	N	0
			14	10	4	
70	AM	1	Total	C	N	0
			14	10	4	
70	Ah	1	Total	C	N	0
			14	10	4	

- Molecule 71 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
71	1	170	Total	Mg	0
			170	170	
71	4	77	Total	Mg	0
			77	77	
71	AA	1	Total	Mg	0
			1	1	
71	AL	2	Total	Mg	0
			2	2	
71	BK	1	Total	Mg	0
			1	1	

- Molecule 72 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
72	AW	1	Total	Zn	0
			1	1	
72	Ad	1	Total	Zn	0
			1	1	
72	Ag	1	Total	Zn	0
			1	1	
72	Ah	1	Total	Zn	0
			1	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
72	Ai	1	Total 1	Zn 1	0
72	BF	1	Total 1	Zn 1	0
72	BP	1	Total 1	Zn 1	0
72	BR	1	Total 1	Zn 1	0
72	BX	1	Total 1	Zn 1	0
72	BY	1	Total 1	Zn 1	0
72	Bc	1	Total 1	Zn 1	0

- Molecule 73 is water.

Mol	Chain	Residues	Atoms		AltConf
73	2	94	Total 94	O 94	0
73	3	4	Total 4	O 4	0
73	1	4730	Total 4730	O 4730	0
73	4	1186	Total 1186	O 1186	0
73	AA	13	Total 13	O 13	0
73	AB	4	Total 4	O 4	0
73	AC	7	Total 7	O 7	0
73	AE	1	Total 1	O 1	0
73	AG	1	Total 1	O 1	0
73	AH	1	Total 1	O 1	0
73	AL	11	Total 11	O 11	0
73	AM	5	Total 5	O 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
73	AN	1	Total 1	O 1	0
73	AQ	1	Total 1	O 1	0
73	AS	1	Total 1	O 1	0
73	AT	3	Total 3	O 3	0
73	AW	1	Total 1	O 1	0
73	AY	1	Total 1	O 1	0
73	Ab	7	Total 7	O 7	0
73	Ad	2	Total 2	O 2	0
73	Ag	1	Total 1	O 1	0
73	Ah	1	Total 1	O 1	0
73	BA	27	Total 27	O 27	0
73	BB	13	Total 13	O 13	0
73	BC	13	Total 13	O 13	0
73	BD	16	Total 16	O 16	0
73	BE	10	Total 10	O 10	0
73	BF	17	Total 17	O 17	0
73	BG	18	Total 18	O 18	0
73	BH	18	Total 18	O 18	0
73	BI	16	Total 16	O 16	0
73	BJ	11	Total 11	O 11	0
73	BK	15	Total 15	O 15	0

Continued on next page...

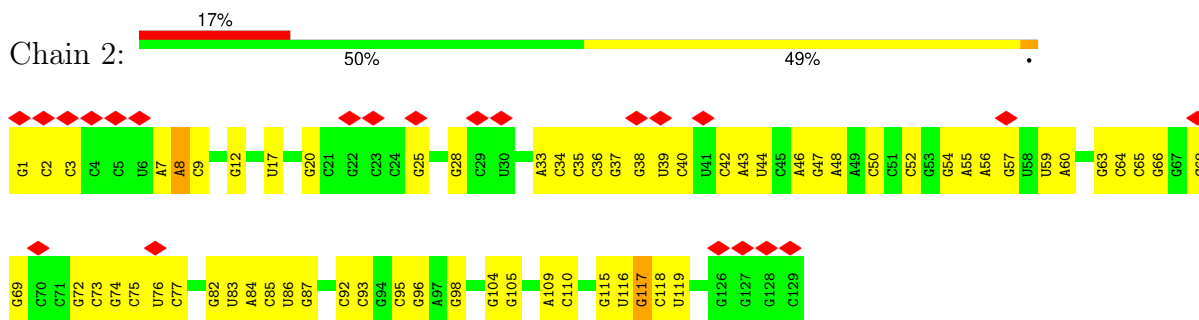
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
73	BL	4	Total 4	O 4	0
73	BM	10	Total 10	O 10	0
73	BN	10	Total 10	O 10	0
73	BO	10	Total 10	O 10	0
73	BP	5	Total 5	O 5	0
73	BQ	6	Total 6	O 6	0
73	BR	9	Total 9	O 9	0
73	BS	4	Total 4	O 4	0
73	BT	12	Total 12	O 12	0
73	BU	11	Total 11	O 11	0
73	BV	3	Total 3	O 3	0
73	BW	11	Total 11	O 11	0
73	BX	7	Total 7	O 7	0
73	BY	6	Total 6	O 6	0
73	BZ	5	Total 5	O 5	0
73	Ba	4	Total 4	O 4	0
73	Bb	11	Total 11	O 11	0
73	Bc	9	Total 9	O 9	0

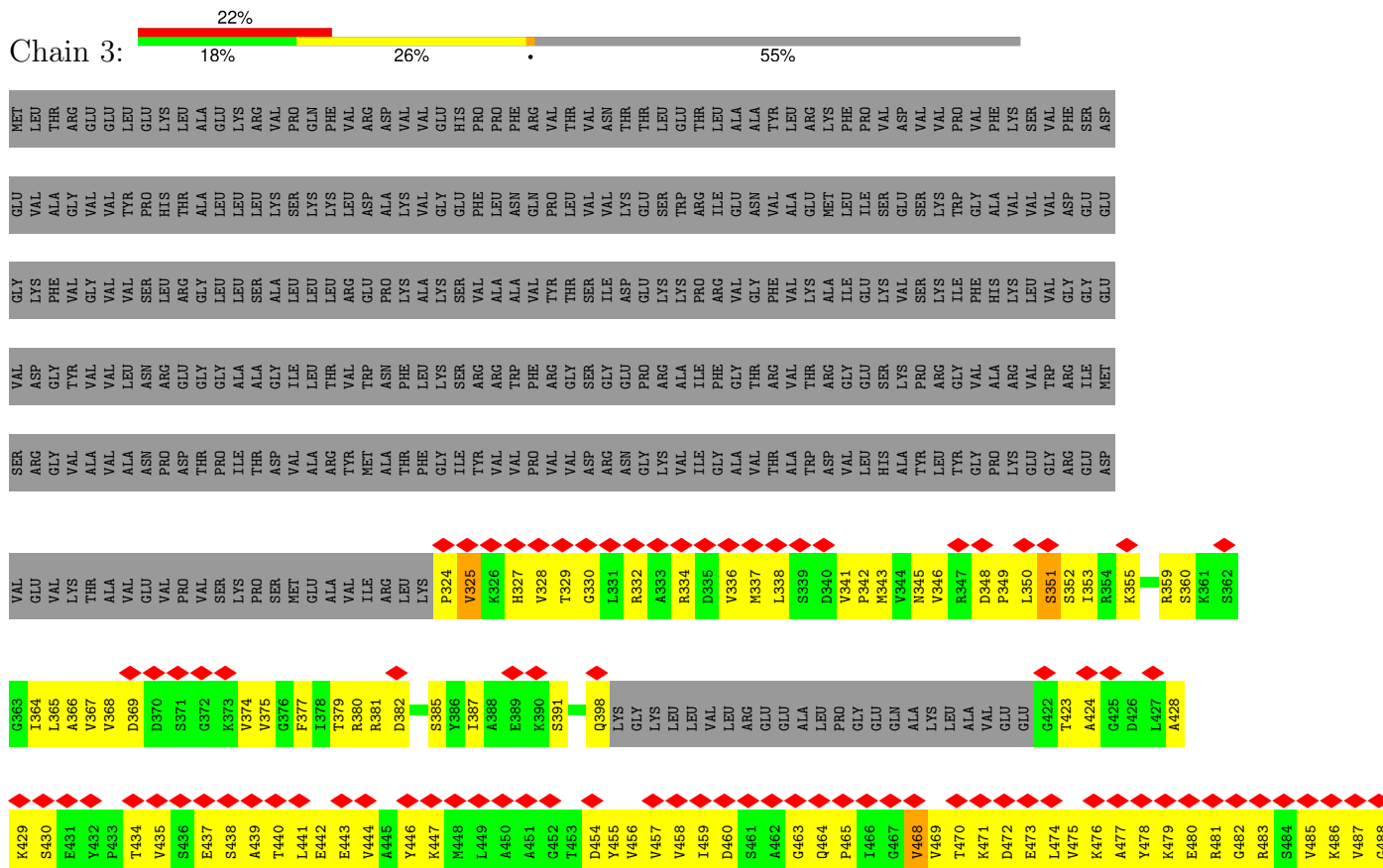
3 Residue-property plots

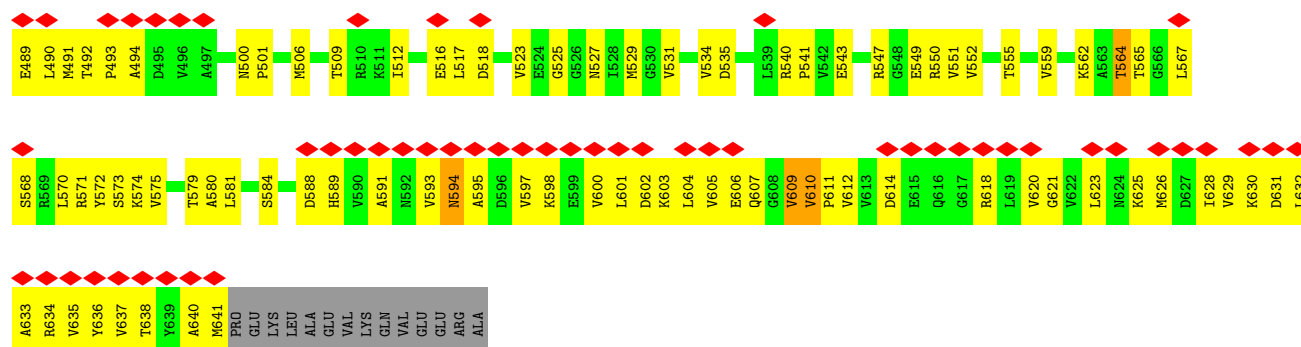
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: 5S rRNA



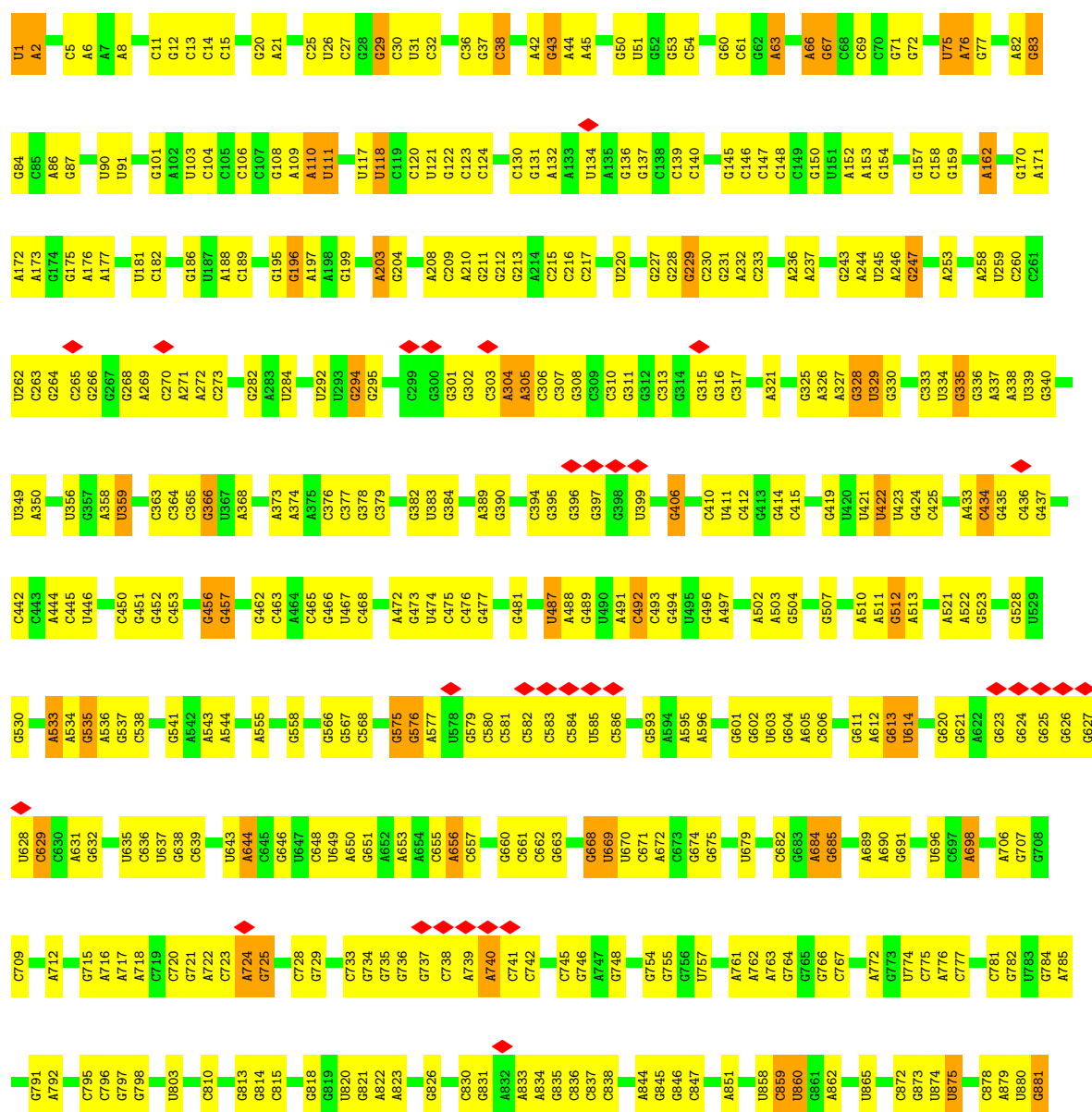
• Molecule 2: Putative signal-transduction protein with CBS domains



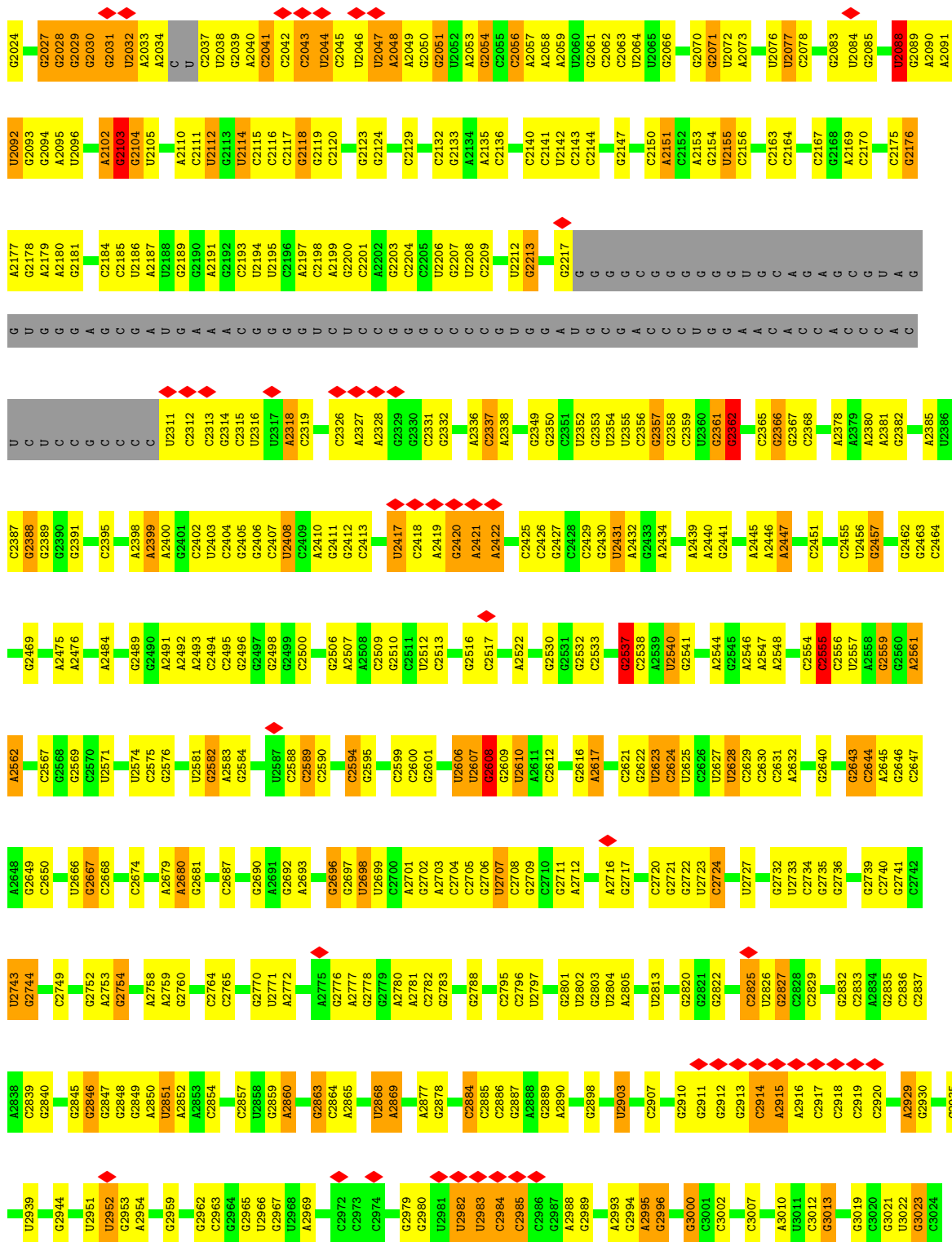


• Molecule 3: 23S rRNA

Chain 1: 48% 38% 8% 6%

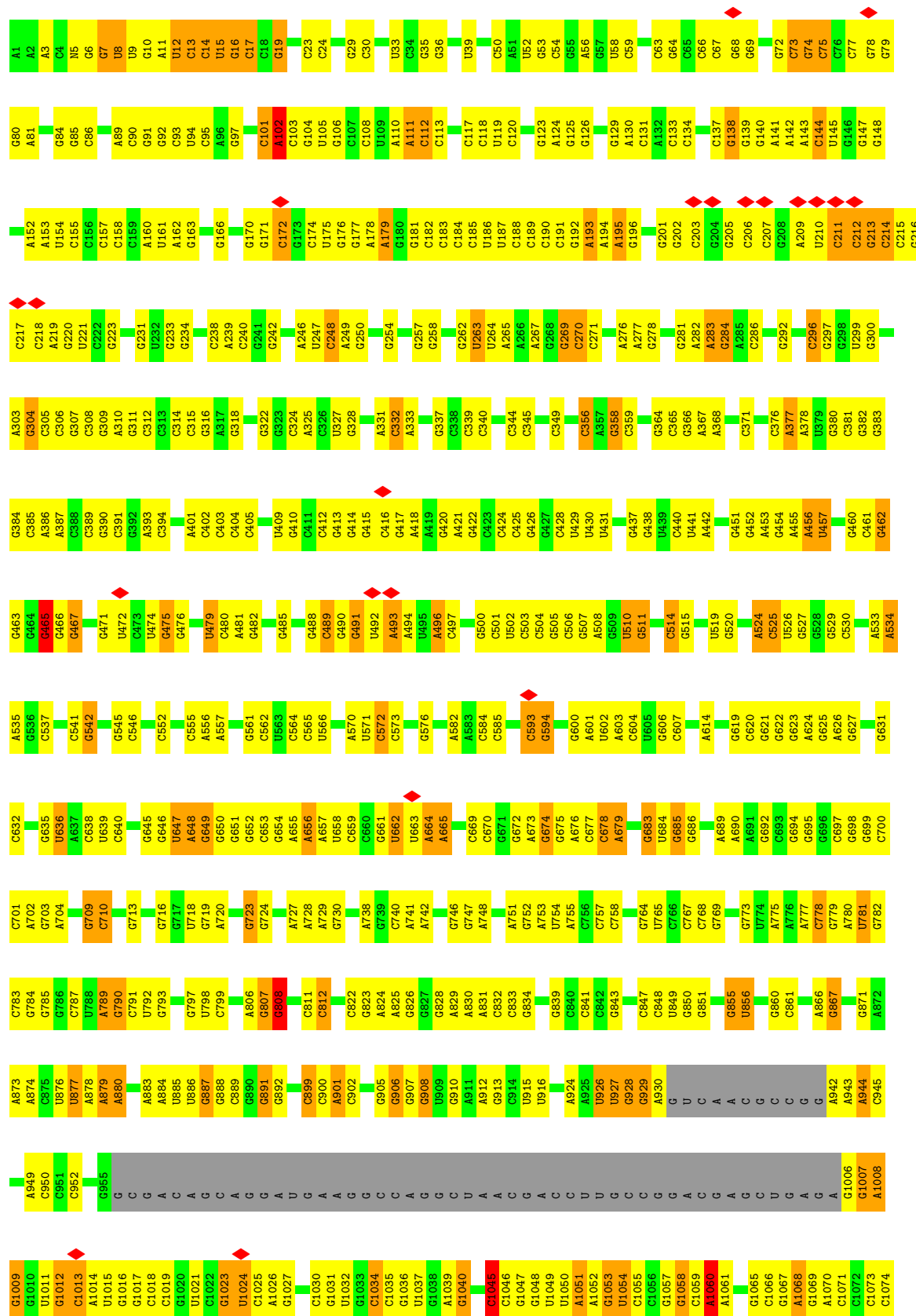


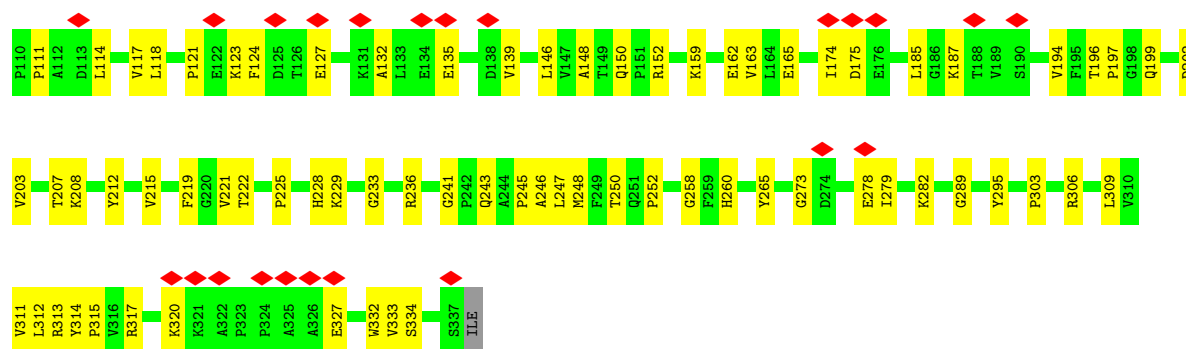
U1930	C1931	C1932	C1933	C1934	C1935	C1936	C1937	A1938	U1944	A1945	A1946	G1947	G1948	G1949	U1954	G1957	G1958	U1963	G1964	G1982	G1985	G1986	G1971	G1975	C1976	C1977	C1978	C1979	C1980	U1983	A1984	U1987	G1988	A1989	A1990	A1999	C2000	A2001	A2002	C2003	G2006	G2007	G2008	G2009	A2010	A2011	G2017	G2018	A2022	G2023	
G1849	U1850	C1853	C1834	U1854	G1855	C1856	G1857	G1858	U1859	C1860	U1861	U1862	G1863	G1864	G1865	G1866	U1867	A1868	U1869	A1870	G1882	G1885	G1886	G1887	G1888	G1889	G1890	A1891	G1892	U1898	G1899	U1906	U1907	G1908	A1909	U1910	U1911	G1912	U1913	U1914	U1915	U1916	G1917	U1918	U1919	A1920	A1921	A1922	A1925	U1926	A1927
G1645	G1646	G1647	A1648	G1649	A1650	A1651	C1657	G1658	A1659	G1662	C1663	G1664	G1665	A1668	U1669	G1674	G1675	G1676	G1677	G1678	U1679	U1680	U1681	C1682	C1683	C1684	G1685	G1686	G1687	U1688	U1698	G1703	A1708	A1712	A1713	A1714	A1715	G1716	G1723	C1728	C1734	A1833	A1834	C1835	C1838	G1839	G1840				
A1752	C1753	C1754	G1755	A1756	C1757	G1758	C1759	A1760	G1764	C1765	U1769	G1770	G1771	A1777	A1778	C1781	C1782	A1783	G1786	G1789	C1790	U1791	C1792	G1793	G1794	G1795	U1796	G1797	A1798	C1801	C1806	C1807	A1808	G1811	A1812	C1816	G1817	A1818	C1819	G1825	A1833	A1834	C1835	C1838	G1839	G1840					
G1564	C1568	U1569	U1570	U1571	C1572	C1573	C1577	G1578	C1579	G1584	G1585	G1586	A1588	A1589	C1592	G1595	G1596	A1600	C1601	U1602	G1603	C1604	G1611	C1612	U1613	U1614	A1615	A1616	G1619	U1620	C1621	G1622	A1623	A1624	G1625	C1628	G1631	G1632	A1633	G1634	U1635	G1636	C1637	C1638	G1639	A1642	U1643	G1644			
A1494	U1495	A1496	G1497	U1498	C1499	A1500	C1501	G1504	C1505	A1508	A1509	A1510	A1514	A1515	A1516	G1517	G1518	A1523	A1524	U1525	A1526	U1527	U1528	C1529	U1533	G1534	C1535	U1536	G1537	C1538	G1539	G1540	G1541	G1542	G1543	U1544	A1545	G1546	G1547	U1548	U1549	C1550	U1551	G1552	G1555	A1556	A1557	A1558	C1559	A1562	G1563
G1396	C1397	A1398	G1401	A1402	A1403	U1410	G1411	A1414	A1415	G1416	C1417	C1418	C1419	C1420	G1424	G1427	G1428	A1429	A1430	A1431	C1435	C1436	G1439	G1440	C1444	G1447	G1448	C1449	U1454	C1455	A1456	A1457	G1468	U1469	U1470	G1473	C1474	C1479	U1480	A1481	A1482	G1483	G1484	G1485	G1486	G1487					
G1297	C1298	C1299	G1300	U1301	U1302	G1303	C1307	G1308	C1309	G1310	U1311	G1312	G1313	G1314	G1315	U1316	A1317	G1318	G1319	G1322	G1323	G1327	G1328	C1337	A1338	G1339	A1340	G1347	G1350	U1351	G1352	A1353	G1354	G1355	U1356	C1357	C1358	A1364	C1365	U1382	C1384	C1385	G1389	G1390	U1391	A1392	G1393	U1394	A1395		
A	C	G	C	G	U	A	C	A	G	C	C	G	A	C	C	C	C	C1234	C1235	G1236	A1237	G1242	G1243	G1244	G1245	G1246	C1247	C1248	A1253	G1254	U1255	G1256	U1257	U1258	A1259	C1260	A1261	G1262	A1265	A1268	A1269	C1279	G1280	C1285	G1289	C1290	C1291	C1292	G1293		
A1152	A1153	A1154	A1155	G1160	U1161	C1162	C1163	C1164	C1165	G1166	G1167	C1168	C1169	C1170	A1171	A1172	A1173	A1174	C1175	A1176	A1177	C	G	G	G	G	C	C	C	U	G	C	G	G	G	C	C	C	A	A	C	C	C	C	C	C	A				
A1037	C1038	C1039	A1044	G1053	A1054	G1067	G1068	G1073	U1074	G1075	G1076	G1077	A1080	A1081	G1082	C1083	C1084	U1085	G1088	C1089	U1090	C1091	A1094	G1095	A1101	A1102	C1103	A1104	G1110	A1120	A1121	G1122	G1123	C1124	C1125	A1129	A1130	G1131	U1132	G1133	G1136	U1145	C1146	A1147	U1151						
C970	C971	G976	G977	G978	U979	A980	A982	G983	U984	A985	C986	U987	A989	G994	G995	U	G	C	C	C	C	C	C	C	A	A	A	G	C	U	C	C	C	C	C1020	C1021	C1022	C1023	G1024	G1025	U1026	C1027	A1028	A1029	A1030	C1031	U1032	C1033	C1034		
G986	G993	G994	G995	A900	A901	G902	A903	A907	U908	C909	A910	G912	G913	C914	C915	G916	G917	U918	U919	A920	U921	A922	G923	C924	U925	C930	C931	C932	C935	G936	A937	A938	G939	U944	C945	U946	C950	C951	C956	U957	C958	G963	A964	G965	G966	G967	G968	G969			



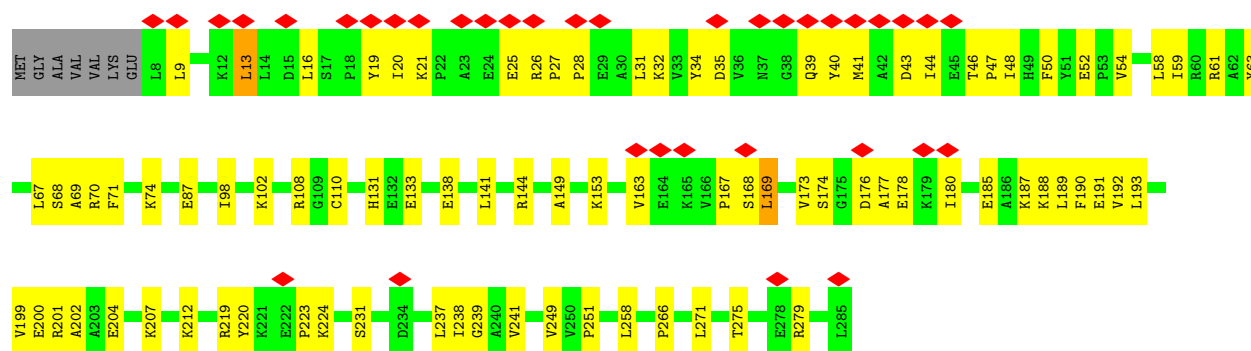
• Molecule 4: 16S rRNA

Chain 4:

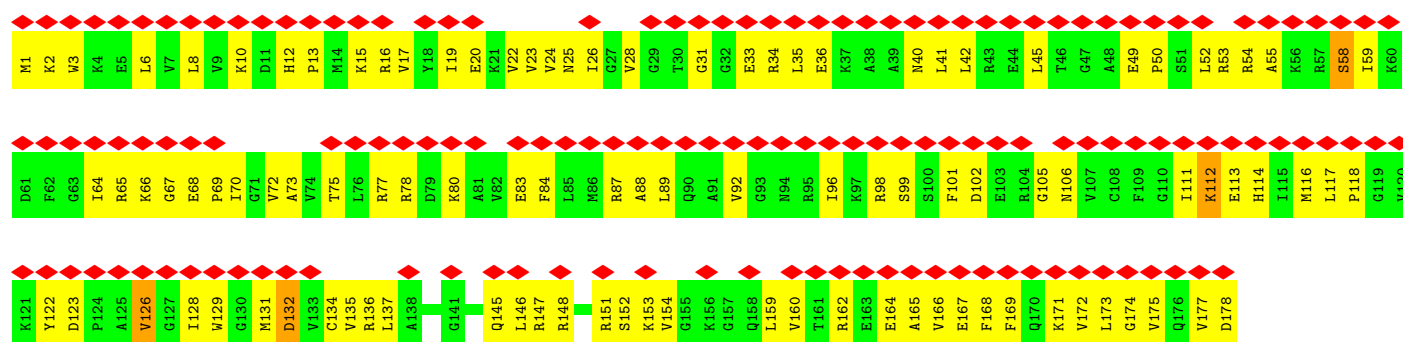
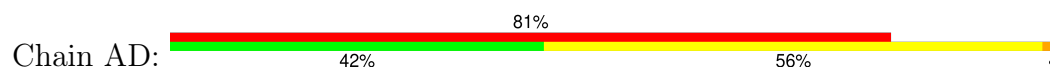




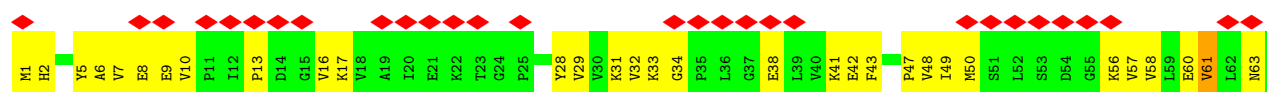
• Molecule 7: Large ribosomal subunit protein uL4

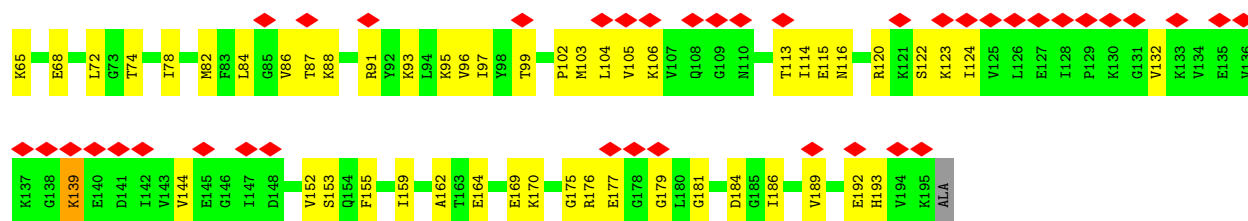


• Molecule 8: Large ribosomal subunit protein uL5

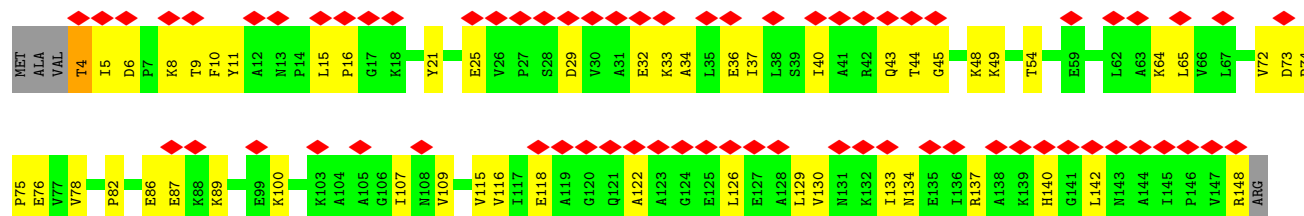


• Molecule 9: Large ribosomal subunit protein uL6

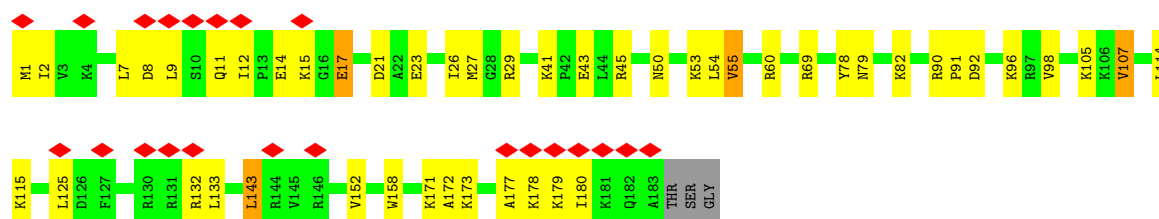
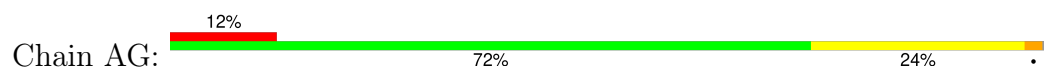




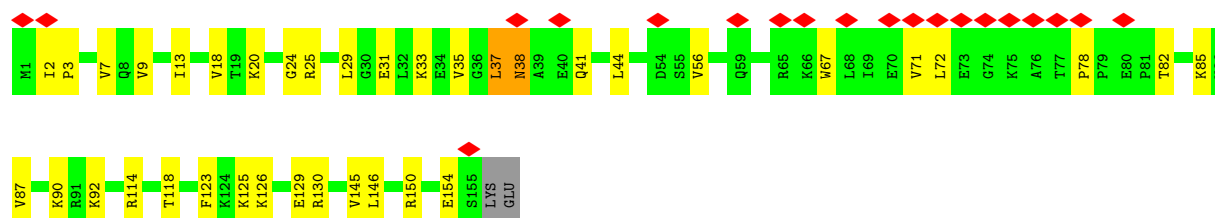
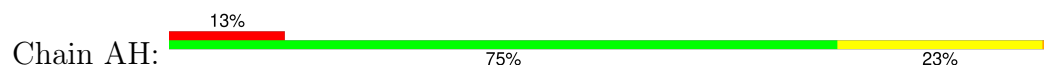
• Molecule 10: Large ribosomal subunit protein eL8



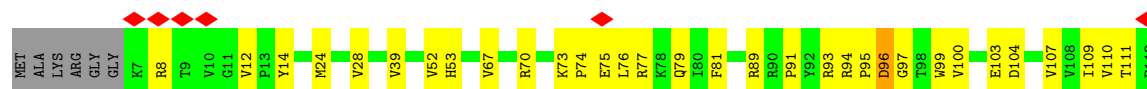
• Molecule 11: Large ribosomal subunit protein uL13

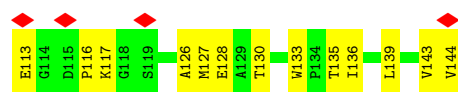


• Molecule 12: Large ribosomal subunit protein eL13

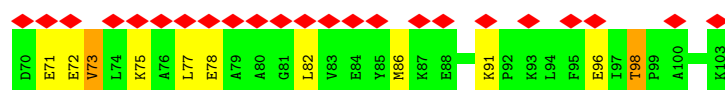
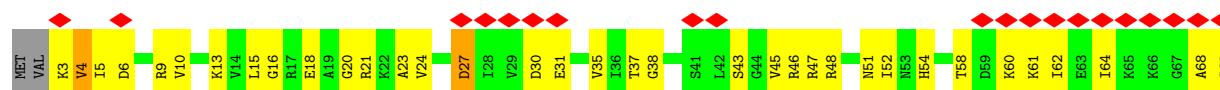
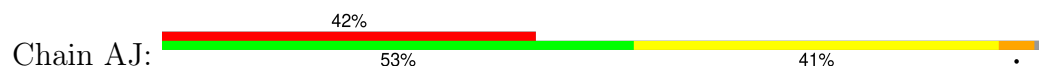


• Molecule 13: Large ribosomal subunit protein uL14

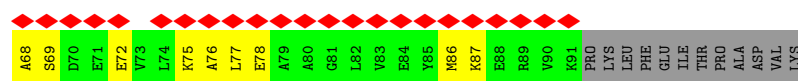
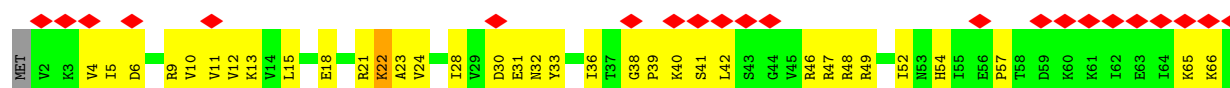




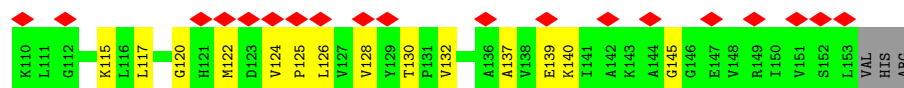
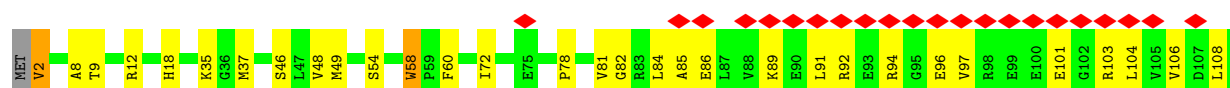
- Molecule 14: Large ribosomal subunit protein eL14



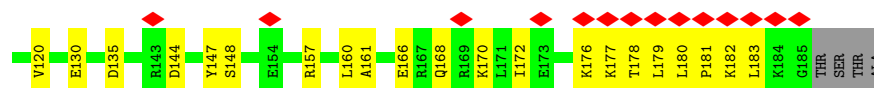
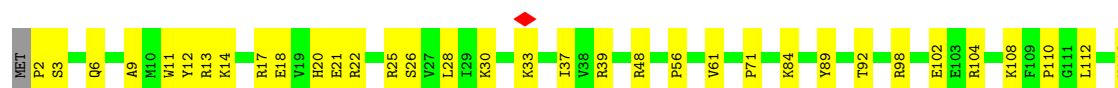
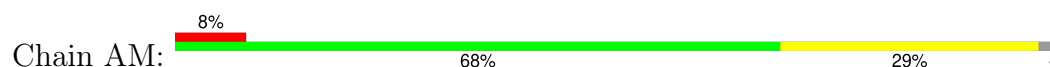
- Molecule 14: Large ribosomal subunit protein eL14



- Molecule 15: Large ribosomal subunit protein uL15

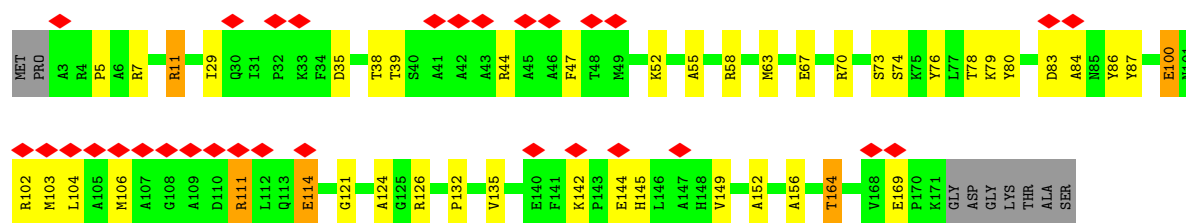


- Molecule 16: 50S ribosomal protein L15e



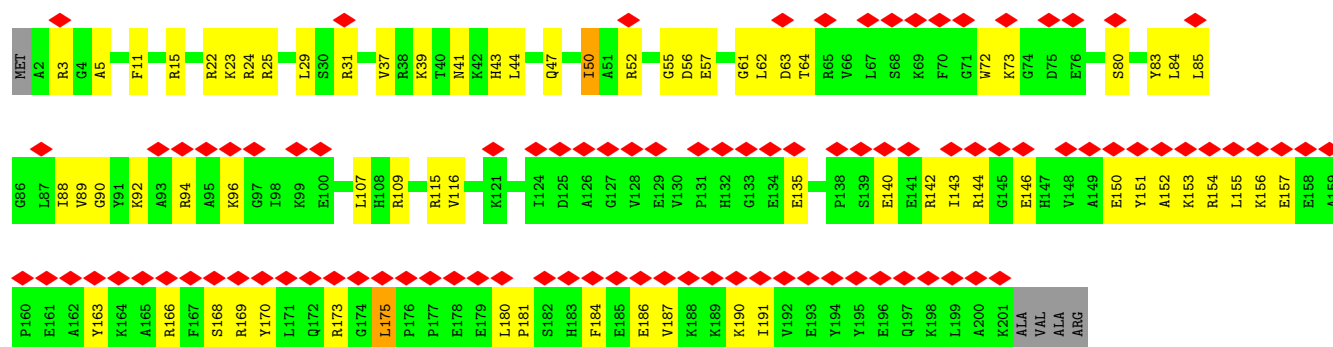
- Molecule 17: Large ribosomal subunit protein uL16

Chain AN: 



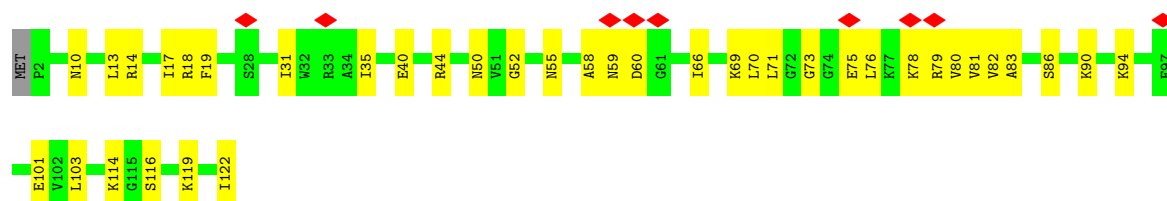
- Molecule 18: Large ribosomal subunit protein uL18

Chain AO: 



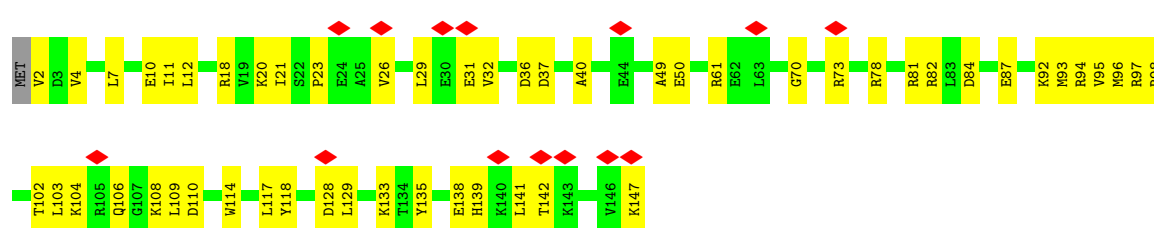
- Molecule 19: Large ribosomal subunit protein eL18

Chain AP: 



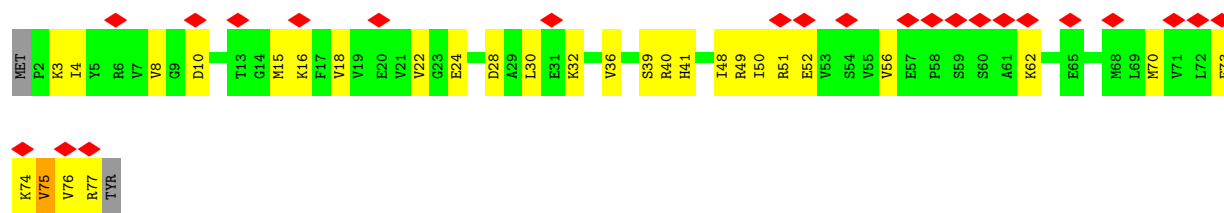
- Molecule 20: Large ribosomal subunit protein eL19

Chain AQ: 

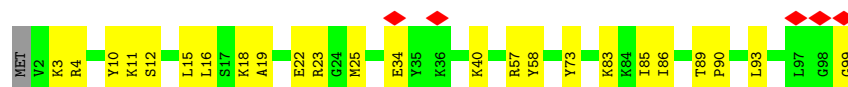
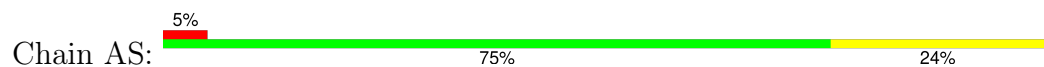


- Molecule 21: Large ribosomal subunit protein eL20

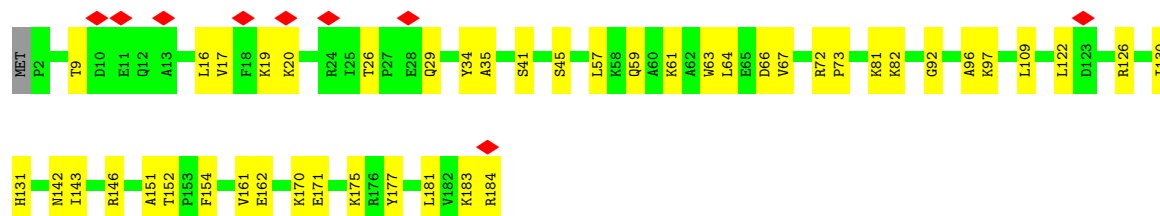
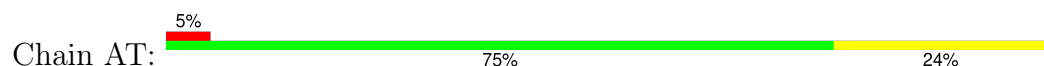
Chain AR: 



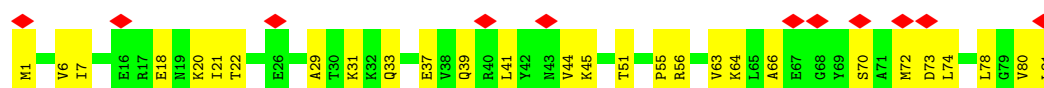
- Molecule 22: Large ribosomal subunit protein eL21



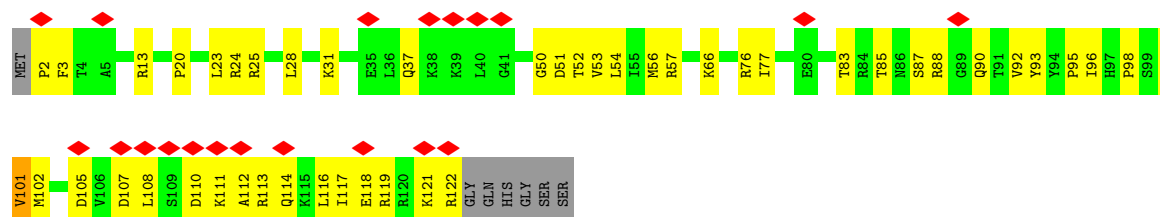
- Molecule 23: Large ribosomal subunit protein uL22



- Molecule 24: Large ribosomal subunit protein uL23

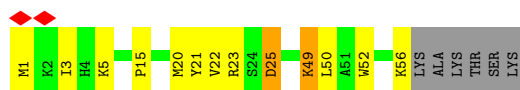


- Molecule 25: Large ribosomal subunit protein uL24

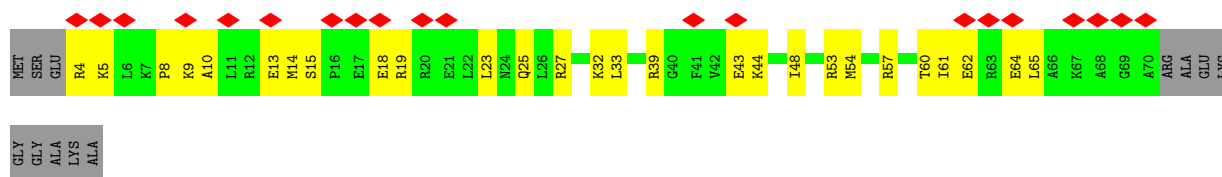


- Molecule 26: Large ribosomal subunit protein eL24

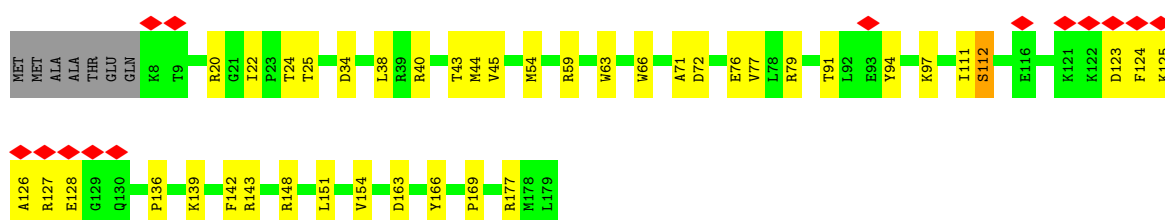
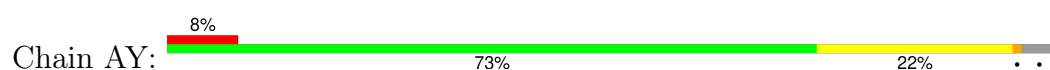




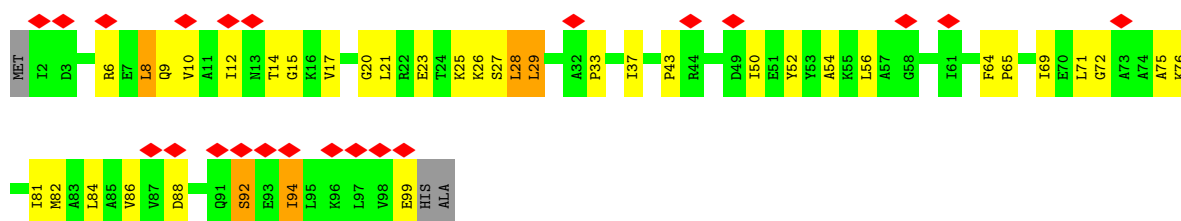
- Molecule 27: Large ribosomal subunit protein uL29



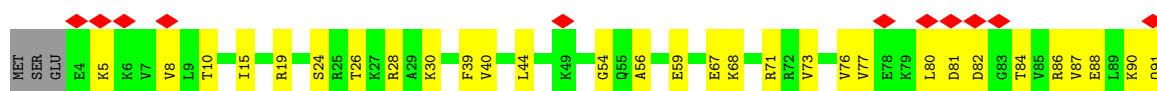
- Molecule 28: Large ribosomal subunit protein uL30



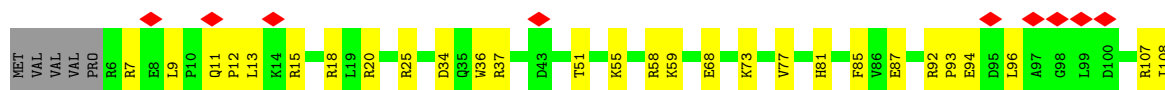
- Molecule 29: Large ribosomal subunit protein eL30



- Molecule 30: Large ribosomal subunit protein eL31



- Molecule 31: Large ribosomal subunit protein eL32

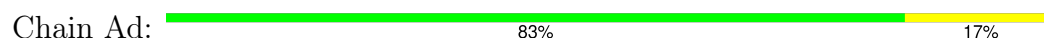




- Molecule 32: Large ribosomal subunit protein eL34



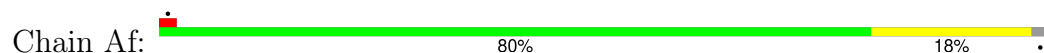
- Molecule 33: Large ribosomal subunit protein eL37



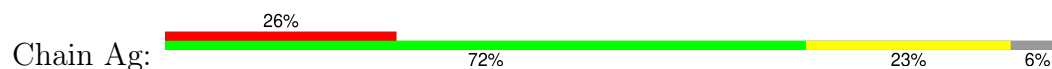
- Molecule 34: LSU ribosomal protein L38E



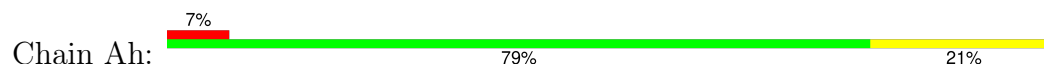
- Molecule 35: Large ribosomal subunit protein eL39



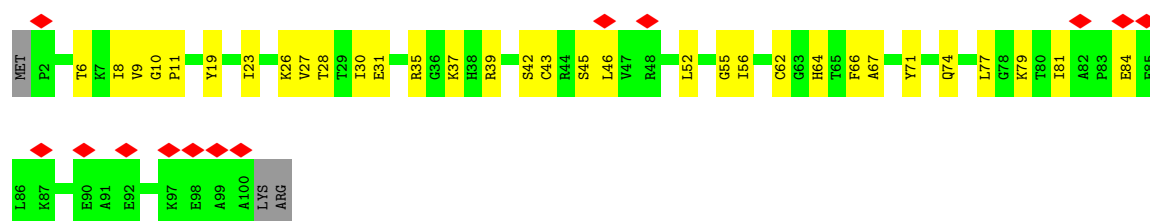
- Molecule 36: Large ribosomal subunit protein eL40



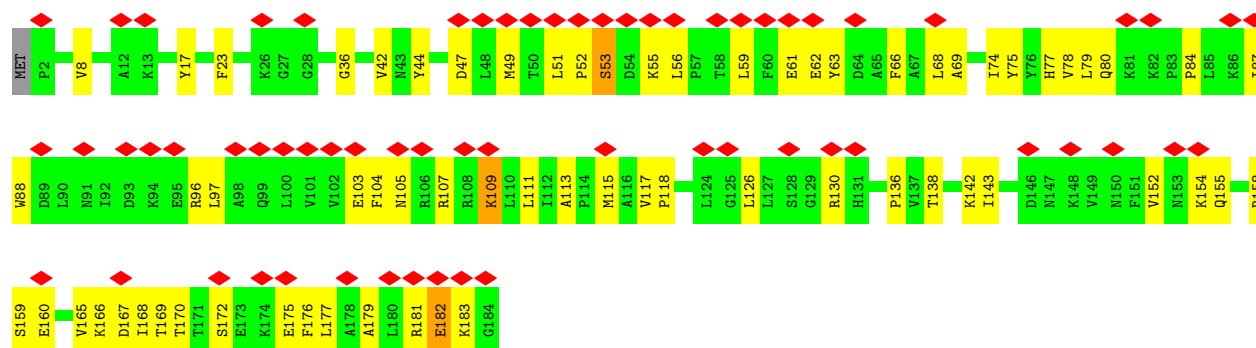
- Molecule 37: eL42



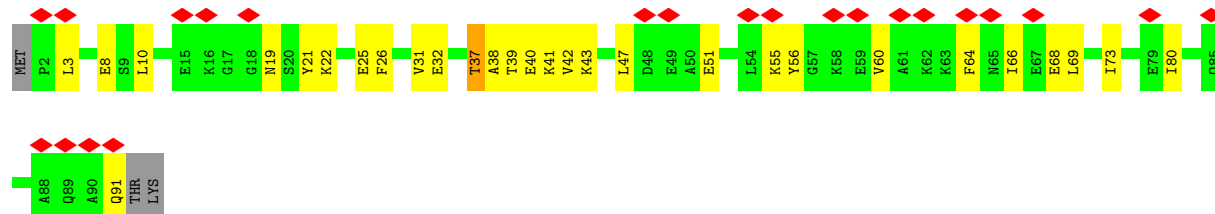
- Molecule 38: Large ribosomal subunit protein eL43



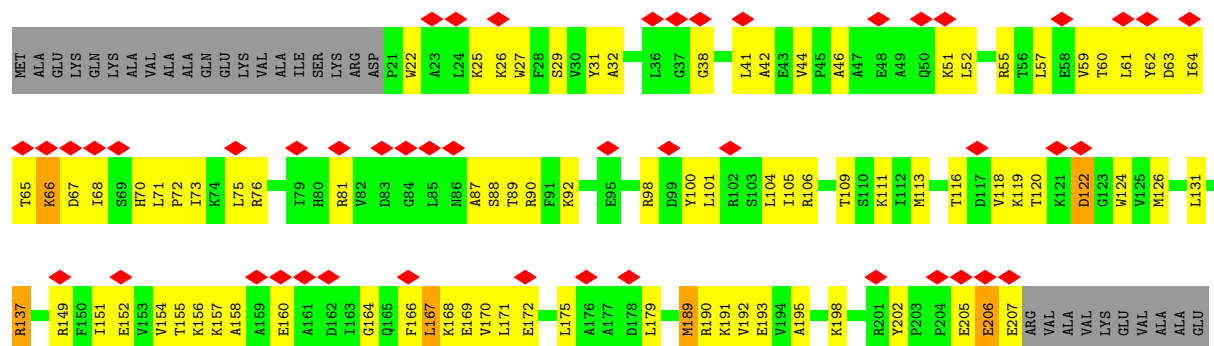
- Molecule 39: DJ-1/PfpI domain-containing protein

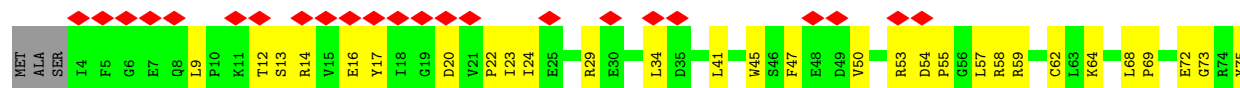


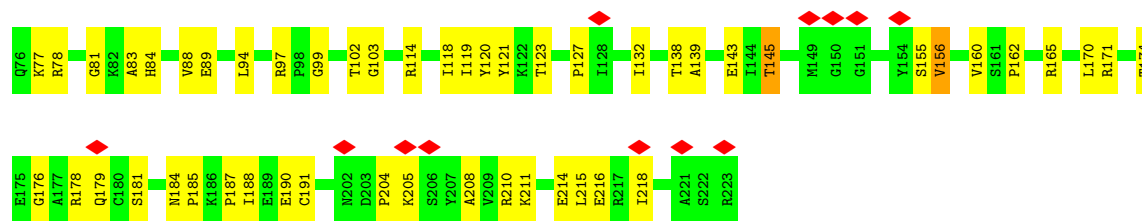
- Molecule 40: PaREP1 domain containing protein



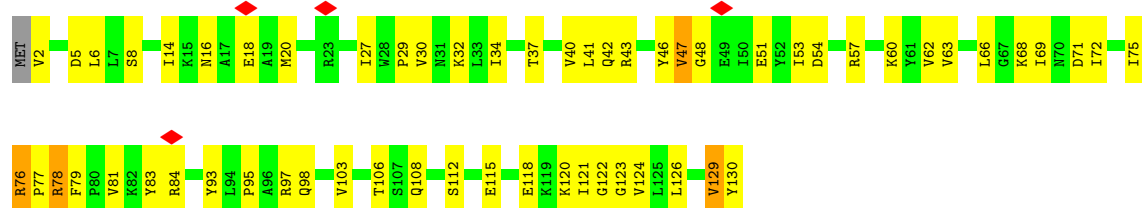
- Molecule 41: Small ribosomal subunit protein eS1



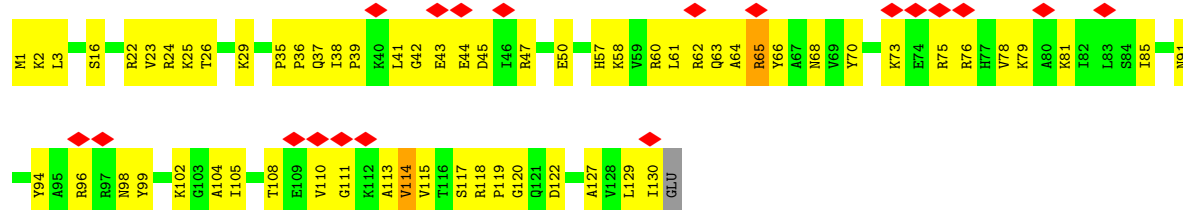




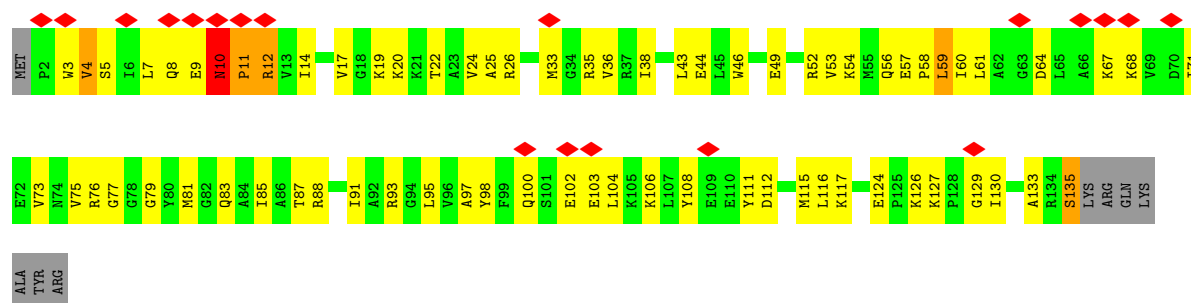
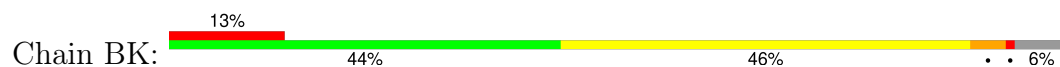
- Molecule 49: Small ribosomal subunit protein uS8



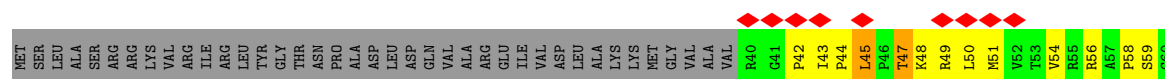
- Molecule 50: Small ribosomal subunit protein eS8

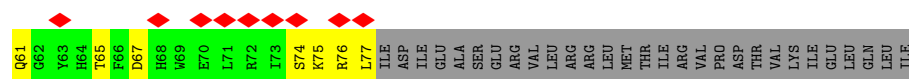


- Molecule 51: Small ribosomal subunit protein uS9

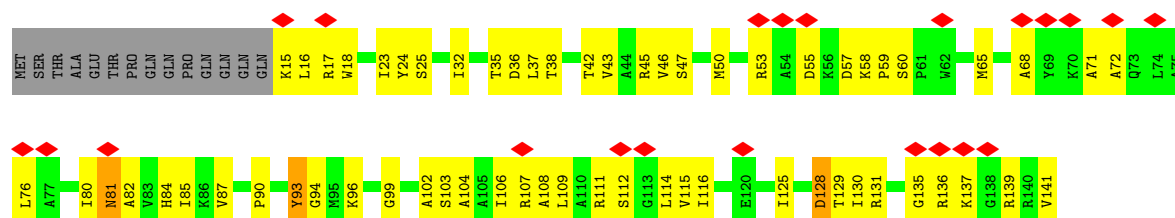


- Molecule 52: Small ribosomal subunit protein uS10

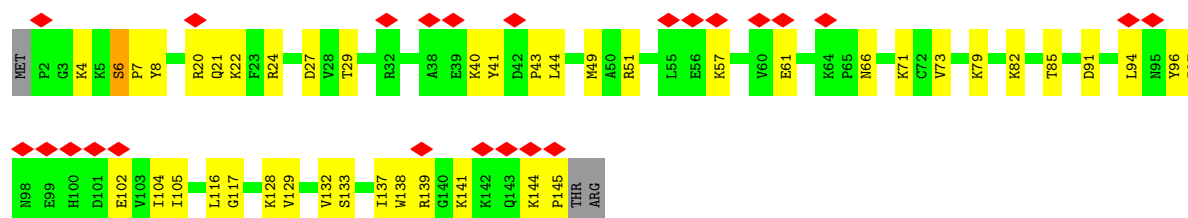




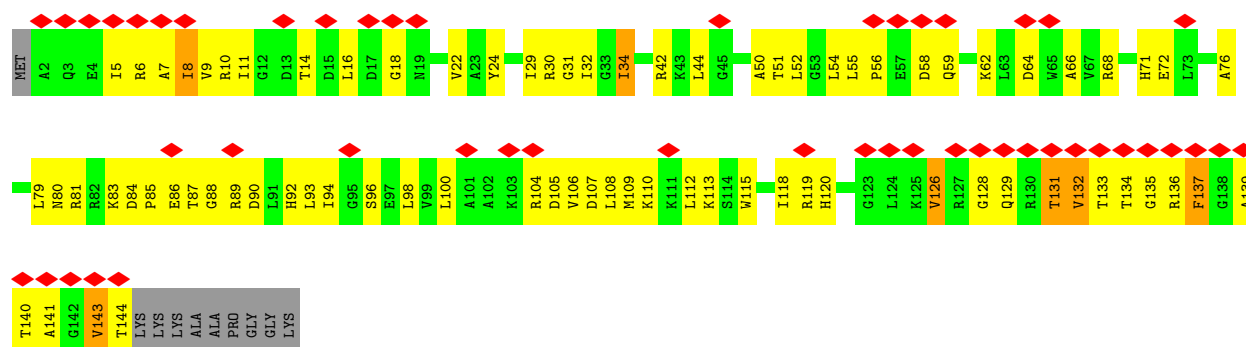
- Molecule 53: Small ribosomal subunit protein uS11



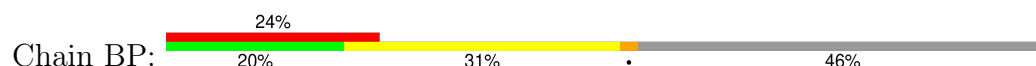
- Molecule 54: Small ribosomal subunit protein uS12



- Molecule 55: Small ribosomal subunit protein uS13

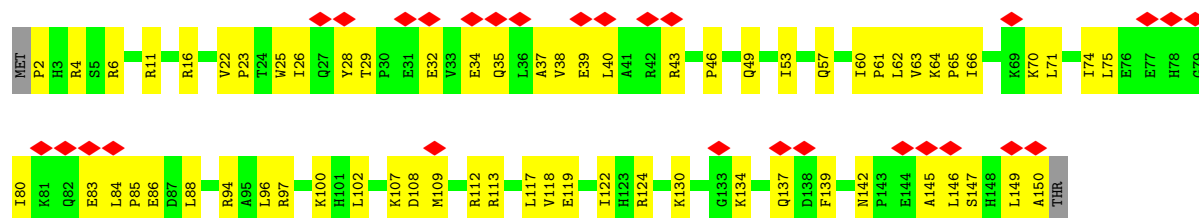


- Molecule 56: Small ribosomal subunit protein uS14



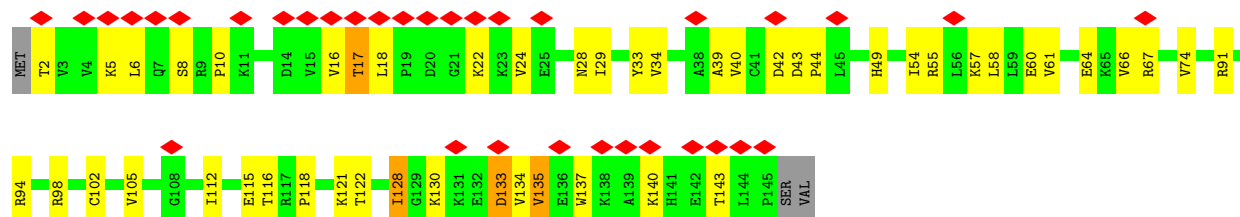
- Molecule 57: Small ribosomal subunit protein uS15

Chain BQ: 



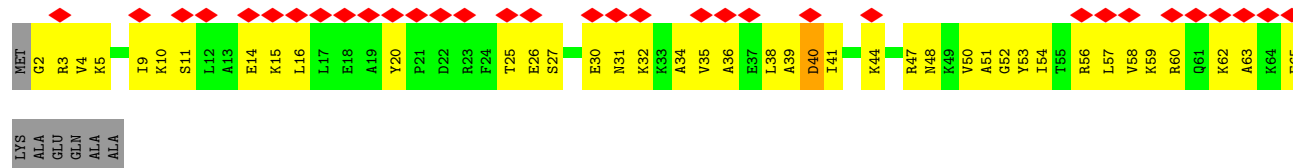
- Molecule 58: Small ribosomal subunit protein uS17

Chain BR: 



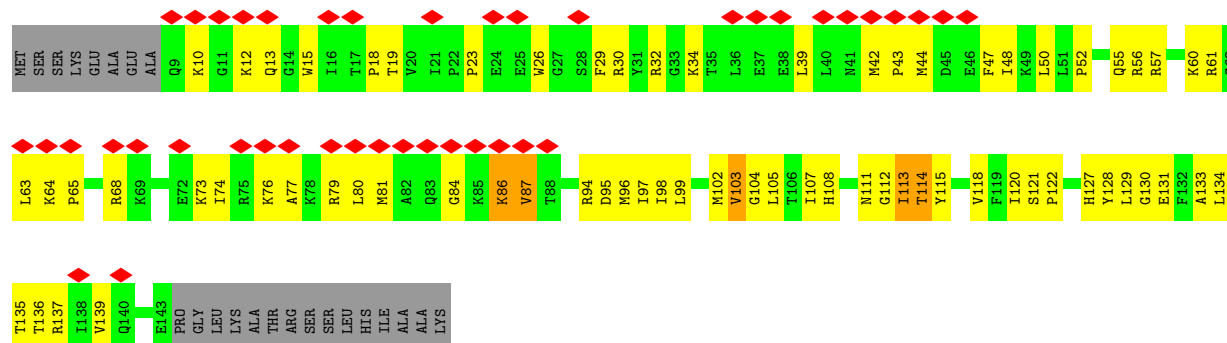
- Molecule 59: Small ribosomal subunit protein eS17

Chain BS: 



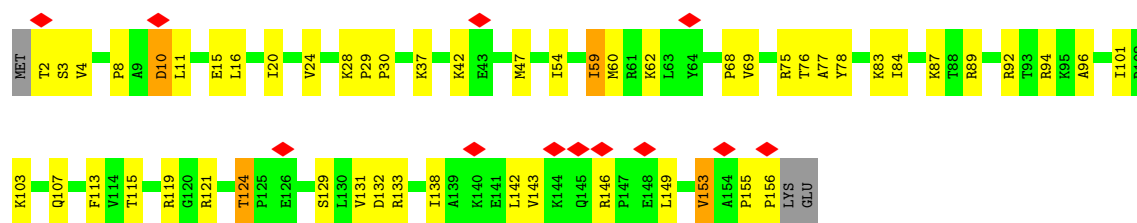
- Molecule 60: Small ribosomal subunit protein uS19

Chain BT: 



- Molecule 61: Small ribosomal subunit protein eS19

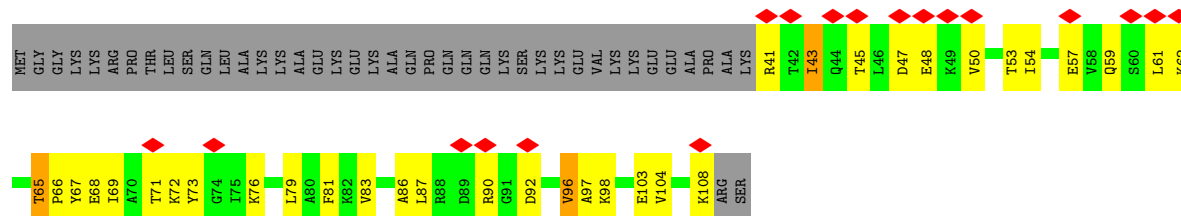
Chain BU: 



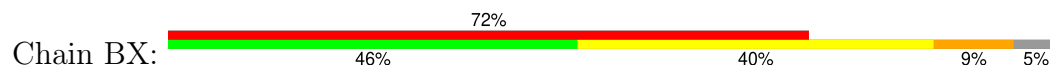
• Molecule 62: Small ribosomal subunit protein eS24



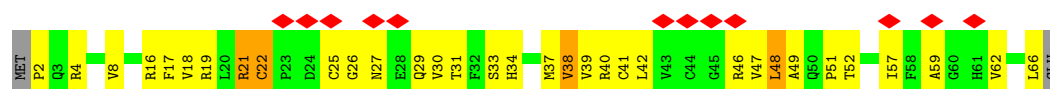
• Molecule 63: SSU ribosomal protein S25E



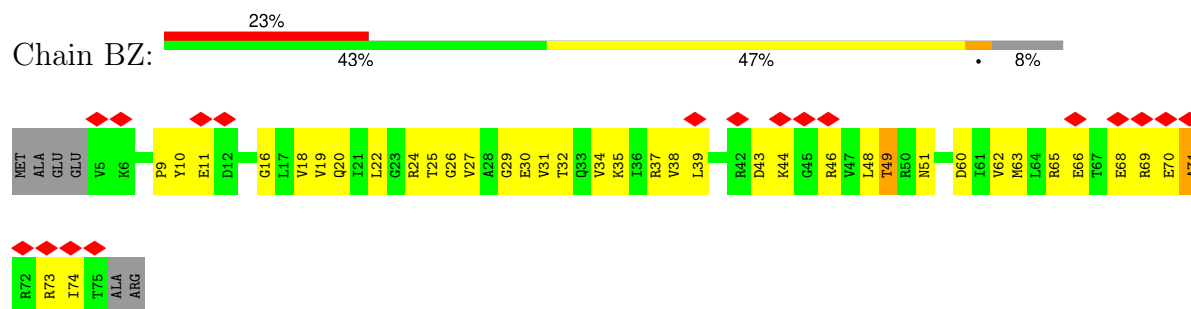
• Molecule 64: SSU ribosomal protein S26E



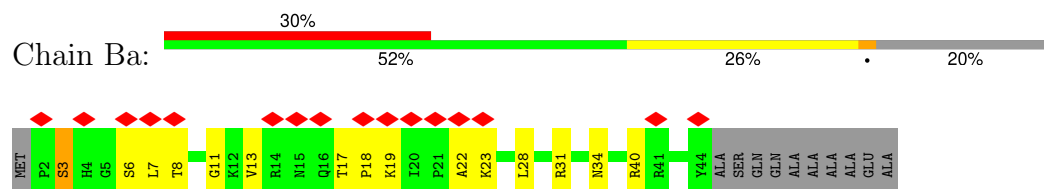
• Molecule 65: Small ribosomal subunit protein eS27



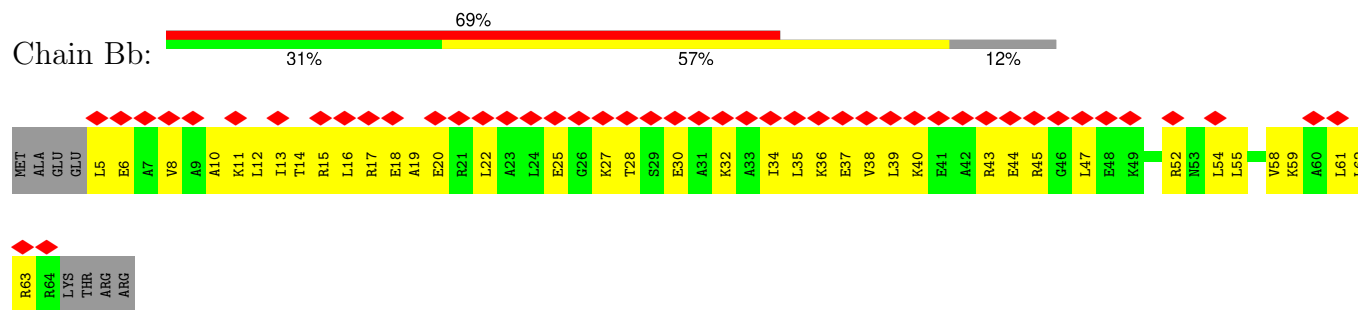
- Molecule 66: Small ribosomal subunit protein eS28



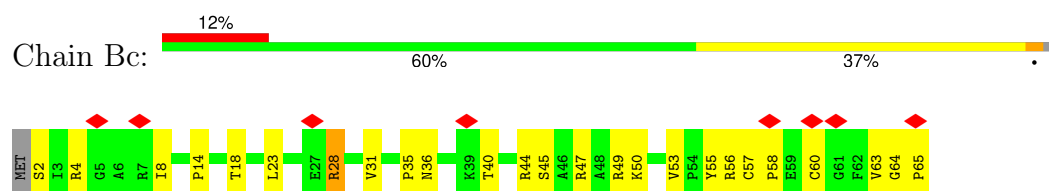
- Molecule 67: SSU ribosomal protein S30E



- Molecule 68: aS35



- Molecule 69: Small zinc finger protein HVO-2753-like zinc-binding pocket domain-containing protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	72157	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.070	Depositor
Minimum map value	-0.389	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.040	Depositor
Recommended contour level	0.188	Depositor
Map size ($\text{\AA}$)	504.2144, 504.2144, 504.2144	wwPDB
Map dimensions	608, 608, 608	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.8293, 0.8293, 0.8293	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PSU, G7M, IAS, OMC, SPM, 4AC, MG, 5MC, MA6, OMU, UR3, B8T, A2M, 6MZ, ZN, OMG, M7A

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	2	0.23	0/3096	0.36	2/4830 (0.0%)
2	3	0.28	0/2279	0.50	0/3084
3	1	0.32	1/67134 (0.0%)	0.35	11/104802 (0.0%)
4	4	0.34	2/33464 (0.0%)	0.39	15/52215 (0.0%)
5	AA	0.29	0/1847	0.44	0/2489
6	AB	0.27	0/2678	0.36	0/3643
7	AC	0.26	0/2234	0.40	0/3024
8	AD	0.19	0/1431	0.43	0/1913
9	AE	0.23	0/1548	0.41	1/2087 (0.0%)
10	AF	0.20	0/1114	0.38	0/1513
11	AG	0.26	0/1542	0.36	0/2076
12	AH	0.23	0/1265	0.35	0/1692
13	AI	0.29	0/1093	0.39	0/1487
14	AJ	0.25	0/795	0.48	0/1068
14	AK	0.27	0/704	0.44	0/944
15	AL	0.25	0/1225	0.40	0/1639
16	AM	0.24	0/1594	0.34	0/2138
17	AN	0.23	0/1365	0.34	0/1841
18	AO	0.20	0/1647	0.37	0/2212
19	AP	0.24	0/933	0.35	0/1263
20	AQ	0.25	0/1233	0.31	0/1645
21	AR	0.22	0/610	0.35	0/817
22	AS	0.25	0/805	0.36	0/1081
23	AT	0.24	0/1536	0.33	0/2075
24	AU	0.28	0/655	0.42	0/877
25	AV	0.25	0/990	0.39	0/1325
26	AW	0.27	0/460	0.33	0/613
27	AX	0.21	0/557	0.29	0/738
28	AY	0.29	0/1407	0.40	0/1905
29	AZ	0.24	0/754	0.42	0/1021
30	Aa	0.25	0/735	0.34	0/986

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	Ab	0.24	0/1209	0.39	0/1621
32	Ac	0.24	0/663	0.37	0/889
33	Ad	0.28	0/442	0.33	0/587
34	Ae	0.25	0/562	0.38	0/753
35	Af	0.24	0/423	0.31	0/566
36	Ag	0.23	0/424	0.40	0/564
37	Ah	0.24	0/753	0.32	0/1001
38	Ai	0.28	0/788	0.44	0/1057
39	Aj	0.24	0/1497	0.43	0/2029
40	Ak	0.22	0/754	0.36	0/1005
41	BA	0.26	0/1515	0.42	0/2043
42	BB	0.29	0/1638	0.47	2/2221 (0.1%)
43	BC	0.27	0/620	0.67	0/831
44	BD	0.25	0/1308	0.40	0/1755
45	BE	0.29	0/1929	0.44	0/2621
46	BF	0.28	0/1522	0.40	2/2059 (0.1%)
47	BG	0.23	0/1087	0.47	0/1465
48	BH	0.30	0/1809	0.45	0/2444
49	BI	0.37	0/1055	0.51	0/1425
50	BJ	0.26	0/1023	0.34	0/1370
51	BK	0.34	0/1079	0.56	1/1452 (0.1%)
52	BL	0.26	0/324	0.61	2/437 (0.5%)
53	BM	0.27	0/951	0.44	1/1288 (0.1%)
54	BN	0.30	0/1157	0.47	0/1551
55	BO	0.26	0/1125	0.45	1/1518 (0.1%)
56	BP	0.28	0/244	0.78	0/324
57	BQ	0.27	0/1254	0.36	0/1692
58	BR	0.29	0/1200	0.35	0/1629
59	BS	0.27	0/524	0.63	1/698 (0.1%)
60	BT	0.27	0/1139	0.47	0/1533
61	BU	0.30	0/1253	0.42	0/1695
62	BV	0.24	0/960	0.47	1/1280 (0.1%)
63	BW	0.28	0/551	0.48	0/741
64	BX	0.27	0/787	0.66	1/1054 (0.1%)
65	BY	0.27	0/511	0.36	0/689
66	BZ	0.30	0/555	0.67	0/745
67	Ba	0.24	0/364	0.38	0/486
68	Bb	0.24	0/478	0.61	0/634
69	Bc	0.24	0/491	0.41	0/670
All	All	0.30	3/174698 (0.0%)	0.39	41/257465 (0.0%)

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
41	BA	0	1
43	BC	0	1
49	BI	0	2
51	BK	0	1
All	All	0	5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	4	496	A2M	O3'-P	5.25	1.61	1.56
3	1	1990	A2M	O3'-P	5.23	1.61	1.56
4	4	880	A2M	O3'-P	5.12	1.61	1.56

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	4	101	C	OP1-P-O3'	-11.32	74.04	108.00
1	2	1	G	OP1-P-O3'	-9.21	80.38	108.00
4	4	1078	C	OP1-P-O3'	-9.19	80.44	108.00
3	1	2952	U	OP2-P-O3'	-9.06	80.82	108.00
4	4	808	G	OP1-P-O3'	-9.04	80.86	108.00
3	1	1679	U	OP1-P-O3'	-8.98	81.07	108.00
4	4	101	C	OP2-P-O3'	-8.77	81.70	108.00
3	1	2903	U	P-O3'-C3'	-8.73	107.11	120.20
4	4	808	G	OP2-P-O3'	-8.64	82.09	108.00
4	4	1177	G	OP1-P-O3'	-8.39	82.81	108.00
4	4	1078	C	OP2-P-O3'	-8.38	82.85	108.00
4	4	812	C	P-O3'-C3'	-8.31	107.73	120.20
3	1	2952	U	OP1-P-O3'	-8.29	83.14	108.00
4	4	1177	G	OP2-P-O3'	-8.15	83.55	108.00
3	1	1679	U	OP2-P-O3'	-8.01	83.97	108.00
4	4	1345	G	P-O3'-C3'	-7.94	108.28	120.20
1	2	1	G	OP2-P-O3'	-7.93	84.20	108.00
4	4	102	A	OP1-P-OP2	7.41	141.82	119.60
3	1	2143	OMC	P-O3'-C3'	-7.02	109.67	120.20
3	1	1564	G	P-O3'-C3'	-7.01	109.69	120.20
4	4	1369	C	P-O3'-C3'	-6.59	110.31	120.20
3	1	328	G	P-O3'-C3'	-6.48	110.48	120.20
46	BF	12	LYS	CA-C-N	6.40	133.22	121.70
46	BF	12	LYS	C-N-CA	6.40	133.22	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	1	1911	PSU	P-O3'-C3'	-6.38	110.62	120.20
3	1	1603	G	P-O3'-C3'	-6.36	110.66	120.20
3	1	1	U	P-O3'-C3'	-6.25	110.83	120.20
4	4	1384	A	P-O3'-C3'	-5.87	111.40	120.20
4	4	1441	A	P-O3'-C3'	-5.69	111.67	120.20
55	BO	132	VAL	N-CA-C	-5.49	107.03	111.91
42	BB	90	CYS	CA-C-N	-5.45	112.42	120.38
42	BB	90	CYS	C-N-CA	-5.45	112.42	120.38
53	BM	93	TYR	CA-CB-CG	5.38	123.58	113.90
52	BL	58	PRO	CA-C-N	5.37	131.79	121.54
52	BL	58	PRO	C-N-CA	5.37	131.79	121.54
51	BK	10	ASN	CB-CA-C	5.34	120.69	110.17
59	BS	41	ILE	CB-CG1-CD1	5.32	124.97	113.80
4	4	1383	G	P-O3'-C3'	-5.30	112.25	120.20
64	BX	20	TYR	CA-CB-CG	5.30	123.43	113.90
62	BV	8	GLN	CB-CG-CD	5.07	121.23	112.60
9	AE	139	LYS	CA-CB-CG	5.02	124.13	114.10

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
41	BA	66	LYS	Peptide
43	BC	184	GLY	Peptide
49	BI	76	ARG	Sidechain
49	BI	78	ARG	Sidechain
51	BK	12	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	2769	0	1405	50	0
2	3	2251	0	2337	188	0
3	1	61386	0	31066	1027	0
4	4	30817	0	15598	768	0
5	AA	1803	0	1849	52	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	AB	2611	0	2737	75	0
7	AC	2178	0	2263	61	0
8	AD	1412	0	1511	106	0
9	AE	1520	0	1607	69	0
10	AF	1095	0	1156	44	0
11	AG	1510	0	1627	42	0
12	AH	1244	0	1346	42	0
13	AI	1068	0	1110	39	0
14	AJ	788	0	853	52	0
14	AK	700	0	760	40	0
15	AL	1198	0	1233	40	0
16	AM	1558	0	1641	45	0
17	AN	1336	0	1378	34	0
18	AO	1615	0	1688	66	0
19	AP	920	0	1010	24	0
20	AQ	1214	0	1272	40	0
21	AR	603	0	647	27	0
22	AS	788	0	832	16	0
23	AT	1496	0	1575	31	0
24	AU	651	0	720	28	0
25	AV	976	0	1073	32	0
26	AW	449	0	465	13	0
27	AX	554	0	613	21	0
28	AY	1374	0	1423	27	0
29	AZ	742	0	796	32	0
30	Aa	726	0	794	21	0
31	Ab	1183	0	1270	34	0
32	Ac	649	0	698	23	0
33	Ad	429	0	430	7	0
34	Ae	552	0	592	25	0
35	Af	415	0	464	9	0
36	Ag	417	0	440	11	0
37	Ah	739	0	782	18	0
38	Ai	769	0	792	30	0
39	Aj	1469	0	1535	56	0
40	Ak	743	0	775	20	0
41	BA	1487	0	1589	77	0
42	BB	1600	0	1645	90	0
43	BC	611	0	648	47	0
44	BD	1284	0	1391	53	0
45	BE	1883	0	1968	72	0
46	BF	1498	0	1557	74	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
47	BG	1065	0	1139	80	0
48	BH	1773	0	1828	66	0
49	BI	1036	0	1090	45	0
50	BJ	1007	0	1086	53	0
51	BK	1058	0	1123	76	0
52	BL	315	0	329	23	0
53	BM	941	0	984	61	0
54	BN	1133	0	1203	38	0
55	BO	1108	0	1163	71	0
56	BP	241	0	251	21	0
57	BQ	1224	0	1287	52	0
58	BR	1171	0	1244	47	0
59	BS	517	0	560	37	0
60	BT	1111	0	1170	61	0
61	BU	1225	0	1301	43	0
62	BV	950	0	1013	81	0
63	BW	544	0	587	27	0
64	BX	772	0	827	54	0
65	BY	501	0	524	24	0
66	BZ	552	0	594	40	0
67	Ba	357	0	394	19	0
68	Bb	479	0	545	47	0
69	Bc	477	0	479	31	0
70	1	602	0	1117	19	0
70	4	252	0	468	9	0
70	AL	14	0	26	2	0
70	AM	14	0	26	0	0
70	Ah	14	0	26	0	0
71	1	170	0	0	0	0
71	4	77	0	0	0	0
71	AA	1	0	0	0	0
71	AL	2	0	0	0	0
71	BK	1	0	0	0	0
72	AW	1	0	0	0	0
72	Ad	1	0	0	0	0
72	Ag	1	0	0	0	0
72	Ah	1	0	0	0	0
72	Ai	1	0	0	0	0
72	BF	1	0	0	0	0
72	BP	1	0	0	0	0
72	BR	1	0	0	0	0
72	BX	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
72	BY	1	0	0	0	0
72	Bc	1	0	0	0	0
73	1	4730	0	0	153	0
73	2	94	0	0	3	0
73	3	4	0	0	3	0
73	4	1186	0	0	46	0
73	AA	13	0	0	0	0
73	AB	4	0	0	1	0
73	AC	7	0	0	0	0
73	AE	1	0	0	0	0
73	AG	1	0	0	0	0
73	AH	1	0	0	0	0
73	AL	11	0	0	1	0
73	AM	5	0	0	0	0
73	AN	1	0	0	0	0
73	AQ	1	0	0	0	0
73	AS	1	0	0	0	0
73	AT	3	0	0	0	0
73	AW	1	0	0	0	0
73	AY	1	0	0	0	0
73	Ab	7	0	0	0	0
73	Ad	2	0	0	0	0
73	Ag	1	0	0	0	0
73	Ah	1	0	0	0	0
73	BA	27	0	0	10	0
73	BB	13	0	0	1	0
73	BC	13	0	0	7	0
73	BD	16	0	0	1	0
73	BE	10	0	0	0	0
73	BF	17	0	0	0	0
73	BG	18	0	0	8	0
73	BH	18	0	0	2	0
73	BI	16	0	0	0	0
73	BJ	11	0	0	0	0
73	BK	15	0	0	3	0
73	BL	4	0	0	1	0
73	BM	10	0	0	5	0
73	BN	10	0	0	2	0
73	BO	10	0	0	1	0
73	BP	5	0	0	2	0
73	BQ	6	0	0	0	0
73	BR	9	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
73	BS	4	0	0	1	0
73	BT	12	0	0	2	0
73	BU	11	0	0	2	0
73	BV	3	0	0	0	0
73	BW	11	0	0	0	0
73	BX	7	0	0	2	0
73	BY	6	0	0	0	0
73	BZ	5	0	0	1	0
73	Ba	4	0	0	0	0
73	Bb	11	0	0	5	0
73	Bc	9	0	0	5	0
All	All	172182	0	123345	4352	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (4352) 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)
47:BG:28:ARG:HA	73:BG:202:HOH:O	1.48	1.13
43:BC:171:ARG:HG3	73:BC:310:HOH:O	1.51	1.08
3:1:2326:C:H1'	73:1:5439:HOH:O	1.53	1.07
3:1:989:A:H1'	73:1:3936:HOH:O	1.56	1.05
3:1:101:G:H4'	73:1:6355:HOH:O	1.52	1.05
3:1:152:A:H5''	73:1:7360:HOH:O	1.57	1.03
2:3:398:GLN:HG2	73:3:701:HOH:O	1.58	1.03
68:Bb:37:GLU:HA	68:Bb:40:LYS:HG2	1.40	1.03
62:BV:29:ILE:HG21	62:BV:37:PRO:HG3	1.39	1.02
56:BP:18:ARG:HA	73:BP:202:HOH:O	1.58	1.02
3:1:2851:OMU:HM21	73:1:5755:HOH:O	1.59	1.02
44:BD:61:LEU:HG	44:BD:92:LEU:HD12	1.42	1.02
41:BA:137:ARG:HD2	73:BA:313:HOH:O	1.60	1.00
3:1:124:C:H4'	73:1:5809:HOH:O	1.60	1.00
41:BA:207:GLU:HG2	73:BA:304:HOH:O	1.63	0.98
55:BO:140:THR:HG21	73:BO:202:HOH:O	1.61	0.98
69:Bc:65:PRO:HA	73:Bc:201:HOH:O	1.64	0.98
41:BA:113:MET:HE2	41:BA:131:LEU:HB3	1.45	0.98
4:4:1112:C:H4'	4:4:1113:A:H5'	1.43	0.97
3:1:1838:C:H5''	38:Ai:9:VAL:HG11	1.47	0.95
4:4:207:C:H5'	73:4:3196:HOH:O	1.63	0.95
54:BN:104:ILE:HB	54:BN:128:LYS:HB2	1.49	0.95

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:551:VAL:HG12	73:3:704:HOH:O	1.67	0.95
46:BF:14:ALA:HA	46:BF:17:ARG:HD2	1.49	0.95
4:4:475:OMG:HM22	4:4:476:G:H5'	1.49	0.94
59:BS:36:ALA:HB2	59:BS:47:ARG:HD2	1.49	0.94
3:1:2538:OMC:H5'	37:Ah:63:LYS:HG2	1.50	0.93
62:BV:93:LEU:HB3	62:BV:97:LEU:HD12	1.47	0.93
3:1:1552:G:H5'	73:1:5162:HOH:O	1.68	0.93
8:AD:1:MET:HE3	8:AD:6:LEU:HG	1.50	0.92
41:BA:131:LEU:HD23	41:BA:195:ALA:HB2	1.50	0.92
46:BF:12:LYS:HD3	46:BF:13:THR:HA	1.48	0.92
2:3:364:ILE:HD11	2:3:377:PHE:HB3	1.50	0.92
52:BL:47:THR:HG22	73:BL:201:HOH:O	1.68	0.91
11:AG:125:LEU:HD21	11:AG:180:ILE:HG12	1.51	0.91
3:1:2356:C:H5'	3:1:2357:G:H5''	1.51	0.91
8:AD:87:ARG:HG3	8:AD:118:PRO:HD2	1.52	0.91
17:AN:63:MET:HE2	17:AN:126:ARG:HB2	1.51	0.90
43:BC:191:ARG:HD3	73:BC:307:HOH:O	1.71	0.90
4:4:1107:G:H1'	73:4:3127:HOH:O	1.70	0.90
59:BS:16:LEU:HD21	59:BS:39:ALA:HB2	1.53	0.90
3:1:679:U:HO2'	15:AL:2:VAL:N	1.69	0.90
60:BT:76:LYS:HA	60:BT:79:ARG:HD3	1.51	0.90
11:AG:7:LEU:HD11	11:AG:12:ILE:HD11	1.52	0.89
73:4:4198:HOH:O	48:BH:73:GLY:HA2	1.72	0.89
62:BV:12:LEU:HB3	62:BV:26:LEU:HG	1.54	0.89
6:AB:36:LEU:HD12	6:AB:40:THR:HG21	1.53	0.89
44:BD:18:LYS:HD2	73:BD:215:HOH:O	1.73	0.88
14:AJ:58:THR:HG23	14:AJ:60:LYS:H	1.39	0.88
41:BA:205:GLU:HB2	73:BA:312:HOH:O	1.72	0.88
60:BT:80:LEU:HD12	60:BT:84:GLY:HA3	1.56	0.88
4:4:465:OMG:HM22	4:4:466:G:H5'	1.54	0.87
3:1:1535:C:H4'	73:1:6919:HOH:O	1.74	0.87
24:AU:70:SER:HB3	24:AU:73:ASP:HB2	1.57	0.87
2:3:435:VAL:HG21	2:3:444:VAL:HG22	1.56	0.87
53:BM:137:LYS:HE2	53:BM:141:VAL:HB	1.56	0.87
3:1:2366:OMG:HM22	3:1:2367:G:H5'	1.57	0.86
3:1:1235:C:H5''	73:1:4890:HOH:O	1.73	0.86
43:BC:128:ARG:HA	43:BC:131:MET:HG2	1.56	0.86
3:1:1151:U:H5''	3:1:1152:A:H5'	1.58	0.86
41:BA:52:LEU:HA	41:BA:55:ARG:HD2	1.56	0.86
59:BS:32:LYS:HD3	59:BS:47:ARG:HH21	1.40	0.85
51:BK:20:LYS:HD3	51:BK:85:ILE:HG21	1.57	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:BG:72:VAL:HG23	47:BG:103:GLY:HA2	1.58	0.85
4:4:1408:G:H1	4:4:1417:U:H3	0.85	0.85
3:1:629:C:H3'	73:1:4192:HOH:O	1.76	0.84
3:1:2469:G:H3'	73:1:5110:HOH:O	1.78	0.84
57:BQ:53:ILE:HG12	65:BY:37:MET:HE1	1.59	0.84
3:1:1790:C:H5'	3:1:1791:U:H5''	1.58	0.84
8:AD:58:SER:HB2	8:AD:65:ARG:HA	1.58	0.84
14:AJ:5:ILE:HG12	29:AZ:29:LEU:HG	1.60	0.84
4:4:1139:C:C5	73:4:4190:HOH:O	2.30	0.84
4:4:493:A:C8	73:4:3280:HOH:O	2.32	0.83
47:BG:8:LEU:HD21	47:BG:117:LEU:HD21	1.61	0.82
43:BC:131:MET:HE2	73:BC:302:HOH:O	1.78	0.82
73:1:4457:HOH:O	24:AU:51:THR:HG21	1.80	0.82
57:BQ:109:MET:HE2	57:BQ:112:ARG:HD2	1.62	0.82
2:3:336:VAL:HG23	2:3:469:VAL:HG21	1.61	0.82
20:AQ:103:LEU:HA	20:AQ:108:LYS:HZ1	1.45	0.82
8:AD:96:ILE:HD11	8:AD:177:VAL:HG22	1.61	0.81
3:1:1242:G:H4'	73:1:7307:HOH:O	1.80	0.81
3:1:2608:OMG:HM22	3:1:2609:G:H5'	1.62	0.81
4:4:1084:U:H3'	4:4:1085:U:H6	1.45	0.81
9:AE:47:PRO:HG3	9:AE:68:GLU:HG2	1.62	0.81
42:BB:140:GLY:HA3	69:Bc:28:ARG:HE	1.46	0.81
52:BL:44:PRO:HB3	52:BL:76:ARG:HH21	1.45	0.81
2:3:442:GLU:HB3	2:3:636:TYR:HB2	1.61	0.81
4:4:1465:U:H1'	53:BM:141:VAL:HG12	1.63	0.81
42:BB:182:LEU:HB3	42:BB:188:LEU:HD23	1.62	0.81
3:1:378:G:H4'	73:1:6172:HOH:O	1.81	0.81
15:AL:49:MET:HE1	15:AL:54:SER:HA	1.63	0.80
3:1:162:A:H1'	3:1:467:U:H5'	1.62	0.80
3:1:2426:C:H5'	8:AD:23:VAL:HG21	1.63	0.80
64:BX:47:PRO:HA	64:BX:49:LEU:HD23	1.63	0.80
6:AB:111:PRO:HD2	6:AB:114:LEU:HD12	1.63	0.80
47:BG:69:HIS:HB3	47:BG:72:VAL:HG22	1.63	0.80
3:1:2739:G:H5'	23:AT:92:GLY:HA2	1.64	0.80
3:1:2851:OMU:HM22	3:1:2852:A:H5'	1.64	0.80
30:Aa:40:VAL:HG21	30:Aa:87:VAL:HG21	1.61	0.79
51:BK:124:GLU:HG2	51:BK:133:ALA:HB1	1.65	0.79
3:1:2417:U:H1'	8:AD:112:LYS:HD2	1.63	0.79
5:AA:80:VAL:HG22	5:AA:91:VAL:HB	1.65	0.79
53:BM:135:GLY:CA	73:BM:201:HOH:O	2.30	0.79
47:BG:141:GLY:HA2	73:BG:216:HOH:O	1.82	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:AJ:72:GLU:HA	14:AJ:75:LYS:HE3	1.64	0.79
4:4:1153:G:H5'	51:BK:127:LYS:HD2	1.63	0.78
58:BR:16:VAL:HG11	58:BR:40:VAL:HG21	1.66	0.78
23:AT:66:ASP:HB3	23:AT:72:ARG:HG3	1.65	0.78
50:BJ:65:ARG:HD3	50:BJ:81:LYS:HE3	1.64	0.78
36:Ag:21:LYS:HZ1	36:Ag:34:ALA:H	1.30	0.78
3:1:229:G:H5'	3:1:230:C:H5''	1.65	0.78
47:BG:5:LYS:HD2	73:BG:217:HOH:O	1.83	0.78
3:1:1435:C:H4'	32:Ac:3:ARG:HB2	1.66	0.78
8:AD:25:ASN:HB3	8:AD:132:ASP:HB2	1.64	0.77
2:3:337:MET:HE1	2:3:458:VAL:HG11	1.66	0.77
3:1:2555:OMC:HM22	3:1:2556:C:H5'	1.63	0.77
4:4:1016:G:H1'	43:BC:185:ILE:HG21	1.64	0.77
60:BT:55:GLN:HG3	60:BT:97:ILE:HD13	1.65	0.77
3:1:2088:OMU:HM22	3:1:2089:G:H5'	1.65	0.77
39:Aj:68:LEU:HD21	39:Aj:97:LEU:HD11	1.66	0.77
48:BH:23:ILE:HG21	48:BH:58:ARG:HH21	1.50	0.77
73:4:3567:HOH:O	55:BO:136:ARG:CG	2.31	0.77
53:BM:137:LYS:HB3	53:BM:141:VAL:HG23	1.65	0.77
55:BO:106:VAL:HG12	55:BO:110:LYS:HE2	1.67	0.77
8:AD:173:LEU:HB3	8:AD:175:VAL:HG23	1.67	0.77
42:BB:139:MET:HB3	42:BB:141:ILE:HD12	1.66	0.77
57:BQ:23:PRO:HG3	57:BQ:61:PRO:HG2	1.66	0.77
60:BT:99:LEU:H	60:BT:102:MET:HG3	1.47	0.77
69:Bc:65:PRO:CA	73:Bc:201:HOH:O	2.24	0.76
51:BK:10:ASN:HB2	51:BK:11:PRO:CD	2.15	0.76
62:BV:25:VAL:HG12	62:BV:75:VAL:HB	1.67	0.76
62:BV:43:ARG:HG3	62:BV:59:VAL:HG23	1.65	0.76
4:4:1145:A:H5''	51:BK:117:LYS:HE3	1.68	0.76
8:AD:87:ARG:HG2	8:AD:117:LEU:HD12	1.67	0.76
3:1:2327:A:C2	73:1:4607:HOH:O	2.39	0.76
8:AD:22:VAL:HG22	8:AD:135:VAL:HG23	1.66	0.76
2:3:398:GLN:C	73:3:701:HOH:O	2.29	0.76
4:4:1212:OMG:HM22	4:4:1213:G:H5'	1.66	0.76
5:AA:40:VAL:HG21	5:AA:72:LEU:HD11	1.67	0.76
60:BT:32:ARG:HG3	60:BT:50:LEU:HD22	1.66	0.76
69:Bc:18:THR:HG21	69:Bc:55:TYR:HA	1.65	0.76
4:4:1443:G:H2'	4:4:1444:G:H5''	1.67	0.76
49:BI:20:MET:HE2	49:BI:20:MET:HA	1.67	0.76
61:BU:2:THR:HG22	61:BU:153:VAL:HG12	1.68	0.76
68:Bb:12:LEU:HD22	68:Bb:38:VAL:HG13	1.67	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1:2851:OMU:CM2	73:1:5755:HOH:O	2.22	0.76
47:BG:120:PRO:HG2	47:BG:123:TYR:HB2	1.67	0.76
57:BQ:146:LEU:HB3	57:BQ:149:LEU:HD12	1.68	0.76
55:BO:11:ILE:HD12	55:BO:16:LEU:HD12	1.68	0.75
39:Aj:167:ASP:HB3	39:Aj:170:THR:HG22	1.68	0.75
3:1:646:G:H5''	31:Ab:51:THR:HG21	1.68	0.75
62:BV:60:ARG:HB2	62:BV:74:GLU:HG2	1.69	0.75
64:BX:32:ARG:HD2	73:BX:206:HOH:O	1.86	0.75
61:BU:84:ILE:HD12	61:BU:92:ARG:HB2	1.69	0.75
70:AL:201:SPM:N1	73:AL:301:HOH:O	2.20	0.75
14:AJ:37:THR:HB	14:AJ:47:ARG:HG3	1.67	0.75
2:3:487:VAL:HG12	2:3:597:VAL:HG12	1.69	0.75
57:BQ:26:ILE:HD11	57:BQ:60:ILE:HD12	1.67	0.75
67:Ba:6:SER:HG	67:Ba:8:THR:HG1	1.35	0.74
73:1:5336:HOH:O	14:AJ:13:LYS:HE2	1.86	0.74
3:1:1976:OMC:HM22	3:1:1977:U:H5'	1.69	0.74
4:4:1171:U:H1'	43:BC:185:ILE:HD11	1.68	0.74
16:AM:71:PRO:HB3	16:AM:92:THR:HG22	1.68	0.74
73:4:3567:HOH:O	55:BO:136:ARG:HG3	1.88	0.74
7:AC:202:ALA:HA	7:AC:223:PRO:HG2	1.70	0.73
73:4:3469:HOH:O	58:BR:57:LYS:HD3	1.87	0.73
21:AR:30:LEU:HD21	21:AR:50:ILE:HG12	1.70	0.73
47:BG:52:GLY:HA3	47:BG:120:PRO:HG3	1.70	0.73
4:4:102:A:H61	4:4:242:G:H1	1.34	0.73
46:BF:103:THR:HG22	46:BF:107:LYS:HE3	1.68	0.73
50:BJ:38:ILE:HD12	50:BJ:99:TYR:HB3	1.71	0.73
37:Ah:2:LYS:HD2	37:Ah:91:VAL:HG21	1.69	0.73
11:AG:55:VAL:HG11	11:AG:143:LEU:HD22	1.70	0.73
8:AD:88:ALA:HA	8:AD:117:LEU:HD11	1.70	0.73
3:1:2427:G:H4'	8:AD:136:ARG:HH21	1.53	0.73
3:1:2885:OMC:HM22	3:1:2886:C:H5'	1.70	0.73
13:AI:109:ILE:HG22	13:AI:117:LYS:HB2	1.70	0.73
49:BI:66:LEU:HB2	49:BI:68:LYS:HG2	1.71	0.73
50:BJ:47:ARG:HG2	50:BJ:61:LEU:HD13	1.71	0.73
62:BV:8:GLN:HB3	62:BV:30:LEU:HB3	1.71	0.73
2:3:355:LYS:HD2	2:3:359:ARG:HH21	1.54	0.72
14:AJ:77:LEU:HD12	14:AJ:82:LEU:HB2	1.70	0.72
4:4:440:C:H5''	62:BV:61:LYS:HG2	1.70	0.72
54:BN:4:LYS:HG3	73:BN:202:HOH:O	1.89	0.72
31:Ab:9:LEU:HD12	31:Ab:13:LEU:HB3	1.72	0.72
41:BA:62:TYR:HB2	41:BA:71:LEU:HD22	1.70	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1:696:U:C2	73:1:5045:HOH:O	2.43	0.72
57:BQ:2:PRO:HB3	57:BQ:113:ARG:HH12	1.54	0.72
2:3:435:VAL:HG13	2:3:447:LYS:HD3	1.71	0.71
15:AL:108:LEU:HD12	15:AL:130:THR:HB	1.72	0.71
43:BC:131:MET:HA	43:BC:131:MET:HE3	1.71	0.71
45:BE:126:THR:HG22	45:BE:134:GLN:HB3	1.71	0.71
55:BO:30:ARG:HH22	55:BO:144:THR:HA	1.53	0.71
7:AC:59:ILE:HD13	7:AC:266:PRO:HB3	1.71	0.71
47:BG:6:LEU:HD12	47:BG:21:ILE:HD11	1.71	0.71
14:AJ:47:ARG:NH2	14:AJ:68:ALA:O	2.24	0.71
42:BB:159:MET:HE3	69:Bc:65:PRO:HB3	1.72	0.71
54:BN:20:ARG:HB3	73:BN:204:HOH:O	1.91	0.71
4:4:572:OMC:HM22	4:4:573:C:H5'	1.71	0.71
3:1:1:U:H2'	3:1:2:A:C8	2.25	0.71
4:4:1055:C:O2'	59:BS:10:LYS:NZ	2.24	0.71
14:AK:65:LYS:HE3	14:AK:68:ALA:HA	1.71	0.71
3:1:266:G:H1'	73:1:7270:HOH:O	1.91	0.71
59:BS:54:ILE:HA	59:BS:57:LEU:HD23	1.73	0.71
46:BF:28:ASP:OD1	46:BF:84:TYR:OH	2.08	0.71
47:BG:32:LEU:HD22	47:BG:36:GLU:HG2	1.72	0.71
2:3:491:MET:HE1	2:3:620:VAL:HG12	1.72	0.71
18:AO:150:GLU:HA	18:AO:153:LYS:HE3	1.72	0.71
2:3:325:VAL:HB	2:3:635:VAL:HG22	1.72	0.70
4:4:1118:A:H5''	52:BL:47:THR:HG23	1.72	0.70
4:4:481:A:H1'	67:Ba:13:VAL:HG23	1.72	0.70
3:1:813:G:H5'	32:Ac:8:SER:HA	1.73	0.70
3:1:2104:OMG:HM22	3:1:2105:U:H5'	1.73	0.70
5:AA:75:GLY:HA2	14:AJ:98:THR:HG21	1.72	0.70
7:AC:9:LEU:HD21	7:AC:48:ILE:HD11	1.74	0.70
8:AD:123:ASP:HB3	8:AD:126:VAL:HG22	1.74	0.70
55:BO:5:ILE:HG13	55:BO:54:LEU:HD21	1.72	0.70
3:1:2077:OMU:HM22	3:1:2078:C:H5'	1.73	0.70
4:4:282:A:H5'	4:4:284:G:H5'	1.71	0.70
38:Ai:11:PRO:HD2	38:Ai:28:THR:HG23	1.74	0.70
4:4:1107:G:N2	73:4:3109:HOH:O	2.24	0.70
4:4:1416:G:H3'	4:4:1417:U:H5''	1.73	0.70
49:BI:60:LYS:NZ	65:BY:8:VAL:O	2.24	0.70
8:AD:114:HIS:HB3	8:AD:131:MET:HE1	1.73	0.70
43:BC:174:ARG:HH21	43:BC:176:VAL:HG21	1.57	0.70
53:BM:87:VAL:HG11	53:BM:106:ILE:HD11	1.73	0.70
2:3:610:VAL:HG23	2:3:623:LEU:HB3	1.74	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:1070:A:H2'	4:4:1071:C:H5'	1.74	0.70
10:AF:37:ILE:HG23	10:AF:122:ALA:HB1	1.72	0.70
41:BA:119:LYS:HE3	73:BA:320:HOH:O	1.91	0.70
42:BB:67:ARG:HH22	69:Bc:35:PRO:HA	1.57	0.69
4:4:1099:A:O2'	4:4:1101:G:N2	2.25	0.69
20:AQ:129:LEU:HG	20:AQ:133:LYS:HE3	1.75	0.69
4:4:514:OMC:HM22	4:4:515:G:H5'	1.74	0.69
24:AU:80:VAL:HG12	27:AX:32:LYS:HG3	1.75	0.69
51:BK:97:ALA:O	51:BK:100:GLN:NE2	2.25	0.69
73:4:3567:HOH:O	55:BO:136:ARG:HB2	1.92	0.69
9:AE:49:ILE:HB	9:AE:60:GLU:HG2	1.74	0.69
9:AE:97:ILE:HG12	36:Ag:9:LYS:HD3	1.73	0.69
2:3:337:MET:HE1	2:3:458:VAL:HG21	1.73	0.69
3:1:2179:A:H5'	73:1:7883:HOH:O	1.92	0.69
4:4:1115:A:H1'	51:BK:26:ARG:HH11	1.56	0.69
17:AN:100:GLU:HG2	17:AN:124:ALA:HB2	1.74	0.69
3:1:754:G:N7	73:1:3474:HOH:O	2.25	0.69
3:1:1171:A:H5''	3:1:1172:A:H4'	1.73	0.69
9:AE:84:LEU:HA	9:AE:87:THR:HG22	1.73	0.69
28:AY:38:LEU:HD21	28:AY:45:VAL:HG22	1.72	0.69
57:BQ:142:ASN:HB3	57:BQ:145:ALA:HB3	1.75	0.69
3:1:894:G:N7	73:1:3488:HOH:O	2.26	0.69
4:4:1139:C:H5	73:4:4190:HOH:O	1.71	0.69
42:BB:189:LYS:HB2	42:BB:192:GLN:HB2	1.74	0.69
2:3:490:LEU:HD12	2:3:597:VAL:HG11	1.74	0.69
4:4:648:A:O2'	4:4:662:U:O4	2.08	0.69
42:BB:183:ARG:NH2	42:BB:192:GLN:O	2.26	0.69
53:BM:46:VAL:HG13	53:BM:50:MET:HE2	1.73	0.69
3:1:42:A:N7	73:1:3481:HOH:O	2.26	0.69
3:1:2028:G:H1	3:1:2044:PSU:HN3	1.40	0.69
45:BE:58:ARG:O	45:BE:62:SER:OG	2.09	0.69
69:Bc:56:ARG:HG3	69:Bc:63:VAL:HG12	1.73	0.69
47:BG:37:GLU:HB3	47:BG:54:LYS:HE2	1.73	0.68
54:BN:51:ARG:HD3	54:BN:102:GLU:HG3	1.75	0.68
46:BF:34:ASN:O	69:Bc:28:ARG:NH1	2.26	0.68
55:BO:119:ARG:HB2	55:BO:126:VAL:HG12	1.74	0.68
2:3:470:THR:OG1	2:3:472:ASP:OD1	2.11	0.68
3:1:2042:C:H2'	3:1:2043:C:H1'	1.76	0.68
9:AE:120:ARG:NH2	9:AE:169:GLU:OE2	2.26	0.68
4:4:1178:A:H4'	4:4:1179:A:H5'	1.75	0.68
8:AD:23:VAL:HG22	8:AD:134:CYS:HB2	1.75	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:BH:59:ARG:NH1	66:BZ:60:ASP:OD1	2.27	0.68
51:BK:73:VAL:HG11	51:BK:87:THR:HG23	1.74	0.68
68:Bb:44:GLU:HA	73:Bb:105:HOH:O	1.93	0.68
3:1:1734:C:OP1	34:Ae:41:TYR:OH	2.12	0.68
6:AB:9:ARG:NH2	6:AB:250:THR:O	2.27	0.68
41:BA:68:ILE:HA	41:BA:71:LEU:HD23	1.75	0.68
46:BF:18:MET:HB3	46:BF:24:ILE:HD13	1.76	0.68
4:4:879:A2M:H2'	4:4:880:A2M:H8	1.73	0.68
4:4:1014:A:N3	43:BC:145:LYS:NZ	2.40	0.68
1:2:34:C:H2'	1:2:35:C:H5'	1.75	0.68
2:3:475:VAL:HG22	2:3:628:ILE:HD11	1.76	0.68
3:1:2622:G:HO2'	3:1:2668:C:HO2'	1.40	0.68
9:AE:104:LEU:HB3	9:AE:115:GLU:HB2	1.73	0.68
23:AT:73:PRO:HB2	23:AT:96:ALA:HB1	1.74	0.68
42:BB:197:PRO:HD2	42:BB:200:GLU:HG2	1.76	0.68
2:3:589:HIS:HD2	2:3:603:LYS:HB3	1.58	0.68
4:4:148:G:H4'	47:BG:116:VAL:HG21	1.75	0.68
21:AR:10:ASP:OD1	21:AR:51:ARG:NH1	2.27	0.68
47:BG:34:ILE:HA	47:BG:57:ILE:HG22	1.75	0.68
2:3:478:TYR:HB3	2:3:601:LEU:HD21	1.75	0.68
2:3:529:MET:HE2	2:3:581:LEU:HD13	1.75	0.68
3:1:2038:U:O2'	3:1:2039:G:N7	2.26	0.68
48:BH:16:GLU:OE1	48:BH:58:ARG:NH2	2.27	0.68
70:1:3114:SPM:N14	73:1:3426:HOH:O	2.21	0.67
4:4:1201:U:O2'	4:4:1202:OMG:O5'	2.11	0.67
4:4:1330:A:OP1	61:BU:89:ARG:NH1	2.27	0.67
73:4:3469:HOH:O	58:BR:57:LYS:HG2	1.93	0.67
42:BB:74:LEU:HD23	42:BB:121:LEU:HD12	1.75	0.67
47:BG:49:LEU:HB3	47:BG:53:VAL:HG11	1.75	0.67
58:BR:66:VAL:HG11	58:BR:105:VAL:HG23	1.74	0.67
65:BY:52:THR:HG21	65:BY:57:ILE:HD13	1.76	0.67
1:2:48:A:OP1	8:AD:78:ARG:NH1	2.26	0.67
25:AV:2:PRO:HA	25:AV:23:LEU:HD11	1.76	0.67
39:Aj:136:PRO:HG3	39:Aj:166:LYS:HD2	1.76	0.67
57:BQ:46:PRO:HD2	57:BQ:49:GLN:HB3	1.76	0.67
3:1:2406:G:OP1	8:AD:148:ARG:NH1	2.28	0.67
4:4:1057:G:H2'	4:4:1058:G:H5''	1.76	0.67
2:3:349:PRO:O	2:3:352:SER:OG	2.12	0.67
23:AT:126:ARG:HD2	23:AT:170:LYS:HB3	1.76	0.67
3:1:247:G:OP2	12:AH:25:ARG:NH2	2.27	0.67
3:1:2868:U:H1'	3:1:2869:A:H5''	1.75	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:BG:5:LYS:CD	73:BG:217:HOH:O	2.42	0.67
51:BK:44:GLU:N	51:BK:44:GLU:OE2	2.28	0.67
51:BK:93:ARG:HG2	51:BK:116:LEU:HD23	1.75	0.67
2:3:342:PRO:HG2	2:3:360:SER:HB2	1.75	0.67
3:1:2820:G:N7	73:1:3504:HOH:O	2.27	0.67
4:4:1040:G:OP2	46:BF:91:LYS:NZ	2.27	0.67
10:AF:54:THR:HG23	10:AF:115:VAL:HB	1.77	0.67
60:BT:96:MET:HB3	60:BT:129:LEU:HD12	1.77	0.67
3:1:2050:G:N2	3:1:2050:G:OP2	2.27	0.67
47:BG:92:LYS:HD3	73:BG:208:HOH:O	1.94	0.67
54:BN:132:VAL:HG13	54:BN:137:ILE:HD11	1.75	0.67
1:2:46:A:N3	8:AD:77:ARG:NH2	2.42	0.67
4:4:1163:OMG:N2	52:BL:61:GLN:OE1	2.27	0.67
47:BG:2:PRO:HD2	47:BG:26:ALA:HB1	1.77	0.67
64:BX:10:ARG:HB3	64:BX:34:LYS:HB2	1.77	0.67
4:4:264:U:O4	50:BJ:118:ARG:NH2	2.27	0.67
3:1:106:C:O2'	3:1:118:U:O2'	2.13	0.66
4:4:138:G:OP1	47:BG:18:GLN:NE2	2.27	0.66
17:AN:100:GLU:OE1	17:AN:102:ARG:NE	2.28	0.66
47:BG:107:THR:HG22	47:BG:110:ILE:HD12	1.77	0.66
51:BK:38:ILE:HD13	51:BK:43:LEU:HD13	1.76	0.66
3:1:1801:C:H5''	6:AB:233:GLY:HA3	1.77	0.66
4:4:1006:G:H21	4:4:1180:A:H3'	1.60	0.66
20:AQ:84:ASP:HB3	20:AQ:87:GLU:HB3	1.77	0.66
34:Ae:4:GLU:OE2	34:Ae:44:ARG:NH1	2.28	0.66
48:BH:69:PRO:HB2	48:BH:89:GLU:HB2	1.76	0.66
60:BT:13:GLN:O	60:BT:137:ARG:NH2	2.27	0.66
60:BT:94:ARG:NH1	60:BT:133:ALA:O	2.27	0.66
62:BV:109:ARG:HH11	62:BV:109:ARG:HA	1.59	0.66
63:BW:41:ARG:HA	63:BW:48:GLU:HG2	1.77	0.66
3:1:1978:G:H21	5:AA:212:PRO:HG2	1.59	0.66
4:4:327:U:O4	50:BJ:29:LYS:NZ	2.28	0.66
4:4:1432:G:H2'	4:4:1433:G:H5'	1.77	0.66
12:AH:2:ILE:HD12	12:AH:3:PRO:HD2	1.77	0.66
12:AH:33:LYS:HZ2	12:AH:38:ASN:HA	1.59	0.66
19:AP:81:VAL:HG22	19:AP:101:GLU:HG2	1.77	0.66
36:Ag:21:LYS:NZ	36:Ag:31:PRO:O	2.29	0.66
42:BB:69:PRO:HG2	42:BB:72:ARG:HG3	1.77	0.66
46:BF:11:PRO:O	46:BF:17:ARG:NH1	2.29	0.66
53:BM:57:ASP:O	53:BM:60:SER:OG	2.13	0.66
62:BV:59:VAL:N	62:BV:96:ASN:OD1	2.28	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1:1257:G:H5''	73:1:4301:HOH:O	1.94	0.66
4:4:10:G:N7	73:4:3120:HOH:O	2.29	0.66
4:4:81:A:N3	4:4:133:C:O2'	2.24	0.66
4:4:188:C:O2'	50:BJ:68:ASN:OD1	2.13	0.66
4:4:778:C:O2	64:BX:8:ARG:NH2	2.29	0.66
54:BN:57:LYS:HE2	54:BN:97:ILE:HG22	1.78	0.66
68:Bb:35:LEU:HD23	68:Bb:58:VAL:HG11	1.76	0.66
3:1:246:A:OP1	12:AH:85:LYS:NZ	2.29	0.66
61:BU:68:PRO:HB2	61:BU:119:ARG:HG3	1.77	0.66
66:BZ:68:GLU:N	66:BZ:68:GLU:OE2	2.29	0.66
3:1:1525:U:H2'	3:1:1526:A:H5''	1.77	0.66
7:AC:201:ARG:NH2	7:AC:224:LYS:O	2.29	0.66
49:BI:30:VAL:HA	49:BI:34:ILE:HD12	1.77	0.66
68:Bb:11:LYS:HE3	68:Bb:15:ARG:HH22	1.60	0.66
2:3:455:TYR:HB3	2:3:470:THR:HG22	1.77	0.66
56:BP:25:ARG:O	56:BP:25:ARG:NE	2.23	0.66
69:Bc:47:ARG:HD2	73:Bc:202:HOH:O	1.94	0.66
3:1:2451:C:OP1	8:AD:66:LYS:NZ	2.28	0.66
4:4:828:G:H1'	73:4:3246:HOH:O	1.95	0.66
3:1:989:A:C1'	73:1:3936:HOH:O	2.27	0.65
3:1:2408:OMU:H5'	73:1:3696:HOH:O	1.95	0.65
3:1:2544:A:N7	73:1:3530:HOH:O	2.29	0.65
4:4:1486:C:OP1	64:BX:10:ARG:NH2	2.29	0.65
42:BB:21:VAL:HG13	42:BB:173:ILE:HD11	1.78	0.65
3:1:1:U:H6	3:1:1:U:H5''	1.61	0.65
4:4:1329:A:O2'	4:4:1331:C:N4	2.29	0.65
4:4:482:G:OP2	54:BN:71:LYS:NZ	2.30	0.65
17:AN:52:LYS:HD2	17:AN:135:VAL:HG21	1.78	0.65
18:AO:73:LYS:HG3	18:AO:173:ARG:HB3	1.78	0.65
23:AT:170:LYS:O	23:AT:175:LYS:NZ	2.29	0.65
41:BA:98:ARG:CD	73:BA:307:HOH:O	2.44	0.65
46:BF:188:LEU:O	46:BF:192:ASN:ND2	2.24	0.65
47:BG:141:GLY:CA	73:BG:216:HOH:O	2.41	0.65
59:BS:27:SER:O	59:BS:31:ASN:ND2	2.28	0.65
3:1:321:A:H2'	73:1:3516:HOH:O	1.95	0.65
7:AC:153:LYS:HE2	7:AC:163:VAL:HB	1.77	0.65
3:1:2476:A:OP2	70:1:3140:SPM:N5	2.29	0.65
7:AC:35:ASP:OD1	7:AC:39:GLN:N	2.28	0.65
3:1:148:C:OP1	16:AM:108:LYS:NZ	2.29	0.65
48:BH:119:ILE:O	48:BH:123:THR:OG1	2.10	0.65
61:BU:62:LYS:HE2	61:BU:77:ALA:HB1	1.78	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:BY:25:CYS:SG	65:BY:26:GLY:N	2.70	0.65
4:4:1133:G:N2	4:4:1135:A:O2'	2.29	0.65
5:AA:133:GLU:HG2	5:AA:135:LYS:HG2	1.78	0.65
10:AF:89:LYS:O	10:AF:148:ARG:NH1	2.30	0.65
15:AL:103:ARG:NH1	15:AL:145:GLY:O	2.30	0.65
46:BF:194:LEU:O	46:BF:197:THR:OG1	2.15	0.65
55:BO:83:LYS:HG2	60:BT:32:ARG:HE	1.62	0.65
61:BU:8:PRO:HG2	61:BU:11:LEU:HD13	1.78	0.65
3:1:1080:A:OP1	17:AN:11:ARG:NH2	2.30	0.65
8:AD:58:SER:HB2	8:AD:65:ARG:HD3	1.77	0.65
17:AN:74:SER:O	17:AN:78:THR:OG1	2.13	0.65
29:AZ:72:GLY:HA2	29:AZ:81:ILE:HD12	1.79	0.65
46:BF:92:SER:OG	46:BF:94:GLN:O	2.15	0.65
53:BM:17:ARG:N	53:BM:81:ASN:OD1	2.25	0.65
61:BU:129:SER:OG	61:BU:133:ARG:NH1	2.30	0.65
4:4:461:C:OP1	54:BN:141:LYS:NZ	2.30	0.65
44:BD:106:ARG:HB2	44:BD:146:LEU:HD13	1.78	0.65
3:1:2561:A:N3	73:1:3538:HOH:O	2.29	0.64
4:4:7:OMG:H2'	4:4:8:U:H5''	1.78	0.64
4:4:257:G:OP1	58:BR:122:THR:OG1	2.14	0.64
14:AJ:3:LYS:NZ	14:AJ:5:ILE:O	2.30	0.64
29:AZ:12:ILE:HD11	29:AZ:75:ALA:HB1	1.79	0.64
45:BE:11:TYR:HA	45:BE:17:ARG:HH21	1.62	0.64
51:BK:135:SER:O	51:BK:135:SER:OG	2.14	0.64
64:BX:30:VAL:HG23	64:BX:35:ALA:HB2	1.78	0.64
3:1:761:A:N1	3:1:2484:A:O2'	2.30	0.64
4:4:282:A:H5''	4:4:283:A:H3'	1.78	0.64
4:4:1445:G:H2'	4:4:1446:G:C8	2.33	0.64
45:BE:93:GLU:OE1	45:BE:95:TYR:OH	2.14	0.64
66:BZ:11:GLU:OE1	66:BZ:11:GLU:N	2.30	0.64
3:1:2094:G:N7	73:1:3539:HOH:O	2.30	0.64
18:AO:50:ILE:HG21	18:AO:52:ARG:HH21	1.62	0.64
42:BB:27:LEU:HB2	42:BB:149:THR:HG22	1.80	0.64
49:BI:42:GLN:NE2	49:BI:48:GLY:O	2.30	0.64
60:BT:42:MET:HG2	60:BT:47:PHE:HB2	1.79	0.64
68:Bb:44:GLU:HB2	73:Bb:105:HOH:O	1.97	0.64
3:1:536:A:H5''	3:1:537:G:H3'	1.79	0.64
11:AG:45:ARG:NH2	11:AG:115:LYS:O	2.31	0.64
3:1:1160:G:OP1	36:Ag:36:LYS:NZ	2.30	0.64
73:1:4983:HOH:O	6:AB:241:GLY:HA2	1.97	0.64
4:4:1219:G:H5''	52:BL:51:MET:HE1	1.78	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:BG:102:ARG:NH2	47:BG:109:SER:OG	2.30	0.64
65:BY:39:VAL:HB	65:BY:49:ALA:HB3	1.80	0.64
2:3:327:HIS:HB3	2:3:483:ARG:HH12	1.62	0.64
4:4:1115:A:H5'	51:BK:17:VAL:HG21	1.78	0.64
66:BZ:18:VAL:HG13	66:BZ:34:VAL:HG23	1.80	0.64
2:3:444:VAL:HG13	2:3:456:VAL:HG11	1.80	0.64
2:3:518:ASP:OD2	2:3:625:LYS:NZ	2.30	0.64
3:1:2690:G:O2'	3:1:2693:A:OP2	2.14	0.64
4:4:103:C:OP1	4:4:315:C:O2'	2.15	0.64
10:AF:4:THR:N	10:AF:87:GLU:OE1	2.31	0.64
20:AQ:93:MET:HE2	20:AQ:93:MET:HA	1.79	0.64
45:BE:83:MET:HE3	45:BE:225:MET:HE3	1.80	0.64
3:1:2029:G:H2'	3:1:2030:G:H1'	1.79	0.64
8:AD:31:GLY:O	8:AD:35:LEU:N	2.24	0.64
10:AF:43:GLN:HG3	10:AF:44:THR:HG23	1.80	0.64
42:BB:90:CYS:HB3	42:BB:95:CYS:H	1.63	0.64
58:BR:49:HIS:HE1	58:BR:102:CYS:SG	2.20	0.64
15:AL:115:LYS:HE3	15:AL:132:VAL:HG11	1.80	0.64
48:BH:162:PRO:HD3	66:BZ:62:VAL:HG12	1.79	0.64
60:BT:12:LYS:HG3	60:BT:114:THR:HG22	1.80	0.64
44:BD:64:THR:HB	44:BD:67:GLU:HG2	1.78	0.64
2:3:500:ASN:OD1	4:4:654:G:N2	2.30	0.63
3:1:791:G:N7	73:1:3557:HOH:O	2.30	0.63
11:AG:15:LYS:NZ	11:AG:43:GLU:OE2	2.31	0.63
17:AN:79:LYS:HE2	17:AN:80:TYR:HE1	1.62	0.63
15:AL:106:VAL:HG12	15:AL:126:LEU:HD11	1.78	0.63
24:AU:1:MET:HE1	24:AU:33:GLN:HB3	1.80	0.63
53:BM:129:THR:OG1	53:BM:130:ILE:N	2.29	0.63
3:1:475:C:OP2	7:AC:74:LYS:NZ	2.31	0.63
3:1:2039:G:N2	4:4:1455:C:O4'	2.32	0.63
3:1:2475:A:N7	73:1:3544:HOH:O	2.30	0.63
4:4:1443:G:C2'	4:4:1444:G:H5''	2.28	0.63
7:AC:180:ILE:HG23	7:AC:185:GLU:HB3	1.81	0.63
8:AD:101:PHE:O	8:AD:162:ARG:NH1	2.31	0.63
32:Ac:3:ARG:HB3	32:Ac:4:PRO:HD3	1.80	0.63
41:BA:31:TYR:O	41:BA:89:THR:OG1	2.12	0.63
44:BD:21:ASN:HB3	44:BD:24:LEU:HB3	1.80	0.63
48:BH:20:ASP:OD1	66:BZ:37:ARG:NH2	2.30	0.63
3:1:1358:C:OP1	31:Ab:117:ARG:NH2	2.31	0.63
3:1:1769:U:H3'	73:1:3406:HOH:O	1.97	0.63
4:4:474:U:H2'	4:4:475:OMG:H8	1.64	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:1230:C:OP1	61:BU:121:ARG:NH2	2.32	0.63
10:AF:72:VAL:HG23	10:AF:75:PRO:HA	1.79	0.63
12:AH:78:PRO:HG3	16:AM:172:ILE:HD11	1.81	0.63
44:BD:85:ILE:O	44:BD:149:ARG:NH2	2.32	0.63
51:BK:102:GLU:HG3	51:BK:106:LYS:HE3	1.80	0.63
53:BM:85:ILE:HD11	53:BM:116:ILE:HD12	1.80	0.63
57:BQ:34:GLU:HG2	57:BQ:74:ILE:HG23	1.79	0.63
60:BT:108:HIS:HB3	60:BT:115:TYR:HB3	1.81	0.63
4:4:451:G:OP1	62:BV:33:LYS:NZ	2.32	0.63
73:4:3469:HOH:O	58:BR:57:LYS:CD	2.46	0.63
20:AQ:108:LYS:O	20:AQ:142:THR:OG1	2.13	0.63
41:BA:65:THR:OG1	41:BA:66:LYS:N	2.27	0.63
6:AB:207:THR:OG1	6:AB:258:GLY:O	2.17	0.63
42:BB:90:CYS:O	42:BB:94:GLY:N	2.22	0.63
47:BG:29:PHE:HA	47:BG:32:LEU:HD12	1.79	0.63
3:1:456:G:H3'	73:1:6868:HOH:O	1.99	0.63
4:4:119:U:O2	45:BE:142:ASN:ND2	2.29	0.63
2:3:350:LEU:HA	2:3:353:ILE:HG12	1.80	0.63
3:1:2167:C:OP1	23:AT:82:LYS:N	2.25	0.63
4:4:727:A:OP2	4:4:773:G:N2	2.32	0.63
14:AJ:9:ARG:NH1	14:AJ:58:THR:O	2.31	0.63
56:BP:29:ILE:HG22	56:BP:36:LEU:H	1.63	0.63
62:BV:30:LEU:HD13	62:BV:70:LYS:HG3	1.81	0.63
4:4:552:C:OP2	49:BI:32:LYS:NZ	2.29	0.63
48:BH:120:TYR:HB2	48:BH:127:PRO:HG3	1.80	0.63
68:Bb:20:GLU:HG2	68:Bb:61:LEU:HD12	1.80	0.63
3:1:457:G:OP1	16:AM:116:ASN:ND2	2.30	0.62
14:AJ:23:ALA:HA	14:AJ:38:GLY:HA3	1.81	0.62
23:AT:35:ALA:HB2	23:AT:109:LEU:HD13	1.81	0.62
41:BA:119:LYS:CE	73:BA:320:HOH:O	2.46	0.62
54:BN:6:SER:HB3	54:BN:7:PRO:HD3	1.81	0.62
60:BT:29:PHE:O	60:BT:30:ARG:NH1	2.30	0.62
3:1:236:A:OP1	12:AH:125:LYS:NZ	2.26	0.62
44:BD:79:LEU:HB3	44:BD:85:ILE:HG12	1.81	0.62
48:BH:29:ARG:NH2	48:BH:50:VAL:O	2.32	0.62
50:BJ:60:ARG:NH1	50:BJ:120:GLY:O	2.32	0.62
3:1:2749:C:O2'	6:AB:165:GLU:OE2	2.16	0.62
12:AH:87:VAL:HG23	16:AM:160:LEU:HD11	1.81	0.62
39:Aj:51:LEU:HD22	39:Aj:52:PRO:HD2	1.82	0.62
48:BH:181:SER:OG	48:BH:191:CYS:SG	2.57	0.62
62:BV:11:ILE:HD11	62:BV:49:GLN:HG2	1.81	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:1136:A:OP1	59:BS:60:ARG:NH2	2.32	0.62
46:BF:137:LYS:HD2	46:BF:142:GLU:HG2	1.82	0.62
53:BM:36:ASP:OD1	53:BM:38:THR:OG1	2.15	0.62
4:4:621:G:H2'	4:4:622:G:C8	2.34	0.62
7:AC:238:ILE:HA	7:AC:249:VAL:HG21	1.81	0.62
11:AG:21:ASP:OD1	11:AG:50:ASN:ND2	2.27	0.62
43:BC:162:TYR:OH	43:BC:201:ASP:OD2	2.17	0.62
46:BF:64:THR:OG1	46:BF:67:GLY:O	2.16	0.62
53:BM:139:ARG:NH1	73:BM:202:HOH:O	2.32	0.62
2:3:604:LEU:HG	2:3:610:VAL:HG22	1.82	0.62
3:1:1429:A:O2'	3:1:1765:C:N4	2.30	0.62
4:4:297:G:OP1	4:4:571:U:O2'	2.15	0.62
4:4:1491:U:OP2	64:BX:5:ARG:NH2	2.32	0.62
13:AI:100:VAL:HG13	26:AW:20:MET:HE3	1.81	0.62
54:BN:27:ASP:OD1	54:BN:29:THR:OG1	2.17	0.62
55:BO:5:ILE:HD11	63:BW:45:THR:HA	1.81	0.62
3:1:2027:G:H2'	3:1:2028:G:O4'	1.99	0.62
4:4:503:C:H5''	67:Ba:40:ARG:HH12	1.64	0.62
48:BH:187:PRO:HG2	48:BH:190:GLU:HG3	1.81	0.62
25:AV:114:GLN:HA	25:AV:117:ILE:HD12	1.81	0.62
4:4:11:A:C2'	4:4:12:U:H5'	2.30	0.62
4:4:576:G:OP2	44:BD:78:LYS:NZ	2.27	0.62
4:4:1379:A:H2'	4:4:1380:C:H6	1.64	0.62
4:4:1415:G:C1'	73:4:3227:HOH:O	2.46	0.62
6:AB:88:ARG:NH1	6:AB:165:GLU:OE2	2.32	0.62
39:Aj:66:PHE:HB3	39:Aj:111:LEU:HD23	1.82	0.62
28:AY:94:TYR:OH	28:AY:136:PRO:O	2.13	0.61
50:BJ:105:ILE:HD13	50:BJ:114:VAL:HG13	1.81	0.61
3:1:1085:U:O2'	3:1:2385:A:N3	2.33	0.61
3:1:1870:A:H4'	20:AQ:98:ARG:HD2	1.81	0.61
4:4:377:A:N3	73:4:3128:HOH:O	2.31	0.61
4:4:405:C:O2'	4:4:582:A:N3	2.31	0.61
9:AE:10:VAL:HG12	9:AE:57:VAL:HB	1.83	0.61
39:Aj:155:GLN:HE22	39:Aj:170:THR:HG23	1.65	0.61
42:BB:106:MET:HE3	42:BB:116:LEU:HG	1.81	0.61
45:BE:82:LEU:HG	45:BE:83:MET:HG2	1.81	0.61
46:BF:13:THR:N	46:BF:39:GLU:OE2	2.30	0.61
49:BI:41:LEU:HD21	49:BI:129:VAL:HG21	1.82	0.61
4:4:784:G:HO2'	49:BI:2:VAL:N	1.98	0.61
73:4:3284:HOH:O	46:BF:159:VAL:HG12	2.00	0.61
17:AN:67:GLU:OE1	17:AN:70:ARG:NE	2.30	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1:308:G:H5'	73:1:4417:HOH:O	1.99	0.61
3:1:1292:C:H2'	3:1:1293:G:C8	2.36	0.61
3:1:1988:G:N1	3:1:2010:A:OP2	2.23	0.61
24:AU:31:LYS:HE3	24:AU:51:THR:HG22	1.82	0.61
48:BH:64:LYS:NZ	51:BK:111:TYR:O	2.30	0.61
3:1:1259:A:O4'	11:AG:69:ARG:NH2	2.33	0.61
8:AD:35:LEU:HD11	8:AD:72:VAL:HG23	1.82	0.61
58:BR:6:LEU:HD12	58:BR:10:PRO:HD3	1.83	0.61
3:1:2805:A:OP2	30:Aa:28:ARG:NH1	2.27	0.61
43:BC:194:PRO:HD2	43:BC:197:LEU:HD22	1.82	0.61
45:BE:118:LYS:NZ	45:BE:139:ASP:OD2	2.31	0.61
1:2:8:A:O2'	1:2:63:G:N2	2.27	0.61
19:AP:55:ASN:ND2	19:AP:75:GLU:O	2.34	0.61
28:AY:76:GLU:OE1	28:AY:79:ARG:NH2	2.31	0.61
42:BB:29:ASN:ND2	42:BB:149:THR:O	2.30	0.61
42:BB:79:ARG:NH2	42:BB:125:ASP:OD2	2.34	0.61
43:BC:179:VAL:HG23	43:BC:181:LEU:HD13	1.83	0.61
69:Bc:65:PRO:N	73:Bc:201:HOH:O	2.33	0.61
2:3:327:HIS:H	2:3:483:ARG:HH22	1.48	0.61
2:3:380:ARG:HD3	2:3:535:ASP:HA	1.83	0.61
4:4:380:G:H5'	45:BE:25:VAL:HG22	1.81	0.61
4:4:1477:MA6:H103	4:4:1478:MA6:H92	1.83	0.61
41:BA:52:LEU:HD23	41:BA:55:ARG:HD3	1.83	0.61
57:BQ:2:PRO:HG2	57:BQ:6:ARG:HG3	1.82	0.61
63:BW:41:ARG:HD2	63:BW:47:ASP:HA	1.82	0.61
2:3:474:LEU:HD12	2:3:629:VAL:HG22	1.82	0.61
2:3:589:HIS:CD2	2:3:603:LYS:HB3	2.36	0.61
16:AM:12:TYR:O	16:AM:17:ARG:NH2	2.33	0.61
18:AO:52:ARG:HG3	18:AO:57:GLU:HG2	1.83	0.61
19:AP:66:ILE:HD13	19:AP:70:LEU:HD13	1.83	0.61
25:AV:52:THR:HB	25:AV:105:ASP:HB3	1.82	0.61
3:1:1740:C:N4	73:1:3589:HOH:O	2.32	0.60
3:1:2043:C:H2'	3:1:2044:PSU:C6	2.36	0.60
4:4:500:G:H5''	67:Ba:22:ALA:HB2	1.83	0.60
8:AD:26:ILE:HD11	8:AD:131:MET:HG3	1.83	0.60
14:AK:30:ASP:OD1	14:AK:33:TYR:N	2.31	0.60
42:BB:31:TYR:OH	69:Bc:65:PRO:O	2.15	0.60
48:BH:55:PRO:HD3	66:BZ:9:PRO:HD3	1.82	0.60
61:BU:3:SER:HA	61:BU:132:ASP:OD1	2.01	0.60
62:BV:78:TYR:OH	62:BV:88:GLU:OE2	2.14	0.60
2:3:325:VAL:HG12	2:3:483:ARG:HH21	1.66	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1:32:C:O2'	3:1:698:A:N1	2.32	0.60
3:1:2712:A:H5''	5:AA:203:GLY:HA3	1.81	0.60
49:BI:51:GLU:HG3	49:BI:62:VAL:HB	1.83	0.60
64:BX:87:GLU:HG3	64:BX:90:LYS:HZ1	1.65	0.60
3:1:2420:G:O2'	3:1:2421:A:OP1	2.19	0.60
3:1:2776:G:O6	9:AE:176:ARG:NH2	2.29	0.60
4:4:685:G:OP2	4:4:793:G:N2	2.34	0.60
4:4:826:G:HO2'	4:4:839:G:HO2'	1.50	0.60
6:AB:203:VAL:HG12	6:AB:312:LEU:HD22	1.82	0.60
14:AJ:60:LYS:HZ3	14:AJ:82:LEU:HD13	1.66	0.60
2:3:441:LEU:HG	2:3:632:LEU:HD12	1.84	0.60
3:1:2846:G:H4'	6:AB:320:LYS:HE2	1.84	0.60
4:4:404:C:OP1	44:BD:9:LYS:HE3	2.02	0.60
11:AG:96:LYS:HE3	11:AG:114:LEU:HG	1.83	0.60
31:Ab:94:GLU:OE2	31:Ab:94:GLU:N	2.32	0.60
32:Ac:63:ARG:HD2	32:Ac:74:LEU:HD23	1.84	0.60
3:1:1927:A:H4'	5:AA:169:PHE:O	2.01	0.60
73:1:3413:HOH:O	19:AP:119:LYS:HE2	2.02	0.60
4:4:16:G:H2'	4:4:17:C:C6	2.35	0.60
4:4:147:G:H4'	47:BG:58:THR:HB	1.83	0.60
4:4:1379:A:H2'	4:4:1380:C:C6	2.37	0.60
16:AM:177:LYS:HG2	16:AM:178:THR:HG23	1.81	0.60
53:BM:68:ALA:HB3	53:BM:108:ALA:HB3	1.82	0.60
3:1:620:G:OP1	31:Ab:18:ARG:NH1	2.34	0.60
3:1:1074:U:H3'	3:1:1075:G:C5'	2.31	0.60
3:1:1529:C:O2'	24:AU:18:GLU:OE2	2.18	0.60
3:1:1592:C:OP1	20:AQ:61:ARG:NH1	2.31	0.60
4:4:286:C:OP1	50:BJ:16:SER:OG	2.18	0.60
4:4:384:G:N2	4:4:387:A:OP2	2.35	0.60
16:AM:144:ASP:HB3	16:AM:147:TYR:HB2	1.82	0.60
19:AP:17:ILE:HD13	19:AP:40:GLU:HG3	1.82	0.60
3:1:216:C:O2'	3:1:463:C:N3	2.35	0.60
34:Ae:8:VAL:HG21	34:Ae:53:LEU:HD11	1.82	0.60
62:BV:108:ALA:HA	62:BV:111:ARG:HE	1.66	0.60
3:1:2562:A:N3	73:1:3573:HOH:O	2.31	0.60
4:4:63:C:H2'	4:4:64:G:C8	2.37	0.60
42:BB:90:CYS:O	42:BB:93:VAL:N	2.28	0.60
54:BN:61:GLU:OE2	67:Ba:3:SER:OG	2.19	0.60
55:BO:87:THR:HG23	55:BO:89:ARG:H	1.67	0.60
66:BZ:20:GLN:HB3	66:BZ:35:LYS:HB2	1.84	0.60
4:4:1184:OMC:HM22	4:4:1185:G:H5'	1.84	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:1216:A:H4'	51:BK:77:GLY:HA2	1.83	0.60
6:AB:92:LEU:HD11	11:AG:171:LYS:HE3	1.82	0.60
12:AH:44:LEU:O	16:AM:168:GLN:NE2	2.28	0.60
51:BK:102:GLU:O	51:BK:106:LYS:HD2	2.02	0.60
64:BX:29:VAL:HG22	64:BX:30:VAL:H	1.67	0.60
3:1:624:G:H2'	3:1:625:G:H8	1.67	0.59
3:1:901:A:H2'	3:1:903:A:OP1	2.00	0.59
3:1:1619:G:H2'	3:1:1620:U:C6	2.37	0.59
4:4:1436:C:H3'	4:4:1437:U:H5''	1.84	0.59
4:4:12:U:H2'	4:4:13:C:C6	2.37	0.59
21:AR:74:LYS:HZ1	21:AR:76:VAL:HG22	1.67	0.59
42:BB:11:VAL:HG11	42:BB:15:LYS:HE2	1.84	0.59
43:BC:170:ASN:HB3	43:BC:171:ARG:HD2	1.83	0.59
63:BW:67:TYR:O	63:BW:71:THR:HG23	2.02	0.59
4:4:1082:A:O2'	52:BL:42:PRO:O	2.18	0.59
4:4:1124:A:OP2	59:BS:32:LYS:NZ	2.36	0.59
28:AY:38:LEU:HD23	28:AY:43:THR:HG22	1.84	0.59
3:1:653:A:OP2	31:Ab:55:LYS:NZ	2.31	0.59
3:1:2982:U:H3'	3:1:2983:U:H3'	1.83	0.59
4:4:1077:C:H1'	4:4:1145:A:C4	2.38	0.59
4:4:1263:C:OP1	63:BW:76:LYS:NZ	2.30	0.59
4:4:1390:C:H2'	4:4:1391:C:C6	2.36	0.59
40:Ak:21:TYR:O	40:Ak:25:GLU:HG2	2.02	0.59
63:BW:81:PHE:HE1	63:BW:103:GLU:HG3	1.67	0.59
3:1:363:C:H5''	25:AV:31:LYS:HE3	1.84	0.59
4:4:785:G:O4'	49:BI:2:VAL:N	2.35	0.59
73:4:4029:HOH:O	57:BQ:107:LYS:HE2	2.01	0.59
39:Aj:61:GLU:OE2	39:Aj:107:ARG:NH2	2.35	0.59
41:BA:29:SER:O	41:BA:87:ALA:N	2.31	0.59
41:BA:118:VAL:HG11	41:BA:154:VAL:HG12	1.85	0.59
58:BR:54:ILE:HG22	58:BR:116:THR:HG22	1.83	0.59
68:Bb:44:GLU:CA	73:Bb:105:HOH:O	2.49	0.59
9:AE:87:THR:HG23	9:AE:88:LYS:HD2	1.85	0.59
68:Bb:13:ILE:O	68:Bb:17:ARG:HG2	2.02	0.59
3:1:624:G:H2'	3:1:625:G:C8	2.37	0.59
3:1:1299:C:H2'	3:1:1300:G:H5''	1.84	0.59
3:1:2032:U:H2'	3:1:2033:A:O4'	2.02	0.59
4:4:830:A:H5''	70:4:3017:SPM:H81	1.84	0.59
2:3:455:TYR:HA	2:3:470:THR:HA	1.85	0.59
3:1:1633:A:H4'	73:1:7057:HOH:O	2.02	0.59
3:1:2980:G:O6	3:1:2983:U:H5''	2.03	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:1378:C:H2'	4:4:1379:A:C8	2.38	0.59
14:AJ:31:GLU:OE2	14:AJ:31:GLU:N	2.33	0.59
48:BH:97:ARG:O	48:BH:178:ARG:NH1	2.36	0.59
51:BK:54:LYS:HD2	51:BK:81:MET:HE3	1.84	0.59
61:BU:59:ILE:HD11	61:BU:101:ILE:HD13	1.85	0.59
2:3:475:VAL:HG12	2:3:601:LEU:HG	1.85	0.59
3:1:595:A:H2'	3:1:596:A:H8	1.67	0.59
3:1:1907:U:H2'	3:1:1908:G:C8	2.38	0.59
3:1:2426:C:O2'	8:AD:106:ASN:ND2	2.35	0.59
23:AT:146:ARG:HG3	23:AT:152:THR:HG23	1.83	0.59
31:Ab:9:LEU:HD12	31:Ab:13:LEU:HD23	1.84	0.59
1:2:117:G:H2'	1:2:118:C:C6	2.37	0.59
2:3:552:VAL:HG12	2:3:562:LYS:HG3	1.85	0.59
3:1:199:G:H22	3:1:216:C:H4'	1.68	0.59
3:1:2042:C:H2'	3:1:2043:C:C1'	2.33	0.59
3:1:2716:A:H4'	73:1:4958:HOH:O	2.02	0.59
73:1:6335:HOH:O	32:Ac:15:LYS:HG3	2.02	0.59
4:4:378:A:N1	4:4:394:C:O2'	2.31	0.59
4:4:952:C:H1'	60:BT:112:GLY:O	2.02	0.59
4:4:1093:C:H2'	4:4:1094:U:H6	1.67	0.59
7:AC:189:LEU:HA	7:AC:192:VAL:HG12	1.84	0.59
3:1:120:C:H1'	73:1:3901:HOH:O	2.03	0.58
3:1:1176:A:H2'	3:1:1177:G:O4'	2.02	0.58
3:1:1259:A:N1	73:1:3580:HOH:O	2.32	0.58
55:BO:51:THR:HB	55:BO:54:LEU:HD12	1.85	0.58
3:1:350:A:H5'	3:1:368:A:H1'	1.86	0.58
3:1:1154:A:H2'	3:1:1155:A:C8	2.38	0.58
4:4:892:G:O2'	4:4:1462:A:N7	2.34	0.58
44:BD:32:MET:HE2	67:Ba:34:ASN:ND2	2.18	0.58
45:BE:97:VAL:HG22	45:BE:107:LEU:HD23	1.85	0.58
2:3:470:THR:N	2:3:473:GLU:OE2	2.31	0.58
2:3:471:LYS:O	2:3:475:VAL:HG23	2.04	0.58
3:1:648:C:H2'	3:1:649:U:O4'	2.04	0.58
3:1:1175:C:H2'	3:1:1176:A:H5'	1.85	0.58
3:1:2102:A:O2'	3:1:2103:OMG:OP1	2.18	0.58
3:1:2135:A:H2'	3:1:2136:C:H6	1.68	0.58
4:4:653:C:O2'	4:4:655:A:N7	2.28	0.58
4:4:1007:G:H1'	4:4:1180:A:O2'	2.03	0.58
4:4:1408:G:O6	4:4:1417:U:O4	2.21	0.58
3:1:27:C:OP2	25:AV:13:ARG:NH1	2.36	0.58
3:1:2440:A:H2'	3:1:2441:G:C8	2.39	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:106:G:OP1	4:4:566:U:O2'	2.14	0.58
4:4:1200:C:C2'	4:4:1201:U:H5'	2.33	0.58
8:AD:55:ALA:HB2	8:AD:70:ILE:HD13	1.84	0.58
51:BK:10:ASN:O	51:BK:12:ARG:N	2.36	0.58
51:BK:124:GLU:HG2	51:BK:133:ALA:CB	2.33	0.58
2:3:626:MET:SD	2:3:630:LYS:HD2	2.44	0.58
3:1:1175:C:C2'	3:1:1176:A:H5'	2.33	0.58
4:4:1013:C:O2'	4:4:1014:A:H5''	2.03	0.58
4:4:1423:G:H2'	4:4:1424:A:C8	2.38	0.58
5:AA:88:VAL:HG21	38:AI:81:ILE:O	2.02	0.58
31:Ab:118:LEU:O	31:Ab:122:LYS:HG3	2.04	0.58
48:BH:176:GLY:O	48:BH:179:GLN:NE2	2.36	0.58
51:BK:58:PRO:HB2	51:BK:91:ILE:HG22	1.86	0.58
55:BO:6:ARG:O	55:BO:18:GLY:HA3	2.02	0.58
55:BO:81:ARG:HD2	55:BO:93:LEU:HD23	1.84	0.58
60:BT:103:VAL:HA	60:BT:120:ILE:HG22	1.83	0.58
64:BX:52:GLU:HG3	64:BX:58:ALA:HB1	1.86	0.58
68:Bb:17:ARG:NH2	68:Bb:54:LEU:HD21	2.19	0.58
3:1:1642:A:N1	3:1:1703:G:O2'	2.31	0.58
4:4:332:C:N4	50:BJ:2:LYS:O	2.36	0.58
41:BA:105:ILE:HD12	41:BA:111:LYS:HD2	1.86	0.58
45:BE:48:LEU:HD13	45:BE:88:ILE:HD11	1.85	0.58
46:BF:9:TRP:CD1	46:BF:41:GLU:HG3	2.38	0.58
3:1:1420:C:H5'	20:AQ:21:ILE:O	2.04	0.58
3:1:1922:A:H1'	3:1:2059:A2M:N6	2.17	0.58
3:1:3021:G:H5'	73:1:4210:HOH:O	2.03	0.58
4:4:75:C:C6	4:4:212:C:H2'	2.39	0.58
4:4:211:C:H2'	4:4:212:C:O4'	2.04	0.58
4:4:231:G:H4'	45:BE:32:HIS:O	2.03	0.58
4:4:264:U:OP1	50:BJ:1:MET:N	2.37	0.58
4:4:1391:C:H2'	4:4:1392:C:C6	2.38	0.58
3:1:2051:G:O2'	3:1:2089:G:O6	2.20	0.58
4:4:77:C:H2'	4:4:78:G:H8	1.67	0.58
4:4:912:A:H2'	4:4:913:G:C8	2.39	0.58
4:4:1192:C:H2'	55:BO:131:THR:HB	1.85	0.58
10:AF:73:ASP:HB3	10:AF:74:PRO:HD3	1.84	0.58
13:AI:128:GLU:OE1	13:AI:128:GLU:N	2.30	0.58
15:AL:115:LYS:HG3	15:AL:132:VAL:HG12	1.84	0.58
25:AV:54:LEU:HD23	25:AV:102:MET:HE2	1.85	0.58
55:BO:137:PHE:CE1	55:BO:139:ALA:HB3	2.39	0.58
63:BW:57:GLU:O	63:BW:61:LEU:HD23	2.04	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1:963:G:H1'	3:1:1054:A:N6	2.18	0.58
3:1:2028:G:C2'	3:1:2029:G:H5'	2.34	0.58
15:AL:101:GLU:N	15:AL:101:GLU:OE2	2.36	0.58
18:AO:186:GLU:O	18:AO:190:LYS:NZ	2.31	0.58
66:BZ:38:VAL:O	66:BZ:44:LYS:NZ	2.37	0.58
3:1:2741:G:N2	3:1:2889:G:OP2	2.35	0.58
4:4:129:G:H2'	4:4:130:A:C8	2.39	0.58
6:AB:91:THR:OG1	6:AB:139:VAL:O	2.14	0.58
11:AG:7:LEU:HD21	11:AG:12:ILE:HD13	1.86	0.58
48:BH:12:THR:O	48:BH:14:ARG:NH2	2.36	0.58
48:BH:118:ILE:HG12	63:BW:104:VAL:HG21	1.86	0.58
57:BQ:2:PRO:HA	57:BQ:117:LEU:HD13	1.86	0.58
3:1:75:U:OP2	25:AV:119:ARG:NH2	2.28	0.57
3:1:2040:A:H2'	3:1:2041:C:H5'	1.85	0.57
6:AB:34:VAL:HG13	6:AB:36:LEU:HG	1.86	0.57
10:AF:130:VAL:HA	10:AF:133:ILE:HG12	1.85	0.57
14:AK:39:PRO:HD2	14:AK:42:LEU:HD23	1.86	0.57
18:AO:37:VAL:HG12	18:AO:116:VAL:HG12	1.85	0.57
44:BD:93:ASP:OD1	44:BD:93:ASP:N	2.35	0.57
47:BG:10:ASP:OD2	47:BG:119:TYR:OH	2.14	0.57
49:BI:106:THR:HB	49:BI:121:ILE:HD12	1.84	0.57
61:BU:16:LEU:O	61:BU:20:ILE:HG13	2.04	0.57
65:BY:39:VAL:HG12	65:BY:48:LEU:HB2	1.86	0.57
3:1:313:C:N4	73:1:3634:HOH:O	2.35	0.57
3:1:2029:G:H2'	3:1:2030:G:C1'	2.34	0.57
14:AK:4:VAL:HG22	21:AR:74:LYS:HZ3	1.67	0.57
15:AL:49:MET:CE	15:AL:54:SER:HA	2.32	0.57
19:AP:58:ALA:O	19:AP:78:LYS:NZ	2.31	0.57
44:BD:30:GLN:O	44:BD:34:GLU:HG3	2.03	0.57
53:BM:135:GLY:HA2	73:BM:201:HOH:O	1.98	0.57
2:3:329:THR:HA	2:3:481:ARG:CD	2.34	0.57
10:AF:36:GLU:O	10:AF:40:ILE:HD12	2.04	0.57
29:AZ:10:VAL:O	29:AZ:14:THR:OG1	2.12	0.57
34:Ae:48:ASP:OD1	34:Ae:48:ASP:N	2.36	0.57
42:BB:92:PHE:HE2	42:BB:195:PRO:HG2	1.69	0.57
54:BN:21:GLN:HA	54:BN:24:ARG:HG3	1.87	0.57
57:BQ:57:GLN:NE2	65:BY:40:ARG:O	2.37	0.57
57:BQ:130:LYS:NZ	57:BQ:139:PHE:O	2.31	0.57
1:2:87:G:N7	73:2:205:HOH:O	2.32	0.57
1:2:109:A:H2'	1:2:110:C:O4'	2.05	0.57
2:3:368:VAL:HG12	2:3:374:VAL:HA	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1:763:A:H2'	3:1:764:G:O4'	2.03	0.57
3:1:1310:G:OP1	28:AY:139:LYS:NZ	2.33	0.57
4:4:638:C:H2'	4:4:639:U:C6	2.39	0.57
6:AB:26:PRO:HG2	6:AB:311:VAL:HG23	1.87	0.57
41:BA:32:ALA:O	41:BA:38:GLY:HA2	2.04	0.57
46:BF:12:LYS:HD3	46:BF:13:THR:CA	2.31	0.57
55:BO:64:ASP:OD2	55:BO:68:ARG:NH2	2.38	0.57
55:BO:140:THR:HG23	55:BO:143:VAL:HG12	1.87	0.57
56:BP:18:ARG:HG3	56:BP:19:CYS:H	1.70	0.57
2:3:334:ARG:HH21	2:3:438:SER:HA	1.69	0.57
3:1:1382:U:H5''	3:1:1383:C:H5''	1.85	0.57
4:4:1370:C:H2'	4:4:1371:G:C8	2.39	0.57
9:AE:10:VAL:CG1	9:AE:57:VAL:HB	2.34	0.57
34:Ae:20:VAL:HG23	34:Ae:63:LYS:HG2	1.85	0.57
45:BE:39:PRO:HG2	45:BE:42:VAL:HG23	1.87	0.57
54:BN:44:LEU:O	54:BN:79:LYS:NZ	2.28	0.57
2:3:328:VAL:HG12	2:3:635:VAL:HG11	1.86	0.57
3:1:2431:U:H3'	18:AO:3:ARG:NH2	2.20	0.57
3:1:2911:G:H2'	3:1:2912:G:C8	2.40	0.57
4:4:23:C:O2'	4:4:299:U:OP1	2.22	0.57
16:AM:89:TYR:O	37:Ah:47:TYR:OH	2.15	0.57
18:AO:140:GLU:O	18:AO:144:ARG:HG2	2.05	0.57
22:AS:73:TYR:HE2	22:AS:90:PRO:HG3	1.69	0.57
55:BO:58:ASP:O	55:BO:62:LYS:HD3	2.05	0.57
3:1:1494:A:H2'	3:1:1495:U:C6	2.40	0.57
3:1:2540:U:OP2	37:Ah:60:LYS:HG2	2.04	0.57
4:4:541:C:H2'	4:4:542:G:O4'	2.05	0.57
4:4:662:U:H4'	4:4:664:A:OP2	2.04	0.57
4:4:1396:G:H2'	4:4:1397:C:C6	2.40	0.57
28:AY:40:ARG:HH22	28:AY:143:ARG:HD2	1.70	0.57
46:BF:78:VAL:HG13	46:BF:106:ALA:HB1	1.87	0.57
48:BH:160:VAL:HG23	48:BH:165:ARG:HG2	1.86	0.57
55:BO:22:VAL:HG13	55:BO:52:LEU:HD13	1.87	0.57
3:1:474:U:O2'	3:1:1328:G:O2'	2.13	0.57
3:1:1454:U:OP2	3:1:1758:G:O2'	2.19	0.57
15:AL:104:LEU:O	15:AL:126:LEU:HD12	2.05	0.57
27:AX:14:MET:HE3	27:AX:18:GLU:HB2	1.85	0.57
51:BK:10:ASN:HB2	51:BK:11:PRO:HD3	1.85	0.57
61:BU:15:GLU:HG3	61:BU:138:ILE:HD11	1.87	0.57
3:1:259:U:H2'	3:1:260:C:C6	2.40	0.57
3:1:712:A:N1	3:1:721:G:O2'	2.34	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1:736:G:N2	73:1:3487:HOH:O	2.26	0.57
3:1:2929:A:H2'	3:1:2930:G:O4'	2.04	0.57
5:AA:102:MET:HE1	38:AI:77:LEU:HD21	1.87	0.57
11:AG:8:ASP:HB3	11:AG:11:GLN:HB2	1.87	0.57
17:AN:55:ALA:HA	17:AN:164:THR:HG22	1.86	0.57
41:BA:52:LEU:HD23	41:BA:55:ARG:CD	2.35	0.57
44:BD:137:GLY:O	62:BV:68:ILE:HD12	2.05	0.57
48:BH:94:LEU:HB2	48:BH:174:THR:HG21	1.87	0.57
53:BM:103:SER:HB3	53:BM:107:ARG:HH22	1.69	0.57
2:3:470:THR:O	2:3:474:LEU:HG	2.04	0.57
3:1:2358:G:H2'	3:1:2359:C:H6	1.69	0.57
4:4:187:U:H2'	4:4:188:C:C6	2.40	0.57
4:4:901:A:H2'	4:4:902:C:C6	2.40	0.57
8:AD:114:HIS:HA	8:AD:117:LEU:HD23	1.87	0.57
41:BA:22:TRP:NE1	53:BM:43:VAL:HA	2.20	0.57
45:BE:68:VAL:HG12	45:BE:69:ASP:OD1	2.05	0.57
46:BF:134:VAL:HG12	46:BF:145:LEU:HB2	1.87	0.57
47:BG:29:PHE:O	47:BG:106:ILE:HD12	2.05	0.57
51:BK:112:ASP:HB3	51:BK:115:MET:HE3	1.87	0.57
58:BR:61:VAL:HG21	58:BR:74:VAL:HG21	1.87	0.57
2:3:555:THR:HG23	4:4:891:G:H4'	1.87	0.56
3:1:595:A:H2'	3:1:596:A:C8	2.40	0.56
4:4:381:C:H2'	4:4:382:G:C8	2.39	0.56
10:AF:72:VAL:HG21	10:AF:78:VAL:HG22	1.86	0.56
12:AH:114:ARG:O	12:AH:118:THR:HG23	2.05	0.56
19:AP:69:LYS:HG3	19:AP:86:SER:OG	2.05	0.56
32:AC:35:PRO:HG2	32:AC:47:MET:HE2	1.87	0.56
46:BF:27:ILE:HD12	46:BF:30:ILE:HD12	1.86	0.56
55:BO:44:LEU:HD11	55:BO:66:ALA:HB2	1.86	0.56
59:BS:10:LYS:HG2	59:BS:53:TYR:CE2	2.40	0.56
2:3:442:GLU:CG	2:3:635:VAL:HB	2.35	0.56
3:1:1517:C:H2'	3:1:1518:G:C8	2.40	0.56
3:1:2583:A:H2'	3:1:2584:G:O4'	2.04	0.56
4:4:171:G:H2'	4:4:172:C:H5''	1.86	0.56
6:AB:87:VAL:HG23	6:AB:185:LEU:HD13	1.87	0.56
7:AC:31:LEU:N	7:AC:44:ILE:O	2.28	0.56
7:AC:153:LYS:HD2	7:AC:169:LEU:HD22	1.86	0.56
62:BV:14:LEU:HD21	62:BV:23:LYS:HE3	1.86	0.56
3:1:12:G:H2'	3:1:13:C:C6	2.40	0.56
3:1:1171:A:H5''	3:1:1172:A:C4'	2.36	0.56
3:1:1685:C:H2'	3:1:1686:G:H8	1.71	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1:2073:A:N3	3:1:2674:C:O2'	2.37	0.56
4:4:178:A:O2'	58:BR:28:ASN:O	2.15	0.56
4:4:389:C:O3'	62:BV:115:ARG:NH2	2.38	0.56
4:4:417:G:N1	4:4:420:G:OP2	2.28	0.56
4:4:421:A:H2'	4:4:422:G:O4'	2.06	0.56
4:4:635:G:H2'	4:4:636:U:C6	2.41	0.56
4:4:1098:U:O2'	4:4:1099:A:OP1	2.18	0.56
8:AD:8:LEU:HB3	8:AD:17:VAL:HB	1.87	0.56
8:AD:98:ARG:O	8:AD:162:ARG:NH2	2.38	0.56
9:AE:9:GLU:OE1	9:AE:58:VAL:HG22	2.06	0.56
9:AE:17:LYS:HB3	9:AE:33:LYS:HD3	1.86	0.56
18:AO:43:HIS:HB3	18:AO:63:ASP:OD2	2.05	0.56
31:Ab:92:ARG:HA	31:Ab:120:ILE:HD11	1.87	0.56
45:BE:118:LYS:HE2	45:BE:120:LEU:HD21	1.86	0.56
53:BM:106:ILE:HA	53:BM:109:LEU:HD12	1.87	0.56
57:BQ:62:LEU:O	57:BQ:66:ILE:HD12	2.06	0.56
3:1:1102:A:HO2'	3:1:2156:C:HO2'	1.54	0.56
4:4:296:C:H5'	4:4:570:A:H61	1.71	0.56
70:4:3008:SPM:H22	73:4:3586:HOH:O	2.05	0.56
13:AI:116:PRO:HG2	13:AI:139:LEU:HD13	1.88	0.56
47:BG:107:THR:HG23	47:BG:109:SER:H	1.70	0.56
51:BK:58:PRO:O	51:BK:108:TYR:OH	2.17	0.56
3:1:8:A:N7	73:1:3600:HOH:O	2.32	0.56
3:1:2185:C:H4'	3:1:2362:OMG:HM22	1.88	0.56
3:1:2907:C:H4'	23:AT:171:GLU:OE2	2.06	0.56
4:4:80:G:H2'	4:4:81:A:C8	2.40	0.56
4:4:93:C:H1'	4:4:358:G:H5'	1.86	0.56
9:AE:2:HIS:HA	9:AE:65:LYS:HE2	1.86	0.56
9:AE:61:VAL:HG22	9:AE:72:LEU:HD11	1.88	0.56
9:AE:104:LEU:HD23	9:AE:115:GLU:HG3	1.87	0.56
13:AI:103:GLU:OE1	26:AW:23:ARG:HD2	2.06	0.56
47:BG:34:ILE:HA	47:BG:57:ILE:CG2	2.34	0.56
60:BT:39:LEU:O	60:BT:42:MET:HB3	2.04	0.56
2:3:614:ASP:OD2	2:3:618:ARG:NH1	2.39	0.56
3:1:42:A:H3'	3:1:43:G:H5'	1.88	0.56
3:1:1536:C:H2'	3:1:1537:G:C8	2.41	0.56
3:1:2646:G:O2'	3:1:2772:A:N1	2.37	0.56
3:1:2825:C:OP1	3:1:2827:G:H4'	2.05	0.56
4:4:684:U:OP2	64:BX:11:LYS:HD3	2.06	0.56
4:4:1313:G:N1	48:BH:72:GLU:O	2.38	0.56
9:AE:103:MET:HE1	9:AE:186:ILE:HG13	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:AI:28:VAL:HG11	13:AI:107:VAL:HG13	1.86	0.56
34:Ae:56:GLU:O	34:Ae:60:LYS:HG2	2.05	0.56
42:BB:14:GLU:N	42:BB:14:GLU:OE2	2.38	0.56
2:3:342:PRO:HB2	2:3:365:LEU:HD23	1.87	0.56
3:1:159:G:H5'	33:Ad:44:ARG:HG2	1.86	0.56
3:1:737:G:N2	3:1:740:A:OP2	2.38	0.56
4:4:337:G:H5'	47:BG:95:MET:HE3	1.87	0.56
4:4:1357:U:H2'	4:4:1358:G:C8	2.41	0.56
11:AG:15:LYS:HD3	11:AG:43:GLU:HG3	1.87	0.56
26:AW:50:LEU:HD13	26:AW:52:TRP:HE1	1.71	0.56
52:BL:54:VAL:HG23	56:BP:38:ARG:HG3	1.88	0.56
60:BT:56:ARG:O	60:BT:60:LYS:HG3	2.05	0.56
69:Bc:40:THR:HG21	69:Bc:58:PRO:HG2	1.86	0.56
2:3:329:THR:HG22	2:3:481:ARG:HB3	1.88	0.56
3:1:334:U:H2'	3:1:335:G:O4'	2.06	0.56
3:1:419:G:O2'	3:1:422:U:O2'	2.23	0.56
12:AH:33:LYS:NZ	12:AH:38:ASN:HA	2.21	0.56
18:AO:187:VAL:O	18:AO:191:ILE:HG13	2.05	0.56
31:Ab:96:LEU:HD12	31:Ab:123:LYS:HG2	1.87	0.56
42:BB:61:ALA:O	42:BB:65:ILE:HG13	2.06	0.56
44:BD:101:ARG:O	44:BD:105:GLU:HG2	2.04	0.56
68:Bb:15:ARG:HA	68:Bb:18:GLU:CD	2.30	0.56
3:1:321:A:C2'	73:1:3516:HOH:O	2.51	0.56
3:1:2439:A:H5'	73:1:3774:HOH:O	2.06	0.56
3:1:2646:G:N2	3:1:2778:G:O2'	2.38	0.56
4:4:1162:A:OP1	4:4:1162:A:H3'	2.06	0.56
10:AF:48:LYS:HB2	10:AF:115:VAL:HG12	1.86	0.56
24:AU:39:GLN:HG2	24:AU:44:VAL:O	2.06	0.56
39:Aj:113:ALA:HB1	39:Aj:117:VAL:HG12	1.88	0.56
46:BF:59:LEU:HD22	46:BF:71:GLN:O	2.06	0.56
47:BG:107:THR:H	47:BG:110:ILE:HD13	1.71	0.56
60:BT:107:ILE:HD12	60:BT:120:ILE:HG12	1.87	0.56
68:Bb:5:LEU:HD22	68:Bb:47:LEU:HD11	1.86	0.56
69:Bc:55:TYR:CZ	69:Bc:64:GLY:HA3	2.40	0.56
3:1:1613:U:O2'	3:1:1614:U:H5'	2.06	0.56
73:1:4063:HOH:O	7:AC:207:LYS:HD3	2.05	0.56
4:4:119:U:H2'	4:4:120:C:C6	2.41	0.56
4:4:1104:G:H2'	4:4:1105:A:C8	2.41	0.56
9:AE:139:LYS:HD2	9:AE:139:LYS:O	2.06	0.56
11:AG:23:GLU:HB2	11:AG:53:LYS:HD2	1.88	0.56
14:AK:49:ARG:NH1	21:AR:28:ASP:OD1	2.39	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:BC:131:MET:CE	73:BC:302:HOH:O	2.47	0.56
44:BD:72:GLU:OE1	44:BD:92:LEU:HD23	2.04	0.56
55:BO:59:GLN:HA	55:BO:62:LYS:HE2	1.88	0.56
2:3:442:GLU:HG2	2:3:635:VAL:HB	1.86	0.55
3:1:1797:G:OP2	30:Aa:19:ARG:NH2	2.36	0.55
3:1:1930:U:H2'	3:1:1931:C:C6	2.41	0.55
3:1:1936:C:H4'	3:1:1937:G:H3'	1.88	0.55
4:4:195:A:N1	4:4:223:G:O2'	2.36	0.55
9:AE:17:LYS:HB3	9:AE:33:LYS:CD	2.36	0.55
12:AH:72:LEU:HD22	16:AM:176:LYS:HG3	1.88	0.55
29:AZ:6:ARG:O	29:AZ:10:VAL:HG23	2.06	0.55
37:Ah:37:GLN:O	37:Ah:41:GLU:HG2	2.06	0.55
42:BB:110:PRO:HA	42:BB:115:TYR:CG	2.41	0.55
3:1:1682:C:H4'	73:1:3903:HOH:O	2.05	0.55
3:1:3000:G:H5'	73:1:5161:HOH:O	2.05	0.55
4:4:112:C:H2'	4:4:113:C:C6	2.41	0.55
13:AI:73:LYS:O	13:AI:77:ARG:HG3	2.05	0.55
14:AK:49:ARG:HB3	21:AR:24:GLU:OE1	2.05	0.55
25:AV:20:PRO:O	25:AV:24:ARG:HG3	2.07	0.55
27:AX:57:ARG:O	27:AX:61:ILE:HG12	2.06	0.55
48:BH:205:LYS:O	48:BH:210:ARG:NH1	2.39	0.55
55:BO:7:ALA:O	55:BO:8:ILE:HD13	2.07	0.55
59:BS:56:ARG:NH1	73:BS:102:HOH:O	2.39	0.55
3:1:644:A:O2'	31:Ab:34:ASP:OD2	2.20	0.55
3:1:717:A:H2'	3:1:718:A:C8	2.41	0.55
3:1:1714:A:H2'	3:1:1715:A:C8	2.41	0.55
3:1:2140:C:H2'	3:1:2141:C:O4'	2.06	0.55
3:1:2311:U:H2'	3:1:2312:C:C6	2.41	0.55
4:4:269:G:H3'	58:BR:121:LYS:HB2	1.88	0.55
4:4:694:G:N7	64:BX:32:ARG:NH2	2.50	0.55
4:4:718:U:H2'	4:4:719:G:O4'	2.06	0.55
4:4:1026:A:N6	4:4:1068:A:H5''	2.21	0.55
4:4:1368:OMC:HM22	4:4:1369:C:H5'	1.87	0.55
4:4:1393:U:H2'	4:4:1394:C:C6	2.41	0.55
14:AK:12:VAL:HG22	14:AK:22:LYS:HD2	1.87	0.55
34:Ae:50:ALA:O	34:Ae:54:ILE:HG13	2.05	0.55
44:BD:150:GLU:OE1	44:BD:150:GLU:N	2.38	0.55
57:BQ:29:THR:HG23	57:BQ:32:GLU:OE1	2.06	0.55
2:3:477:ALA:HA	2:3:480:GLU:OE2	2.06	0.55
2:3:630:LYS:O	2:3:634:ARG:HD3	2.07	0.55
3:1:25:C:O2'	3:1:26:U:H5'	2.06	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:AO:135:GLU:OE1	18:AO:135:GLU:N	2.34	0.55
62:BV:27:VAL:HG22	62:BV:73:ALA:HB3	1.88	0.55
1:2:2:C:H2'	1:2:3:C:C6	2.42	0.55
2:3:543:GLU:O	2:3:547:ARG:HB2	2.07	0.55
3:1:670:U:H2'	3:1:671:C:C6	2.41	0.55
3:1:1544:U:H2'	3:1:1545:A:C8	2.41	0.55
3:1:1825:G:N3	3:1:1898:A:H2'	2.21	0.55
3:1:1890:C:N3	3:1:2829:C:O2'	2.38	0.55
3:1:2606:U:H2'	3:1:2607:PSU:O4'	2.06	0.55
3:1:2623:OMU:HM22	3:1:2624:OMC:H5''	1.88	0.55
4:4:192:G:O2'	4:4:193:A:H5''	2.06	0.55
4:4:1084:U:H3'	4:4:1085:U:C6	2.36	0.55
4:4:1492:C:OP1	64:BX:83:ARG:NE	2.28	0.55
12:AH:35:VAL:HG23	12:AH:37:LEU:HD12	1.89	0.55
14:AJ:27:ASP:HB2	14:AJ:35:VAL:HB	1.88	0.55
31:Ab:107:ARG:HB2	31:Ab:132:LEU:HD12	1.89	0.55
41:BA:61:LEU:HB3	41:BA:70:HIS:HB3	1.88	0.55
41:BA:98:ARG:HD2	73:BA:307:HOH:O	2.03	0.55
43:BC:153:PHE:CZ	43:BC:155:LYS:HE3	2.42	0.55
48:BH:17:TYR:CE1	48:BH:22:PRO:HB3	2.42	0.55
50:BJ:42:GLY:HA3	50:BJ:63:GLN:HE21	1.70	0.55
2:3:612:VAL:N	2:3:621:GLY:O	2.37	0.55
3:1:521:A:H2'	3:1:522:A:C8	2.42	0.55
3:1:1292:C:H2'	3:1:1293:G:H8	1.71	0.55
3:1:1516:A:O2'	3:1:1527:U:O2	2.24	0.55
3:1:1559:C:OP2	32:Ac:63:ARG:NH1	2.26	0.55
3:1:3000:G:C5'	73:1:5161:HOH:O	2.55	0.55
4:4:1487:U:OP1	64:BX:8:ARG:HD3	2.07	0.55
45:BE:40:LEU:HD13	45:BE:80:ILE:HD11	1.87	0.55
50:BJ:113:ALA:HB1	50:BJ:127:ALA:HB1	1.89	0.55
66:BZ:71:ALA:HB1	66:BZ:73:ARG:HH22	1.72	0.55
3:1:722:A:O2'	3:1:755:G:O2'	2.14	0.55
3:1:980:A:H2'	3:1:981:G:O4'	2.07	0.55
3:1:1136:G:N2	21:AR:39:SER:HB2	2.21	0.55
4:4:438:G:N2	62:BV:36:THR:OG1	2.37	0.55
4:4:830:A:H2'	4:4:831:A:C8	2.42	0.55
5:AA:5:ILE:HG22	5:AA:198:ALA:O	2.06	0.55
11:AG:2:ILE:HD13	11:AG:133:LEU:HD23	1.87	0.55
14:AK:4:VAL:HG22	21:AR:74:LYS:NZ	2.22	0.55
18:AO:73:LYS:HD3	18:AO:173:ARG:O	2.07	0.55
20:AQ:20:LYS:HG3	20:AQ:50:GLU:HG2	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:Ab:93:PRO:HG3	31:Ab:119:GLU:HG3	1.87	0.55
41:BA:154:VAL:HG23	41:BA:179:LEU:HD21	1.87	0.55
42:BB:185:ARG:NH2	42:BB:187:GLU:OE2	2.39	0.55
47:BG:6:LEU:N	47:BG:19:PHE:O	2.37	0.55
63:BW:72:LYS:HG2	63:BW:73:TYR:CD1	2.42	0.55
3:1:776:A:H2'	3:1:777:C:C6	2.42	0.55
3:1:792:A:N3	3:1:2557:U:O2'	2.34	0.55
3:1:1838:C:H2'	38:Ai:8:ILE:HD11	1.89	0.55
3:1:2046:U:H2'	73:1:4403:HOH:O	2.06	0.55
3:1:2915:A:H2'	3:1:2916:A:C8	2.42	0.55
4:4:674:OMG:H2'	4:4:675:G:C8	2.42	0.55
4:4:1039:A:OP1	46:BF:91:LYS:HE2	2.06	0.55
15:AL:92:ARG:HG3	15:AL:104:LEU:HD21	1.89	0.55
16:AM:177:LYS:CG	16:AM:178:THR:HG23	2.37	0.55
18:AO:72:TRP:HE3	18:AO:187:VAL:HG21	1.72	0.55
28:AY:54:MET:HA	28:AY:54:MET:HE3	1.88	0.55
29:AZ:43:PRO:HD2	29:AZ:82:MET:SD	2.46	0.55
32:Ac:40:THR:HB	32:Ac:42:GLN:OE1	2.06	0.55
34:Ae:54:ILE:HG23	34:Ae:64:VAL:HG11	1.88	0.55
59:BS:50:VAL:O	59:BS:54:ILE:HG13	2.07	0.55
62:BV:16:GLU:OE2	62:BV:23:LYS:HB3	2.07	0.55
66:BZ:48:LEU:HD22	66:BZ:70:GLU:HG2	1.89	0.55
2:3:479:LYS:NZ	2:3:598:LYS:O	2.26	0.55
3:1:1265:A:H5'	11:AG:98:VAL:HG13	1.89	0.55
4:4:77:C:H2'	4:4:78:G:C8	2.41	0.55
4:4:873:A:H2'	4:4:874:A:C8	2.41	0.55
4:4:1397:C:H2'	4:4:1398:G:O4'	2.06	0.55
8:AD:20:GLU:HB3	8:AD:136:ARG:HG2	1.89	0.55
25:AV:108:LEU:HD22	25:AV:117:ILE:HD11	1.88	0.55
38:Ai:39:ARG:HA	38:Ai:45:SER:O	2.07	0.55
41:BA:151:ILE:O	41:BA:155:THR:OG1	2.14	0.55
48:BH:216:GLU:HB3	66:BZ:65:ARG:NH2	2.21	0.55
51:BK:56:GLN:HA	51:BK:59:LEU:HD12	1.88	0.55
51:BK:56:GLN:O	51:BK:60:ILE:HG12	2.07	0.55
53:BM:94:GLY:O	53:BM:96:LYS:HE3	2.07	0.55
3:1:846:G:O2'	3:1:881:G:H4'	2.06	0.55
3:1:1662:G:N2	40:Ak:40:GLU:OE1	2.38	0.55
3:1:2630:C:O2'	3:1:2631:C:H5'	2.07	0.55
4:4:1313:G:O2'	4:4:1339:G:O6	2.17	0.55
8:AD:148:ARG:HD2	18:AO:109:ARG:HH21	1.72	0.55
28:AY:169:PRO:HG3	39:Aj:75:TYR:CZ	2.42	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:Ae:16:GLU:HG2	34:Ae:60:LYS:HE2	1.87	0.55
44:BD:59:ALA:O	44:BD:63:MET:HG3	2.07	0.55
47:BG:32:LEU:O	47:BG:106:ILE:HG13	2.07	0.55
47:BG:50:PRO:O	47:BG:53:VAL:HG12	2.06	0.55
54:BN:91:ASP:OD1	67:Ba:11:GLY:HA2	2.06	0.55
60:BT:65:PRO:HA	60:BT:68:ARG:HG2	1.89	0.55
60:BT:111:ASN:HB2	60:BT:113:ILE:O	2.06	0.55
1:2:37:G:O2'	1:2:38:G:H5'	2.07	0.54
3:1:822:A:O2'	38:Ai:10:GLY:O	2.18	0.54
3:1:2399:A:H62	3:1:2456:U:H3	1.53	0.54
4:4:489:OMC:HM22	4:4:490:G:H5'	1.88	0.54
8:AD:12:HIS:HB2	8:AD:15:LYS:HD2	1.89	0.54
8:AD:80:LYS:HA	8:AD:83:GLU:OE2	2.06	0.54
29:AZ:52:TYR:CE2	32:Ac:83:ARG:HG2	2.42	0.54
41:BA:22:TRP:HE1	53:BM:43:VAL:HA	1.71	0.54
42:BB:19:ALA:CB	42:BB:168:LYS:HD2	2.36	0.54
45:BE:196:GLU:HG3	58:BR:143:THR:OG1	2.07	0.54
49:BI:78:ARG:HB3	49:BI:124:VAL:CG1	2.37	0.54
3:1:720:C:O2'	3:1:757:U:OP1	2.20	0.54
3:1:762:A:H2'	3:1:763:A:C8	2.42	0.54
4:4:481:A:H1'	67:Ba:13:VAL:CG2	2.37	0.54
4:4:1284:A:O2'	60:BT:95:ASP:OD2	2.25	0.54
8:AD:25:ASN:O	8:AD:26:ILE:HD13	2.07	0.54
10:AF:34:ALA:HA	10:AF:37:ILE:HD12	1.89	0.54
20:AQ:109:LEU:HD21	20:AQ:117:LEU:HD12	1.89	0.54
44:BD:115:MET:HE1	44:BD:152:GLU:O	2.08	0.54
51:BK:8:GLN:NE2	51:BK:9:GLU:O	2.39	0.54
2:3:324:PRO:HA	2:3:638:THR:OG1	2.07	0.54
3:1:36:C:H2'	3:1:37:G:C8	2.42	0.54
3:1:145:G:H2'	3:1:146:C:C6	2.43	0.54
3:1:511:A:H5''	25:AV:92:VAL:HG21	1.89	0.54
3:1:1685:C:H2'	3:1:1686:G:C8	2.42	0.54
3:1:2361:G:O2'	3:1:2610:PSU:OP1	2.24	0.54
3:1:2540:U:OP1	37:Ah:59:ALA:N	2.34	0.54
4:4:457:U:H1'	73:4:3289:HOH:O	2.07	0.54
4:4:1475:G:H2'	4:4:1477:MA6:OP2	2.07	0.54
5:AA:60:ASN:OD1	5:AA:62:VAL:HG23	2.07	0.54
8:AD:65:ARG:N	8:AD:68:GLU:OE2	2.29	0.54
41:BA:90:ARG:HD2	41:BA:202:TYR:CZ	2.43	0.54
42:BB:90:CYS:O	42:BB:91:LYS:C	2.45	0.54
45:BE:162:ASP:OD1	45:BE:169:LYS:HB2	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:BM:135:GLY:N	73:BM:201:HOH:O	2.39	0.54
55:BO:113:LYS:HG3	60:BT:19:THR:CG2	2.38	0.54
2:3:604:LEU:HD22	2:3:625:LYS:HG2	1.88	0.54
3:1:1074:U:H3'	3:1:1075:G:H5'	1.87	0.54
3:1:1090:U:H2'	3:1:1091:C:C6	2.42	0.54
3:1:2048:A:H2'	3:1:2049:A:C8	2.42	0.54
3:1:2915:A:O2'	3:1:2916:A:O4'	2.16	0.54
3:1:2963:C:H5'	6:AB:282:LYS:HG3	1.90	0.54
4:4:1012:G:N7	4:4:1165:U:H3'	2.22	0.54
14:AJ:6:ASP:HB3	14:AJ:61:LYS:NZ	2.23	0.54
18:AO:73:LYS:CG	18:AO:173:ARG:HB3	2.37	0.54
23:AT:17:VAL:HG22	23:AT:130:ILE:HG12	1.90	0.54
43:BC:198:ARG:HH22	59:BS:40:ASP:CG	2.14	0.54
47:BG:126:PRO:HB2	68:Bb:10:ALA:HB1	1.90	0.54
49:BI:83:TYR:HB3	49:BI:84:ARG:NH1	2.23	0.54
50:BJ:70:TYR:HE1	50:BJ:75:ARG:HA	1.72	0.54
51:BK:9:GLU:O	51:BK:10:ASN:C	2.49	0.54
57:BQ:11:ARG:O	65:BY:2:PRO:HD2	2.08	0.54
1:2:52:C:OP2	18:AO:115:ARG:NH2	2.33	0.54
2:3:487:VAL:CG2	2:3:593:VAL:HA	2.38	0.54
3:1:2312:C:H2'	3:1:2313:C:H6	1.73	0.54
3:1:2704:OMC:HM22	3:1:2705:C:O4'	2.08	0.54
3:1:2716:A:C4'	73:1:4958:HOH:O	2.55	0.54
4:4:452:G:H2'	4:4:453:A:C8	2.43	0.54
4:4:1425:C:H2'	4:4:1426:G:O4'	2.08	0.54
4:4:1446:G:H2'	4:4:1447:G:H5''	1.89	0.54
9:AE:95:LYS:NZ	36:Ag:12:ILE:HG13	2.23	0.54
41:BA:119:LYS:CD	73:BA:320:HOH:O	2.55	0.54
47:BG:21:ILE:HG23	47:BG:25:LEU:HB2	1.88	0.54
56:BP:19:CYS:HB2	56:BP:22:CYS:O	2.08	0.54
60:BT:104:GLY:O	60:BT:105:LEU:HD23	2.07	0.54
2:3:598:LYS:HE3	2:3:601:LEU:HD22	1.90	0.54
3:1:1796:U:H2'	3:1:1797:G:O4'	2.06	0.54
3:1:2753:A:H2'	3:1:2754:G:O4'	2.08	0.54
4:4:11:A:H2'	4:4:12:U:H5'	1.87	0.54
4:4:318:G:OP1	50:BJ:26:THR:HG23	2.07	0.54
4:4:789:A:H2'	4:4:790:G:O4'	2.07	0.54
73:4:4029:HOH:O	57:BQ:107:LYS:CE	2.55	0.54
8:AD:13:PRO:O	8:AD:16:ARG:HG2	2.07	0.54
45:BE:196:GLU:HB3	45:BE:209:ALA:HB3	1.88	0.54
52:BL:50:LEU:HD12	56:BP:32:TYR:CZ	2.43	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:BN:133:SER:O	54:BN:137:ILE:HD12	2.08	0.54
56:BP:27:ALA:HB3	56:BP:38:ARG:HB3	1.88	0.54
2:3:485:VAL:HG12	2:3:486:LYS:O	2.08	0.54
3:1:1473:C:O2'	3:1:1515:A:H2'	2.08	0.54
3:1:1570:U:H2'	3:1:1571:C:C6	2.43	0.54
3:1:2001:A:H2'	3:1:2002:A:O4'	2.08	0.54
3:1:2040:A:C2'	3:1:2041:C:H5'	2.37	0.54
3:1:2194:U:H2'	3:1:2195:U:C6	2.43	0.54
4:4:14:C:H5'	46:BF:140:SER:OG	2.08	0.54
14:AJ:37:THR:CB	14:AJ:47:ARG:HG3	2.37	0.54
43:BC:173:ARG:NH2	73:BC:301:HOH:O	2.37	0.54
44:BD:80:TYR:HB2	44:BD:85:ILE:HD11	1.90	0.54
54:BN:132:VAL:CG1	54:BN:137:ILE:HD11	2.38	0.54
2:3:460:ASP:OD1	2:3:464:GLN:N	2.28	0.54
3:1:338:A:O2'	3:1:339:U:H2'	2.08	0.54
3:1:2537:OMG:HM22	3:1:2538:OMC:O4'	2.08	0.54
3:1:2849:G:H2'	3:1:2850:A:C8	2.43	0.54
73:1:4981:HOH:O	31:Ab:58:ARG:HD2	2.07	0.54
73:1:5207:HOH:O	19:AP:44:ARG:HG3	2.07	0.54
4:4:507:G:N1	67:Ba:28:LEU:O	2.40	0.54
4:4:1171:U:C1'	43:BC:185:ILE:HD11	2.38	0.54
6:AB:92:LEU:HB3	11:AG:172:ALA:HB2	1.89	0.54
11:AG:27:MET:HA	11:AG:54:LEU:HD22	1.89	0.54
13:AI:103:GLU:HG3	26:AW:21:TYR:OH	2.07	0.54
40:Ak:10:LEU:HD13	40:Ak:26:PHE:CE1	2.43	0.54
41:BA:60:THR:HG22	41:BA:62:TYR:H	1.71	0.54
44:BD:80:TYR:HB2	44:BD:88:PRO:HB3	1.89	0.54
45:BE:229:THR:HG22	45:BE:230:GLU:H	1.73	0.54
48:BH:216:GLU:HB3	66:BZ:65:ARG:HH22	1.73	0.54
66:BZ:31:VAL:HG11	66:BZ:51:ASN:HB3	1.89	0.54
2:3:329:THR:HA	2:3:481:ARG:HD3	1.90	0.54
3:1:1563:G:H4'	3:1:1564:G:O5'	2.08	0.54
3:1:1663:C:H2'	3:1:1664:G:H8	1.72	0.54
3:1:1989:A:OP2	3:1:2009:G:N2	2.33	0.54
4:4:7:OMG:HM22	4:4:8:U:H5''	1.90	0.54
4:4:129:G:H2'	4:4:130:A:H8	1.73	0.54
4:4:689:A:H2'	4:4:690:A:C8	2.43	0.54
4:4:1050:U:O2'	4:4:1052:A:OP2	2.15	0.54
21:AR:74:LYS:NZ	21:AR:76:VAL:HG22	2.23	0.54
45:BE:26:ARG:O	45:BE:77:LYS:HD2	2.08	0.54
46:BF:153:GLY:N	46:BF:171:ASP:OD1	2.22	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:BG:107:THR:HG22	47:BG:110:ILE:CD1	2.38	0.54
2:3:455:TYR:CB	2:3:470:THR:HG22	2.37	0.54
3:1:651:G:H2'	3:1:2150:C:C5	2.42	0.54
3:1:1234:C:H2'	3:1:1235:C:C6	2.43	0.54
4:4:677:C:O2'	53:BM:128:IAS:HB3	2.08	0.54
4:4:879:A2M:H2'	4:4:880:A2M:C8	2.38	0.54
18:AO:144:ARG:HD3	18:AO:146:GLU:OE2	2.08	0.54
41:BA:41:LEU:CD2	41:BA:59:VAL:HG11	2.38	0.54
41:BA:76:ARG:HG3	41:BA:92:LYS:HB3	1.90	0.54
47:BG:64:GLU:OE2	47:BG:64:GLU:N	2.30	0.54
51:BK:8:GLN:NE2	51:BK:11:PRO:HD2	2.23	0.54
2:3:346:VAL:HG23	2:3:368:VAL:O	2.08	0.53
2:3:603:LYS:O	2:3:606:GLU:HG2	2.08	0.53
3:1:186:G:H5''	12:AH:123:PHE:CD1	2.43	0.53
3:1:265:C:H1'	73:1:4001:HOH:O	2.08	0.53
3:1:602:G:N2	3:1:605:A:OP2	2.39	0.53
3:1:741:C:H2'	3:1:742:C:H6	1.74	0.53
3:1:878:C:H2'	3:1:879:A:O4'	2.08	0.53
3:1:886:G:H1'	3:1:1510:A:N6	2.23	0.53
3:1:931:C:H2'	3:1:932:C:C6	2.43	0.53
3:1:2114:U:H2'	3:1:2115:OMC:O4'	2.08	0.53
3:1:2358:G:H2'	3:1:2359:C:C6	2.42	0.53
3:1:2836:C:OP1	6:AB:208:LYS:NZ	2.38	0.53
4:4:684:U:O4'	64:BX:11:LYS:HB2	2.08	0.53
4:4:901:A:H2'	4:4:902:C:H6	1.71	0.53
4:4:1118:A:H5''	52:BL:47:THR:CG2	2.38	0.53
14:AJ:62:ILE:CD1	14:AJ:64:ILE:HG12	2.38	0.53
43:BC:182:LYS:O	43:BC:182:LYS:NZ	2.30	0.53
3:1:1859:U:H2'	3:1:1860:C:O4'	2.07	0.53
3:1:2667:OMG:O4'	3:1:2696:G:O2'	2.20	0.53
5:AA:147:GLU:N	5:AA:147:GLU:OE1	2.42	0.53
18:AO:151:TYR:OH	18:AO:166:ARG:NH1	2.41	0.53
20:AQ:103:LEU:HA	20:AQ:108:LYS:NZ	2.22	0.53
21:AR:36:VAL:HG13	21:AR:40:ARG:HD2	1.90	0.53
25:AV:77:ILE:HD11	25:AV:101:VAL:HG11	1.90	0.53
39:Aj:105:ASN:HB2	39:Aj:111:LEU:HD11	1.90	0.53
3:1:172:A:H2'	3:1:173:A:H8	1.73	0.53
3:1:465:C:H2'	3:1:466:G:C8	2.43	0.53
3:1:2627:U:H2'	3:1:2628:OMU:H6	1.89	0.53
4:4:8:U:H5	4:4:880:A2M:N7	2.06	0.53
4:4:17:C:OP1	4:4:850:G:H5'	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:385:C:H2'	4:4:386:A:O4'	2.08	0.53
4:4:402:C:H2'	4:4:403:C:C6	2.44	0.53
4:4:1243:G:H1'	4:4:1248:C:O2	2.09	0.53
4:4:1435:G:H2'	4:4:1436:C:H6	1.74	0.53
8:AD:96:ILE:CD1	8:AD:177:VAL:HG22	2.34	0.53
8:AD:147:ARG:O	8:AD:151:ARG:HG3	2.07	0.53
9:AE:28:TYR:CE2	9:AE:50:MET:HG3	2.44	0.53
9:AE:32:VAL:HG12	9:AE:86:VAL:HG21	1.91	0.53
14:AJ:16:GLY:O	32:Ac:63:ARG:HG3	2.07	0.53
14:AK:75:LYS:HA	14:AK:78:GLU:HG3	1.89	0.53
18:AO:52:ARG:CG	18:AO:57:GLU:HG2	2.38	0.53
32:Ac:84:ARG:HB2	32:Ac:84:ARG:HH11	1.73	0.53
41:BA:166:PHE:O	41:BA:170:VAL:HG23	2.09	0.53
42:BB:127:ARG:HD3	42:BB:150:ASP:O	2.08	0.53
45:BE:193:GLN:OE1	45:BE:211:ARG:NH1	2.40	0.53
46:BF:201:LYS:NZ	49:BI:18:GLU:OE2	2.40	0.53
49:BI:78:ARG:HB3	49:BI:124:VAL:HG13	1.91	0.53
57:BQ:25:TRP:CD1	65:BY:30:VAL:HG11	2.43	0.53
62:BV:88:GLU:HB2	62:BV:93:LEU:HD21	1.90	0.53
1:2:82:G:N2	1:2:83:U:O4	2.29	0.53
2:3:435:VAL:HB	2:3:439:ALA:CB	2.38	0.53
2:3:442:GLU:HG3	2:3:632:LEU:O	2.09	0.53
2:3:549:GLU:HA	2:3:565:THR:OG1	2.09	0.53
3:1:976:G:O2'	3:1:977:G:H5'	2.09	0.53
4:4:29:G:H2'	4:4:30:C:C6	2.43	0.53
4:4:75:C:OP2	4:4:213:G:H5''	2.08	0.53
4:4:314:C:H5''	45:BE:8:LEU:HD11	1.90	0.53
4:4:507:G:P	44:BD:39:ASN:HB2	2.48	0.53
4:4:790:G:C5'	42:BB:30:LYS:HD2	2.38	0.53
4:4:1089:A:H2'	4:4:1090:C:H5'	1.89	0.53
4:4:1250:C:OP2	4:4:1251:G:O2'	2.25	0.53
4:4:1258:C:H2'	4:4:1259:C:C6	2.43	0.53
4:4:1402:C:H2'	4:4:1403:C:C6	2.43	0.53
73:4:3663:HOH:O	55:BO:129:GLN:HA	2.08	0.53
23:AT:29:GLN:HA	23:AT:122:LEU:HD21	1.90	0.53
28:AY:44:MET:HE2	28:AY:142:PHE:CD2	2.43	0.53
40:Ak:8:GLU:HG2	40:Ak:64:PHE:CE2	2.43	0.53
52:BL:43:ILE:HG22	52:BL:45:LEU:HD23	1.90	0.53
61:BU:16:LEU:HD22	61:BU:60:MET:HE1	1.90	0.53
1:2:115:G:O2'	1:2:116:U:H5'	2.09	0.53
3:1:284:U:H3	10:AF:74:PRO:HD2	1.72	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1:603:U:OP2	14:AK:48:ARG:HD2	2.09	0.53
3:1:709:C:O2'	3:1:774:U:OP1	2.24	0.53
3:1:977:G:N3	3:1:2380:A:H2'	2.22	0.53
3:1:1514:A:H2'	3:1:1515:A:C8	2.43	0.53
4:4:501:C:OP1	67:Ba:23:LYS:HG2	2.07	0.53
8:AD:64:ILE:O	8:AD:65:ARG:NH1	2.41	0.53
9:AE:63:ASN:HB2	14:AK:31:GLU:OE1	2.08	0.53
9:AE:144:VAL:HG12	9:AE:152:VAL:HG13	1.90	0.53
12:AH:72:LEU:O	16:AM:176:LYS:HG2	2.09	0.53
15:AL:81:VAL:CG1	15:AL:122:MET:HB2	2.38	0.53
46:BF:11:PRO:HG3	46:BF:20:LYS:HD3	1.90	0.53
51:BK:76:ARG:HD3	73:BK:311:HOH:O	2.08	0.53
60:BT:77:ALA:O	60:BT:81:MET:N	2.40	0.53
3:1:1572:C:H2'	3:1:1573:C:C6	2.44	0.53
3:1:1668:A:OP2	34:Ae:26:TYR:OH	2.23	0.53
3:1:2017:OMG:HM22	3:1:2018:OMC:H5''	1.89	0.53
4:4:53:G:H2'	4:4:54:C:C6	2.43	0.53
4:4:652:G:O2'	4:4:653:C:H5'	2.09	0.53
5:AA:83:ASP:OD1	5:AA:83:ASP:N	2.27	0.53
11:AG:14:GLU:HG3	11:AG:41:LYS:HE3	1.91	0.53
14:AJ:71:GLU:O	14:AJ:75:LYS:HG3	2.08	0.53
27:AX:43:GLU:HG2	27:AX:44:LYS:HG2	1.90	0.53
47:BG:45:GLU:HG2	47:BG:46:LEU:HD12	1.90	0.53
50:BJ:65:ARG:HG2	50:BJ:66:TYR:CE1	2.43	0.53
55:BO:42:ARG:NH2	61:BU:47:MET:O	2.42	0.53
64:BX:18:GLU:OE1	64:BX:33:SER:OG	2.16	0.53
68:Bb:32:LYS:HG3	68:Bb:62:LEU:HD22	1.90	0.53
3:1:1075:G:H5''	3:1:1076:G:OP2	2.09	0.53
3:1:1416:G:OP1	3:1:1417:C:N4	2.37	0.53
3:1:2163:C:H2'	3:1:2164:C:C6	2.44	0.53
3:1:2367:G:O2'	3:1:2368:C:H5'	2.09	0.53
3:1:2425:C:OP1	8:AD:53:ARG:HD2	2.09	0.53
73:1:4216:HOH:O	23:AT:81:LYS:HD2	2.08	0.53
4:4:104:G:H2'	4:4:105:U:C6	2.44	0.53
4:4:171:G:C2'	4:4:172:C:H5''	2.38	0.53
4:4:1111:G:O2'	4:4:1112:C:H5'	2.09	0.53
4:4:1164:G:H2'	4:4:1165:U:C6	2.43	0.53
24:AU:18:GLU:O	24:AU:64:LYS:NZ	2.42	0.53
29:AZ:99:GLU:N	29:AZ:99:GLU:OE2	2.41	0.53
38:Ai:23:ILE:O	38:Ai:27:VAL:HG23	2.09	0.53
51:BK:33:MET:HE2	51:BK:35:ARG:NH1	2.23	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:BQ:96:LEU:HD13	57:BQ:150:ALA:HB2	1.91	0.53
63:BW:50:VAL:O	63:BW:54:ILE:HG13	2.07	0.53
3:1:230:C:OP2	3:1:2509:C:O2'	2.25	0.53
3:1:911:A:OP2	3:1:2191:A:O2'	2.27	0.53
3:1:1414:A:H1'	3:1:1416:G:OP2	2.08	0.53
3:1:1930:U:H2'	3:1:1931:C:H6	1.73	0.53
3:1:1963:U:H2'	3:1:1964:G:O4'	2.08	0.53
4:4:262:G:H2'	4:4:263:PSU:C6	2.43	0.53
4:4:409:U:OP2	67:Ba:31:ARG:NH1	2.40	0.53
4:4:860:G:H2'	4:4:861:C:C6	2.43	0.53
10:AF:37:ILE:CD1	10:AF:129:LEU:HD22	2.39	0.53
15:AL:85:ALA:O	15:AL:89:LYS:HG3	2.08	0.53
17:AN:79:LYS:HE2	17:AN:80:TYR:CE1	2.44	0.53
25:AV:76:ARG:HG3	25:AV:95:PRO:HB2	1.91	0.53
47:BG:45:GLU:HG2	47:BG:46:LEU:CD1	2.38	0.53
47:BG:64:GLU:OE1	47:BG:102:ARG:NH1	2.42	0.53
55:BO:100:LEU:O	55:BO:104:ARG:HG3	2.09	0.53
55:BO:119:ARG:HB2	55:BO:126:VAL:CG1	2.39	0.53
57:BQ:2:PRO:HA	57:BQ:117:LEU:CD1	2.38	0.53
3:1:340:G:H5'	3:1:359:U:O2'	2.08	0.53
3:1:860:U:OP1	6:AB:229:LYS:HD3	2.08	0.53
3:1:1290:C:H2'	3:1:1291:C:C6	2.43	0.53
4:4:664:A:H4'	4:4:665:A:C5'	2.39	0.53
11:AG:60:ARG:HG3	11:AG:152:VAL:HG11	1.91	0.53
13:AI:96:ASP:OD1	13:AI:96:ASP:N	2.31	0.53
13:AI:126:ALA:O	13:AI:130:THR:HG23	2.09	0.53
18:AO:39:LYS:HD2	18:AO:115:ARG:NH2	2.24	0.53
23:AT:34:TYR:CE2	23:AT:162:GLU:HB3	2.44	0.53
30:Aa:5:LYS:HD3	30:Aa:82:ASP:OD2	2.09	0.53
44:BD:80:TYR:HA	44:BD:85:ILE:HG13	1.90	0.53
51:BK:11:PRO:HA	73:BK:305:HOH:O	2.08	0.53
58:BR:34:VAL:HG11	58:BR:128:ILE:HG22	1.90	0.53
62:BV:46:LEU:HD23	62:BV:57:ILE:CG2	2.39	0.53
68:Bb:59:LYS:HB3	68:Bb:63:ARG:HH21	1.74	0.53
3:1:1631:G:O2'	3:1:1632:G:H5'	2.09	0.53
3:1:1833:A:H2'	3:1:1834:A:C8	2.43	0.53
3:1:2031:G:C2'	3:1:2032:U:H5'	2.40	0.53
3:1:2418:C:OP2	3:1:2419:A:O2'	2.15	0.53
18:AO:11:PHE:CD2	22:AS:25:MET:HE3	2.44	0.53
19:AP:66:ILE:CD1	19:AP:70:LEU:HD13	2.39	0.53
39:Aj:84:PRO:HD2	39:Aj:88:TRP:CE3	2.44	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:BG:26:ALA:O	47:BG:30:VAL:HG23	2.09	0.53
47:BG:74:GLY:O	47:BG:103:GLY:HA3	2.09	0.53
53:BM:25:SER:O	53:BM:99:GLY:N	2.37	0.53
66:BZ:31:VAL:CG1	66:BZ:51:ASN:HB3	2.38	0.53
3:1:1075:G:O2'	3:1:2378:A:OP2	2.22	0.52
3:1:1337:C:H5''	3:1:1339:G:O4'	2.09	0.52
4:4:1334:G:OP2	51:BK:126:LYS:HD3	2.09	0.52
4:4:1485:G:N7	53:BM:136:ARG:NH2	2.56	0.52
7:AC:28:PRO:O	7:AC:46:THR:OG1	2.16	0.52
14:AK:52:ILE:HB	21:AR:77:ARG:HH12	1.74	0.52
15:AL:103:ARG:CG	15:AL:125:PRO:HB2	2.39	0.52
31:Ab:15:ARG:HG3	31:Ab:18:ARG:HH12	1.74	0.52
42:BB:31:TYR:O	42:BB:35:ARG:HG2	2.09	0.52
45:BE:38:LEU:HD23	45:BE:43:VAL:HG23	1.89	0.52
50:BJ:85:ILE:HD12	50:BJ:98:ASN:HA	1.90	0.52
62:BV:36:THR:HG22	62:BV:37:PRO:HD2	1.91	0.52
64:BX:87:GLU:HA	64:BX:90:LYS:NZ	2.23	0.52
68:Bb:55:LEU:O	68:Bb:59:LYS:HG3	2.08	0.52
2:3:346:VAL:HG23	2:3:369:ASP:HA	1.92	0.52
3:1:83:G:C5	35:Af:32:LYS:HD2	2.44	0.52
3:1:237:A:O3'	12:AH:114:ARG:NH2	2.43	0.52
3:1:329:U:C6	25:AV:56:MET:HE3	2.44	0.52
3:1:2184:C:H2'	3:1:2185:C:C6	2.43	0.52
3:1:2863:G:N7	73:1:3765:HOH:O	2.40	0.52
4:4:481:A:N3	67:Ba:13:VAL:HG21	2.24	0.52
4:4:1137:G:H5'	59:BS:4:VAL:HG22	1.91	0.52
4:4:1243:G:H2'	4:4:1244:C:H5''	1.91	0.52
4:4:1380:C:H2'	4:4:1381:C:C6	2.44	0.52
70:4:3005:SPM:H122	73:4:3862:HOH:O	2.08	0.52
10:AF:37:ILE:HD12	10:AF:129:LEU:HD22	1.91	0.52
17:AN:78:THR:HG23	17:AN:83:ASP:OD1	2.09	0.52
25:AV:57:ARG:HB2	25:AV:100:LYS:HD2	1.92	0.52
45:BE:98:VAL:HG21	45:BE:108:LYS:HG3	1.91	0.52
45:BE:209:ALA:O	45:BE:210:LEU:HD23	2.09	0.52
45:BE:219:THR:HG22	45:BE:220:ILE:H	1.74	0.52
47:BG:7:VAL:HB	47:BG:114:ASN:HD22	1.74	0.52
55:BO:44:LEU:HD11	55:BO:66:ALA:CB	2.39	0.52
66:BZ:66:GLU:HG2	73:BZ:102:HOH:O	2.08	0.52
69:Bc:55:TYR:CZ	69:Bc:65:PRO:HD2	2.43	0.52
2:3:367:VAL:HG11	2:3:428:ALA:HB2	1.92	0.52
3:1:1557:A:N3	3:1:1628:C:O2'	2.37	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1:2041:C:H2'	3:1:2042:C:C6	2.43	0.52
3:1:2382:G:N7	73:1:3625:HOH:O	2.34	0.52
73:1:5424:HOH:O	12:AH:13:ILE:HD11	2.09	0.52
4:4:1273:U:O2'	55:BO:141:ALA:O	2.21	0.52
4:4:1298:A:O2'	55:BO:139:ALA:HB1	2.09	0.52
5:AA:102:MET:CE	38:Ai:77:LEU:HD21	2.40	0.52
8:AD:154:VAL:HB	8:AD:159:LEU:HD21	1.90	0.52
13:AI:144:VAL:HG21	26:AW:22:VAL:HG21	1.90	0.52
14:AJ:30:ASP:HB2	14:AJ:31:GLU:OE2	2.09	0.52
18:AO:62:LEU:HD11	18:AO:92:LYS:NZ	2.24	0.52
46:BF:12:LYS:O	46:BF:39:GLU:HG2	2.09	0.52
48:BH:138:THR:CG2	48:BH:208:ALA:HB1	2.40	0.52
54:BN:43:PRO:HA	54:BN:82:LYS:NZ	2.24	0.52
3:1:1790:C:C5'	3:1:1791:U:H5''	2.35	0.52
3:1:2840:G:H4'	13:AI:99:TRP:HH2	1.75	0.52
3:1:2959:G:H1'	73:1:6804:HOH:O	2.10	0.52
4:4:825:A:H2'	4:4:826:G:O4'	2.09	0.52
4:4:1486:C:O2'	4:4:1487:U:H5'	2.08	0.52
7:AC:173:VAL:HB	7:AC:271:LEU:HD11	1.91	0.52
9:AE:88:LYS:HB3	9:AE:193:HIS:HB3	1.92	0.52
41:BA:101:LEU:HD21	41:BA:131:LEU:HD22	1.91	0.52
42:BB:54:ILE:O	42:BB:58:LEU:HG	2.10	0.52
44:BD:87:ASP:HB3	44:BD:90:VAL:HG13	1.92	0.52
45:BE:38:LEU:HD23	45:BE:43:VAL:CG2	2.40	0.52
49:BI:40:VAL:HG22	49:BI:43:ARG:NH2	2.24	0.52
50:BJ:91:ASN:HB3	50:BJ:94:TYR:CD2	2.44	0.52
58:BR:60:GLU:OE1	58:BR:60:GLU:N	2.42	0.52
66:BZ:43:ASP:HB3	66:BZ:46:ARG:HG3	1.91	0.52
68:Bb:18:GLU:O	68:Bb:22:LEU:HG	2.09	0.52
1:2:50:C:H4'	18:AO:109:ARG:HD3	1.90	0.52
3:1:668:G:H4'	3:1:669:U:O5'	2.09	0.52
3:1:1469:U:C4	24:AU:55:PRO:HG3	2.44	0.52
3:1:1533:U:H5'	73:1:3685:HOH:O	2.09	0.52
3:1:2403:U:O2'	3:1:2489:G:N3	2.42	0.52
4:4:92:G:H21	4:4:358:G:H5'	1.75	0.52
4:4:1059:C:OP2	42:BB:101:ARG:HD2	2.09	0.52
4:4:1282:G:N2	4:4:1284:A:H3'	2.24	0.52
6:AB:132:ALA:O	6:AB:135:GLU:HG2	2.10	0.52
14:AK:5:ILE:HD13	14:AK:57:PRO:HG3	1.91	0.52
14:AK:13:LYS:HD3	14:AK:18:GLU:HG2	1.90	0.52
38:Ai:39:ARG:NH2	38:Ai:46:LEU:HB2	2.25	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:BB:19:ALA:HB2	42:BB:168:LYS:HD2	1.89	0.52
48:BH:75:TYR:HB3	48:BH:81:GLY:O	2.09	0.52
50:BJ:38:ILE:CD1	50:BJ:99:TYR:HB3	2.39	0.52
55:BO:6:ARG:NH1	55:BO:9:VAL:HG22	2.25	0.52
59:BS:59:LYS:O	59:BS:63:ALA:N	2.42	0.52
60:BT:103:VAL:HA	60:BT:120:ILE:CG2	2.39	0.52
3:1:215:C:H2'	3:1:216:C:C6	2.45	0.52
3:1:1663:C:H2'	3:1:1664:G:C8	2.44	0.52
3:1:2628:OMU:HM22	3:1:2629:C:O4'	2.10	0.52
3:1:2752:G:H4'	6:AB:98:TYR:CE1	2.44	0.52
4:4:949:A:H5'	4:4:950:C:OP2	2.09	0.52
10:AF:72:VAL:CG2	10:AF:75:PRO:HA	2.40	0.52
27:AX:23:LEU:O	27:AX:27:ARG:HG3	2.10	0.52
49:BI:27:ILE:HG22	49:BI:30:VAL:HG12	1.90	0.52
60:BT:23:PRO:HA	60:BT:26:TRP:CD2	2.45	0.52
62:BV:27:VAL:CG2	62:BV:73:ALA:HB3	2.40	0.52
64:BX:54:GLU:O	64:BX:55:LYS:HG2	2.09	0.52
65:BY:52:THR:CG2	65:BY:57:ILE:HD13	2.39	0.52
2:3:391:SER:O	2:3:391:SER:OG	2.26	0.52
3:1:444:A:H1'	3:1:2001:A:C2	2.45	0.52
3:1:1398:A:N3	3:1:2124:G:O2'	2.36	0.52
3:1:2217:G:H1	3:1:2311:U:H3	1.58	0.52
4:4:193:A:H2'	4:4:194:A:C8	2.45	0.52
4:4:1463:G:OP1	4:4:1466:A:H4'	2.10	0.52
7:AC:61:ARG:NH1	7:AC:138:GLU:OE2	2.43	0.52
14:AJ:18:GLU:OE2	14:AJ:45:VAL:HG13	2.09	0.52
14:AJ:21:ARG:HD3	14:AJ:43:SER:O	2.10	0.52
14:AK:72:GLU:O	14:AK:75:LYS:HG3	2.10	0.52
51:BK:64:ASP:HA	51:BK:67:LYS:HD2	1.92	0.52
58:BR:5:LYS:O	58:BR:6:LEU:HD23	2.09	0.52
63:BW:83:VAL:O	63:BW:87:LEU:HG	2.10	0.52
3:1:646:G:H5''	31:Ab:51:THR:CG2	2.38	0.52
3:1:669:U:H2'	3:1:670:U:C6	2.44	0.52
3:1:1751:A:H1'	35:Af:45:ARG:HH22	1.75	0.52
3:1:2561:A:H1'	73:1:3538:HOH:O	2.10	0.52
4:4:157:C:H2'	4:4:158:C:H6	1.75	0.52
4:4:1019:C:H4'	52:BL:56:ARG:O	2.10	0.52
4:4:1252:U:O2'	61:BU:76:THR:HG22	2.10	0.52
4:4:1409:C:H2'	4:4:1410:C:C6	2.45	0.52
8:AD:111:ILE:HD13	8:AD:117:LEU:HD21	1.92	0.52
9:AE:1:MET:HG3	9:AE:2:HIS:O	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:AF:48:LYS:HB2	10:AF:115:VAL:CG1	2.39	0.52
17:AN:73:SER:HB3	17:AN:156:ALA:HB2	1.92	0.52
27:AX:60:THR:O	27:AX:64:GLU:HG3	2.09	0.52
34:Ae:8:VAL:HG12	34:Ae:9:GLU:OE1	2.10	0.52
59:BS:44:LYS:O	59:BS:48:ASN:ND2	2.43	0.52
3:1:510:A:H1'	3:1:512:G:H5''	1.92	0.52
3:1:971:C:H42	3:1:1044:A:H61	1.58	0.52
3:1:1121:A:H2'	3:1:1122:G:O4'	2.10	0.52
3:1:1915:U:OP2	3:1:1920:A:N6	2.35	0.52
4:4:183:C:H4'	45:BE:128:VAL:O	2.09	0.52
6:AB:246:ALA:HB3	11:AG:78:TYR:CE2	2.45	0.52
11:AG:15:LYS:CD	11:AG:43:GLU:HG3	2.40	0.52
28:AY:91:THR:HG23	28:AY:94:TYR:H	1.73	0.52
65:BY:4:ARG:O	65:BY:8:VAL:HG12	2.10	0.52
3:1:130:C:H2'	3:1:131:G:O4'	2.09	0.52
3:1:1588:A:H2'	3:1:1589:G:O4'	2.10	0.52
3:1:2405:G:H2'	3:1:2406:G:C8	2.45	0.52
4:4:90:C:H2'	4:4:91:G:O4'	2.09	0.52
4:4:479:U:OP2	4:4:491:G:O2'	2.20	0.52
4:4:780:A:H3'	4:4:781:U:H5'	1.91	0.52
4:4:1226:G:H4'	4:4:1249:C:O2'	2.10	0.52
7:AC:32:LYS:HG2	7:AC:40:TYR:CE1	2.44	0.52
10:AF:130:VAL:O	10:AF:134:ASN:HB2	2.11	0.52
14:AJ:91:LYS:NZ	32:Ac:65:TYR:OH	2.34	0.52
32:Ac:50:LYS:HE2	32:Ac:50:LYS:HA	1.92	0.52
51:BK:10:ASN:HB2	51:BK:11:PRO:HD2	1.89	0.52
64:BX:30:VAL:HG11	64:BX:34:LYS:HD3	1.92	0.52
2:3:516:GLU:O	2:3:626:MET:HE2	2.10	0.51
3:1:1308:G:H2'	3:1:1309:C:C6	2.45	0.51
4:4:474:U:H2'	4:4:475:OMG:C8	2.44	0.51
4:4:1115:A:H1'	51:BK:26:ARG:NH1	2.24	0.51
9:AE:47:PRO:CG	9:AE:68:GLU:HG2	2.39	0.51
13:AI:133:TRP:CB	13:AI:136:ILE:HD13	2.39	0.51
22:AS:3:LYS:NZ	22:AS:4:ARG:O	2.43	0.51
40:Ak:66:ILE:HG22	40:Ak:69:LEU:H	1.75	0.51
46:BF:61:GLN:OE1	46:BF:68:GLU:HG3	2.09	0.51
50:BJ:3:LEU:HD12	50:BJ:35:PRO:HD3	1.91	0.51
60:BT:44:MET:O	60:BT:48:ILE:HD13	2.10	0.51
62:BV:57:ILE:HG12	62:BV:77:VAL:HG13	1.90	0.51
3:1:186:G:OP1	12:AH:130:ARG:NH2	2.40	0.51
3:1:2117:C:H4'	3:1:2118:G:OP1	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1:2588:C:OP2	3:1:2589:C:N4	2.26	0.51
3:1:2886:C:H2'	3:1:2887:G:O4'	2.10	0.51
70:1:3103:SPM:H62	73:1:7782:HOH:O	2.09	0.51
4:4:218:C:H2'	4:4:219:A:C8	2.45	0.51
4:4:380:G:H2'	4:4:381:C:C6	2.45	0.51
4:4:1080:C:H2'	4:4:1081:U:C6	2.45	0.51
4:4:1391:C:H2'	4:4:1392:C:H6	1.75	0.51
6:AB:332:TRP:CH2	6:AB:334:SER:HA	2.45	0.51
8:AD:89:LEU:HD11	8:AD:173:LEU:HD23	1.92	0.51
8:AD:166:VAL:CG1	8:AD:177:VAL:HG11	2.41	0.51
9:AE:91:ARG:N	9:AE:192:GLU:O	2.38	0.51
18:AO:150:GLU:HA	18:AO:153:LYS:CE	2.38	0.51
27:AX:14:MET:HE3	27:AX:18:GLU:CB	2.40	0.51
45:BE:203:ARG:O	45:BE:221:LEU:HD23	2.11	0.51
68:Bb:27:LYS:HB3	68:Bb:30:GLU:CD	2.36	0.51
2:3:355:LYS:HD2	2:3:359:ARG:NH2	2.24	0.51
3:1:433:A:H2'	3:1:434:C:C6	2.45	0.51
3:1:601:G:H4'	39:Aj:17:TYR:CE2	2.46	0.51
3:1:2705:C:H2'	3:1:2706:G:C8	2.45	0.51
3:1:2917:C:H2'	3:1:2918:C:C6	2.45	0.51
4:4:887:G:H4'	46:BF:64:THR:HA	1.91	0.51
4:4:1006:G:O2'	4:4:1181:C:OP2	2.15	0.51
4:4:1045:OMC:HM22	4:4:1046:C:O4'	2.11	0.51
4:4:1065:G:H2'	4:4:1066:C:C6	2.45	0.51
4:4:1143:G:H2'	4:4:1144:G:O4'	2.10	0.51
8:AD:23:VAL:HG12	8:AD:75:THR:HG22	1.92	0.51
14:AK:40:LYS:C	14:AK:42:LEU:H	2.18	0.51
15:AL:103:ARG:HG2	15:AL:125:PRO:HB2	1.92	0.51
18:AO:85:LEU:O	18:AO:89:VAL:HG22	2.10	0.51
21:AR:16:LYS:HE3	21:AR:18:VAL:HG23	1.93	0.51
24:AU:72:MET:HE1	24:AU:81:LEU:HD11	1.93	0.51
39:Aj:78:VAL:HG12	39:Aj:143:ILE:HD13	1.92	0.51
39:Aj:103:GLU:O	39:Aj:107:ARG:HG3	2.11	0.51
49:BI:51:GLU:CG	49:BI:62:VAL:HB	2.39	0.51
50:BJ:108:THR:N	50:BJ:111:GLY:O	2.42	0.51
51:BK:20:LYS:HE2	51:BK:85:ILE:HD13	1.93	0.51
56:BP:18:ARG:O	56:BP:28:VAL:HG23	2.10	0.51
56:BP:29:ILE:HG23	56:BP:34:LEU:O	2.11	0.51
57:BQ:34:GLU:O	57:BQ:38:VAL:HG23	2.10	0.51
62:BV:114:GLU:OE1	62:BV:114:GLU:N	2.44	0.51
1:2:73:C:OP1	18:AO:5:ALA:HB2	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:437:GLU:OE1	2:3:460:ASP:HA	2.10	0.51
2:3:637:VAL:HG22	2:3:641:MET:CE	2.40	0.51
3:1:487:U:OP1	35:Af:34:ARG:NH1	2.40	0.51
3:1:2312:C:H2'	3:1:2313:C:C6	2.45	0.51
3:1:2405:G:H2'	3:1:2406:G:H8	1.75	0.51
3:1:2617:A:N6	73:1:3597:HOH:O	2.32	0.51
4:4:479:U:H4'	4:4:480:C:O2	2.10	0.51
5:AA:42:GLU:OE1	5:AA:44:LEU:HD21	2.11	0.51
8:AD:23:VAL:CG2	8:AD:134:CYS:HB2	2.41	0.51
14:AJ:10:VAL:O	14:AJ:58:THR:HG22	2.10	0.51
24:AU:56:ARG:HG2	35:Af:18:ASN:OD1	2.10	0.51
31:Ab:96:LEU:CD1	31:Ab:123:LYS:HG2	2.40	0.51
60:BT:127:HIS:HB3	60:BT:131:GLU:OE1	2.10	0.51
64:BX:21:VAL:HG22	64:BX:22:TYR:H	1.75	0.51
3:1:582:C:H2'	3:1:583:C:C6	2.45	0.51
3:1:584:C:O2'	3:1:585:U:H5'	2.10	0.51
3:1:621:G:OP2	31:Ab:18:ARG:NH2	2.36	0.51
3:1:741:C:H2'	3:1:742:C:C6	2.46	0.51
3:1:1402:A:O2'	3:1:1403:A:H2'	2.09	0.51
3:1:1866:G:H2'	3:1:1868:A:H62	1.75	0.51
3:1:2028:G:O2'	3:1:2029:G:H5'	2.11	0.51
3:1:2594:C:H2'	3:1:2595:G:H5'	1.92	0.51
4:4:424:C:O2'	4:4:425:C:H5'	2.10	0.51
4:4:1100:C:O2'	4:4:1101:G:O5'	2.28	0.51
4:4:1432:G:C2'	4:4:1433:G:H5'	2.39	0.51
14:AK:65:LYS:CE	14:AK:68:ALA:HA	2.38	0.51
39:Aj:115:MET:O	39:Aj:118:PRO:HD2	2.09	0.51
41:BA:60:THR:O	41:BA:64:ILE:HG12	2.11	0.51
41:BA:90:ARG:NH1	41:BA:206:GLU:OE2	2.43	0.51
42:BB:90:CYS:C	42:BB:92:PHE:N	2.67	0.51
49:BI:72:ILE:HD12	49:BI:129:VAL:HG13	1.92	0.51
55:BO:6:ARG:NH1	55:BO:8:ILE:O	2.41	0.51
57:BQ:22:VAL:HG22	57:BQ:66:ILE:HG13	1.92	0.51
58:BR:2:THR:HA	58:BR:42:ASP:OD1	2.10	0.51
62:BV:117:GLU:O	62:BV:120:ARG:HB3	2.11	0.51
3:1:172:A:H2'	3:1:173:A:C8	2.45	0.51
3:1:1029:A:H4'	70:1:3106:SPM:H72	1.92	0.51
3:1:2644:C:O2'	3:1:2646:G:OP2	2.26	0.51
3:1:2709:G:N2	3:1:2712:A:OP2	2.41	0.51
70:1:3117:SPM:H41	73:1:7377:HOH:O	2.11	0.51
7:AC:178:GLU:HA	7:AC:237:LEU:HB2	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:AD:162:ARG:O	8:AD:166:VAL:HG23	2.11	0.51
13:AI:100:VAL:HG22	26:AW:20:MET:HE2	1.93	0.51
16:AM:157:ARG:HH11	16:AM:161:ALA:HB2	1.76	0.51
17:AN:76:TYR:HD2	17:AN:152:ALA:HB2	1.74	0.51
43:BC:171:ARG:HG2	73:BC:311:HOH:O	2.11	0.51
48:BH:143:GLU:HB2	48:BH:160:VAL:CG1	2.41	0.51
51:BK:14:ILE:HD12	51:BK:98:TYR:HA	1.92	0.51
57:BQ:84:LEU:HD13	57:BQ:88:LEU:CD2	2.40	0.51
63:BW:65:THR:OG1	63:BW:68:GLU:HG3	2.11	0.51
3:1:1909:A:N6	38:AI:19:TYR:HA	2.26	0.51
3:1:2914:C:O2'	3:1:2915:A:H3'	2.10	0.51
4:4:29:G:H4'	54:BN:133:SER:HB3	1.91	0.51
4:4:1211:OMG:HM22	4:4:1212:OMG:H5'	1.93	0.51
6:AB:246:ALA:HB3	11:AG:78:TYR:HE2	1.76	0.51
9:AE:33:LYS:HG3	9:AE:38:GLU:OE2	2.10	0.51
9:AE:106:LYS:HG2	9:AE:113:THR:OG1	2.11	0.51
14:AK:77:LEU:CD1	14:AK:86:MET:HG3	2.41	0.51
18:AO:144:ARG:HG3	18:AO:146:GLU:HG3	1.92	0.51
19:AP:59:ASN:HA	19:AP:78:LYS:NZ	2.26	0.51
20:AQ:103:LEU:HD23	20:AQ:108:LYS:NZ	2.26	0.51
20:AQ:138:GLU:HG2	20:AQ:139:HIS:ND1	2.25	0.51
23:AT:63:TRP:O	23:AT:67:VAL:HG23	2.10	0.51
27:AX:9:LYS:O	27:AX:13:GLU:HG2	2.10	0.51
44:BD:118:ALA:HB2	44:BD:127:LEU:HD12	1.91	0.51
55:BO:85:PRO:HA	60:BT:32:ARG:NH1	2.25	0.51
61:BU:16:LEU:HD22	61:BU:60:MET:CE	2.40	0.51
65:BY:29:GLN:OE1	65:BY:41:CYS:HA	2.11	0.51
68:Bb:19:ALA:HB2	68:Bb:34:ILE:HB	1.92	0.51
3:1:243:G:H21	3:1:462:G:H2'	1.76	0.51
3:1:1415:A:O2'	3:1:1416:G:H5'	2.11	0.51
3:1:1798:A:O2'	6:AB:212:TYR:O	2.27	0.51
4:4:138:G:N2	47:BG:112:GLN:OE1	2.36	0.51
4:4:306:C:O2'	4:4:307:G:H5'	2.09	0.51
4:4:651:G:H2'	4:4:652:G:C8	2.46	0.51
4:4:1152:G:H4'	51:BK:124:GLU:OE1	2.11	0.51
4:4:1338:U:H2'	4:4:1339:G:O4'	2.11	0.51
4:4:1494:C:O2	64:BX:39:THR:HG23	2.10	0.51
6:AB:65:LEU:HD11	13:AI:95:PRO:HB2	1.92	0.51
11:AG:8:ASP:CG	11:AG:11:GLN:HB2	2.36	0.51
17:AN:39:THR:HG22	17:AN:87:TYR:CE1	2.46	0.51
24:AU:21:ILE:HD12	24:AU:21:ILE:O	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:Aj:126:LEU:O	39:Aj:130:ARG:NH1	2.44	0.51
41:BA:149:ARG:NH2	73:BA:306:HOH:O	2.43	0.51
42:BB:90:CYS:C	42:BB:93:VAL:H	2.17	0.51
51:BK:8:GLN:HE22	51:BK:11:PRO:CD	2.24	0.51
52:BL:49:ARG:O	52:BL:50:LEU:HD13	2.10	0.51
57:BQ:108:ASP:O	57:BQ:112:ARG:HG3	2.11	0.51
60:BT:18:PRO:HG3	60:BT:118:VAL:HG22	1.93	0.51
3:1:689:A:H2'	3:1:690:A:C8	2.46	0.51
3:1:931:C:H2'	3:1:932:C:H6	1.75	0.51
3:1:1486:G:H2'	3:1:1487:G:C8	2.46	0.51
3:1:2919:C:H2'	3:1:2920:C:C6	2.46	0.51
3:1:3002:C:O3'	6:AB:289:GLY:HA2	2.11	0.51
4:4:502:U:H2'	4:4:503:C:C6	2.46	0.51
4:4:718:U:OP1	4:4:783:C:O2'	2.24	0.51
4:4:1067:G:H2'	4:4:1068:A:H5'	1.92	0.51
4:4:1093:C:H2'	4:4:1094:U:C6	2.45	0.51
4:4:1200:C:H2'	4:4:1201:U:H5'	1.93	0.51
4:4:1377:C:O2'	4:4:1378:C:H5'	2.11	0.51
4:4:1483:C:H2'	4:4:1484:G:C8	2.46	0.51
73:4:3143:HOH:O	44:BD:18:LYS:NZ	2.43	0.51
6:AB:203:VAL:HG12	6:AB:312:LEU:CD2	2.41	0.51
11:AG:26:ILE:HG22	11:AG:29:ARG:H	1.76	0.51
16:AM:108:LYS:O	16:AM:110:PRO:HD3	2.11	0.51
20:AQ:70:GLY:HA2	20:AQ:73:ARG:NH1	2.26	0.51
24:AU:70:SER:HB3	24:AU:73:ASP:CB	2.36	0.51
36:Ag:21:LYS:HG2	36:Ag:47:PRO:HA	1.91	0.51
46:BF:97:GLN:O	46:BF:101:LYS:HG3	2.10	0.51
48:BH:62:CYS:HB2	48:BH:83:ALA:O	2.10	0.51
53:BM:15:LYS:HD3	53:BM:16:LEU:H	1.75	0.51
66:BZ:25:THR:OG1	66:BZ:26:GLY:N	2.44	0.51
68:Bb:25:GLU:HB2	68:Bb:27:LYS:NZ	2.25	0.51
3:1:1500:A:O2'	3:1:1501:C:H5'	2.10	0.51
3:1:1615:A:H2'	3:1:1616:A:C8	2.46	0.51
3:1:1989:A:H2'	3:1:1990:A2M:C8	2.41	0.51
3:1:2319:C:O2'	3:1:2338:A:N1	2.39	0.51
3:1:2739:G:H2'	3:1:2740:C:C6	2.46	0.51
3:1:2764:C:H2'	3:1:2765:C:C6	2.46	0.51
70:1:3128:SPM:H92	73:1:6313:HOH:O	2.11	0.51
4:4:265:A:OP2	50:BJ:58:LYS:NZ	2.44	0.51
4:4:1149:A:H5'	59:BS:2:GLY:HA2	1.93	0.51
4:4:1435:G:H3'	4:4:1436:C:H5''	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AC:54:VAL:HG13	7:AC:149:ALA:HB2	1.93	0.51
10:AF:25:GLU:OE1	10:AF:140:HIS:NE2	2.44	0.51
41:BA:179:LEU:HB3	41:BA:192:VAL:HG11	1.93	0.51
42:BB:77:THR:OG1	42:BB:124:VAL:HB	2.10	0.51
42:BB:182:LEU:CB	42:BB:188:LEU:HD23	2.38	0.51
44:BD:139:ARG:NH1	62:BV:67:GLY:HA2	2.25	0.51
48:BH:68:LEU:HD23	51:BK:57:GLU:OE2	2.11	0.51
3:1:188:A:H2'	3:1:189:C:O4'	2.12	0.50
3:1:815:C:O2'	3:1:851:A:N6	2.43	0.50
3:1:1338:A:C4	31:Ab:115:ARG:HB2	2.45	0.50
3:1:2046:U:H5''	3:1:2047:U:OP1	2.11	0.50
3:1:2410:A:H2'	3:1:2411:G:O4'	2.11	0.50
8:AD:6:LEU:O	8:AD:172:VAL:HG11	2.10	0.50
8:AD:87:ARG:CG	8:AD:118:PRO:HD2	2.33	0.50
9:AE:17:LYS:O	9:AE:33:LYS:HD2	2.11	0.50
17:AN:39:THR:HG22	17:AN:87:TYR:HE1	1.76	0.50
39:Aj:138:THR:O	39:Aj:142:LYS:HE2	2.11	0.50
44:BD:109:GLN:HE21	44:BD:121:ILE:HG13	1.76	0.50
51:BK:4:VAL:HG21	51:BK:97:ALA:HB3	1.92	0.50
54:BN:73:VAL:HG11	54:BN:97:ILE:HG21	1.93	0.50
54:BN:132:VAL:HG11	54:BN:145:PRO:HD3	1.93	0.50
3:1:2623:OMU:H5	70:1:3128:SPM:H82	1.93	0.50
4:4:147:G:H2'	4:4:148:G:H8	1.76	0.50
4:4:485:G:H5''	54:BN:116:LEU:HD11	1.92	0.50
4:4:1097:C:H2'	4:4:1098:U:O4'	2.12	0.50
73:4:3772:HOH:O	55:BO:140:THR:HB	2.11	0.50
5:AA:196:PRO:HG3	5:AA:203:GLY:HA2	1.92	0.50
6:AB:146:LEU:HG	6:AB:163:VAL:HG13	1.93	0.50
9:AE:78:ILE:O	9:AE:82:MET:HG3	2.11	0.50
14:AJ:5:ILE:CG1	29:AZ:29:LEU:HG	2.36	0.50
18:AO:180:LEU:HB3	18:AO:181:PRO:HD3	1.92	0.50
39:Aj:167:ASP:HB3	39:Aj:170:THR:CG2	2.39	0.50
42:BB:27:LEU:HB2	42:BB:149:THR:CG2	2.40	0.50
45:BE:2:VAL:HG22	45:BE:26:ARG:HD3	1.92	0.50
45:BE:90:PRO:HG2	62:BV:19:LEU:HD23	1.93	0.50
45:BE:164:GLU:HG2	45:BE:165:ASN:OD1	2.11	0.50
46:BF:16:GLY:HA2	46:BF:42:ILE:HD11	1.93	0.50
47:BG:85:PRO:HG2	47:BG:86:PRO:HD3	1.93	0.50
48:BH:187:PRO:CG	48:BH:190:GLU:HG3	2.40	0.50
51:BK:57:GLU:OE1	51:BK:88:ARG:NH1	2.27	0.50
53:BM:137:LYS:HE2	53:BM:141:VAL:CB	2.36	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:BQ:28:TYR:CD2	57:BQ:60:ILE:HD11	2.47	0.50
62:BV:30:LEU:CD1	62:BV:70:LYS:HG3	2.41	0.50
65:BY:22:CYS:SG	65:BY:46:ARG:HD3	2.50	0.50
1:2:39:U:H2'	1:2:40:C:C6	2.47	0.50
3:1:365:C:H2'	3:1:366:G:O4'	2.12	0.50
3:1:1253:A:O2'	3:1:1254:G:H5''	2.12	0.50
4:4:381:C:H2'	4:4:382:G:H8	1.75	0.50
4:4:1402:C:H2'	4:4:1403:C:H6	1.76	0.50
8:AD:23:VAL:CG1	8:AD:75:THR:HG22	2.42	0.50
9:AE:99:THR:N	9:AE:184:ASP:OD2	2.40	0.50
14:AK:66:LYS:HD2	21:AR:73:GLU:OE2	2.10	0.50
17:AN:111:ARG:HH21	17:AN:121:GLY:HA2	1.75	0.50
18:AO:52:ARG:HB2	18:AO:55:GLY:O	2.12	0.50
45:BE:109:PRO:O	45:BE:235:LYS:NZ	2.30	0.50
48:BH:45:TRP:CE2	48:BH:127:PRO:HG2	2.47	0.50
49:BI:112:SER:OG	49:BI:115:GLU:HG3	2.11	0.50
53:BM:135:GLY:C	73:BM:201:HOH:O	2.53	0.50
57:BQ:35:GLN:O	57:BQ:39:GLU:HG3	2.11	0.50
62:BV:61:LYS:NZ	62:BV:63:LYS:HB2	2.26	0.50
69:Bc:36:ASN:ND2	69:Bc:60:CYS:SG	2.85	0.50
1:2:12:G:O2'	18:AO:56:ASP:OD1	2.30	0.50
3:1:30:C:H2'	3:1:31:U:C6	2.47	0.50
3:1:181:U:H2'	3:1:182:C:H5'	1.94	0.50
3:1:656:A:H2'	3:1:657:C:C6	2.46	0.50
3:1:862:A:N6	73:1:3523:HOH:O	2.28	0.50
3:1:1556:C:O2'	14:AJ:54:HIS:ND1	2.30	0.50
3:1:1642:A:H2'	3:1:1643:U:C6	2.47	0.50
3:1:2083:G:OP2	3:1:2083:G:N2	2.31	0.50
3:1:2185:C:H2'	3:1:2186:U:C6	2.47	0.50
3:1:2724:C:H3'	73:1:4085:HOH:O	2.11	0.50
4:4:52:U:H2'	4:4:53:G:C8	2.46	0.50
4:4:162:A:H2'	4:4:163:G:O4'	2.12	0.50
4:4:664:A:H4'	4:4:665:A:H5'	1.92	0.50
4:4:689:A:OP1	57:BQ:2:PRO:HG3	2.11	0.50
4:4:1202:OMG:H2'	4:4:1203:C:C6	2.46	0.50
5:AA:120:GLY:HA2	5:AA:159:VAL:HG12	1.93	0.50
7:AC:9:LEU:HD21	7:AC:48:ILE:CD1	2.41	0.50
25:AV:56:MET:SD	25:AV:102:MET:HB2	2.50	0.50
38:Ai:26:LYS:O	38:Ai:30:ILE:HD12	2.10	0.50
51:BK:61:LEU:HD11	51:BK:111:TYR:CD2	2.47	0.50
57:BQ:130:LYS:HE2	57:BQ:137:GLN:O	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:BR:58:LEU:HD11	58:BR:128:ILE:HD12	1.92	0.50
60:BT:34:LYS:NZ	60:BT:42:MET:HE1	2.25	0.50
60:BT:98:ILE:HD11	60:BT:129:LEU:HD23	1.92	0.50
2:3:435:VAL:HB	2:3:439:ALA:HB2	1.93	0.50
3:1:150:G:N2	3:1:153:A:OP2	2.31	0.50
3:1:737:G:N2	3:1:739:A:H3'	2.26	0.50
3:1:874:U:H2'	3:1:875:OMU:H6	1.93	0.50
3:1:1649:G:O6	29:AZ:23:GLU:HG2	2.11	0.50
3:1:2736:G:O2'	3:1:2944:G:N7	2.43	0.50
4:4:441:U:OP2	62:BV:95:ARG:NH1	2.40	0.50
4:4:843:G:OP2	54:BN:4:LYS:HE3	2.12	0.50
13:AI:39:VAL:HB	13:AI:67:VAL:HB	1.94	0.50
18:AO:37:VAL:HG11	18:AO:116:VAL:HA	1.93	0.50
22:AS:90:PRO:HA	22:AS:93:LEU:HD12	1.94	0.50
30:Aa:5:LYS:HG2	30:Aa:81:ASP:OD1	2.12	0.50
43:BC:166:TYR:O	43:BC:171:ARG:HD3	2.12	0.50
47:BG:127:PRO:HD2	68:Bb:10:ALA:HA	1.93	0.50
49:BI:115:GLU:HA	49:BI:118:GLU:HG2	1.92	0.50
50:BJ:43:GLU:HA	50:BJ:65:ARG:HE	1.76	0.50
55:BO:84:ASP:HB3	55:BO:87:THR:HG22	1.93	0.50
55:BO:132:VAL:HG13	55:BO:133:THR:HG23	1.92	0.50
59:BS:54:ILE:HA	59:BS:57:LEU:CD2	2.40	0.50
62:BV:103:LYS:O	62:BV:107:GLU:HG2	2.11	0.50
2:3:342:PRO:HB2	2:3:365:LEU:CD2	2.41	0.50
2:3:435:VAL:CG1	2:3:447:LYS:HD3	2.41	0.50
3:1:231:G:H2'	3:1:232:A:C8	2.47	0.50
3:1:1932:C:O2'	5:AA:228:SER:HB3	2.12	0.50
3:1:1934:C:O2'	3:1:1938:A:N3	2.38	0.50
73:1:4257:HOH:O	32:Ac:59:ARG:HD2	2.11	0.50
4:4:393:A:H3'	4:4:394:C:H6	1.76	0.50
4:4:848:C:O2'	4:4:849:U:H5'	2.11	0.50
4:4:1013:C:H1'	4:4:1162:A:C5	2.47	0.50
4:4:1289:OMG:HM22	4:4:1290:C:O4'	2.10	0.50
5:AA:217:ALA:O	5:AA:222:LYS:HE2	2.12	0.50
10:AF:25:GLU:OE1	10:AF:25:GLU:N	2.42	0.50
29:AZ:27:SER:O	29:AZ:33:PRO:HD3	2.12	0.50
49:BI:41:LEU:CD2	49:BI:129:VAL:HG21	2.42	0.50
60:BT:34:LYS:HZ3	60:BT:42:MET:HE1	1.76	0.50
61:BU:42:LYS:HG2	73:BU:204:HOH:O	2.11	0.50
62:BV:89:PRO:O	62:BV:93:LEU:HG	2.10	0.50
62:BV:107:GLU:O	62:BV:111:ARG:HG3	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:50:C:O2'	18:AO:109:ARG:HD3	2.12	0.50
2:3:327:HIS:HB3	2:3:483:ARG:NH1	2.27	0.50
2:3:368:VAL:HG12	2:3:374:VAL:CA	2.41	0.50
2:3:593:VAL:HG13	2:3:594:ASN:OD1	2.10	0.50
3:1:120:C:C1'	73:1:3901:HOH:O	2.60	0.50
3:1:585:U:O2'	3:1:586:C:H5'	2.11	0.50
3:1:1569:G:H2'	3:1:1570:U:C6	2.46	0.50
3:1:2439:A:H2'	3:1:2440:A:C8	2.46	0.50
3:1:2860:A:H1'	9:AE:74:THR:OG1	2.11	0.50
4:4:249:A:N1	4:4:281:G:O2'	2.43	0.50
4:4:1378:C:H2'	4:4:1379:A:H8	1.77	0.50
10:AF:21:TYR:OH	10:AF:72:VAL:HG22	2.12	0.50
14:AK:28:ILE:HD12	21:AR:75:VAL:HG23	1.93	0.50
16:AM:37:ILE:HD11	16:AM:104:ARG:HB3	1.93	0.50
32:Ac:26:HIS:HB3	32:Ac:28:GLU:OE1	2.11	0.50
42:BB:84:LYS:HB3	42:BB:85:PRO:HD3	1.94	0.50
46:BF:9:TRP:CZ2	46:BF:11:PRO:HA	2.47	0.50
47:BG:39:ASP:O	47:BG:42:VAL:HG12	2.11	0.50
61:BU:68:PRO:CB	61:BU:119:ARG:HG3	2.42	0.50
66:BZ:19:VAL:HG22	66:BZ:35:LYS:O	2.12	0.50
2:3:487:VAL:HG22	2:3:593:VAL:HA	1.92	0.50
2:3:564:THR:HG22	2:3:567:LEU:HD23	1.94	0.50
3:1:272:A:H2'	3:1:273:C:O4'	2.12	0.50
3:1:1659:A:H4'	32:Ac:50:LYS:HG3	1.93	0.50
3:1:2031:G:H2'	3:1:2032:U:H5'	1.93	0.50
4:4:327:U:H2'	4:4:328:G:O4'	2.12	0.50
4:4:790:G:H5'	42:BB:30:LYS:HD2	1.93	0.50
4:4:811:C:H2'	4:4:812:C:H6	1.77	0.50
4:4:1137:G:H5''	59:BS:3:ARG:O	2.12	0.50
4:4:1163:OMG:H5'	4:4:1164:G:OP2	2.11	0.50
4:4:1417:U:H2'	4:4:1418:G:C8	2.47	0.50
70:4:3012:SPM:C9	57:BQ:11:ARG:HG2	2.42	0.50
5:AA:95:GLY:HA2	5:AA:129:GLN:NE2	2.27	0.50
6:AB:273:GLY:HA3	6:AB:295:TYR:CE1	2.47	0.50
7:AC:187:LYS:NZ	7:AC:191:GLU:OE2	2.40	0.50
14:AK:77:LEU:HD13	14:AK:86:MET:HG3	1.92	0.50
18:AO:156:LYS:HB2	18:AO:163:TYR:CD1	2.46	0.50
29:AZ:9:GLN:HB3	29:AZ:76:LYS:HZ3	1.76	0.50
39:Aj:105:ASN:HD22	39:Aj:126:LEU:HD13	1.76	0.50
45:BE:31:PRO:O	45:BE:139:ASP:HB2	2.12	0.50
55:BO:84:ASP:HB2	55:BO:89:ARG:O	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:BQ:37:ALA:HA	57:BQ:40:LEU:HD12	1.94	0.50
62:BV:114:GLU:HA	62:BV:117:GLU:OE2	2.12	0.50
3:1:1356:U:H2'	3:1:1357:C:C6	2.46	0.50
3:1:1444:C:O2'	3:1:1523:A:N3	2.38	0.50
3:1:1578:G:H2'	3:1:1579:C:C6	2.47	0.50
4:4:639:U:H2'	4:4:640:C:C6	2.47	0.50
4:4:1396:G:H2'	4:4:1397:C:H6	1.77	0.50
8:AD:24:VAL:HA	8:AD:132:ASP:O	2.11	0.50
8:AD:96:ILE:HD12	8:AD:96:ILE:O	2.11	0.50
9:AE:176:ARG:HG2	9:AE:177:GLU:HG2	1.93	0.50
16:AM:182:LYS:O	16:AM:182:LYS:HD3	2.12	0.50
18:AO:83:TYR:CD2	18:AO:143:ILE:HD12	2.47	0.50
22:AS:12:SER:HB3	22:AS:16:LEU:HG	1.93	0.50
41:BA:67:ASP:OD1	41:BA:68:ILE:N	2.45	0.50
47:BG:53:VAL:HA	47:BG:118:VAL:O	2.12	0.50
2:3:336:VAL:HG23	2:3:469:VAL:CG2	2.37	0.49
2:3:485:VAL:O	2:3:597:VAL:HG13	2.12	0.49
3:1:308:G:C5'	73:1:4417:HOH:O	2.57	0.49
3:1:414:G:H2'	3:1:415:C:C6	2.47	0.49
3:1:2132:C:H2'	3:1:2133:G:O4'	2.12	0.49
3:1:2935:C:O2	3:1:3010:A:O2'	2.26	0.49
4:4:310:A:O2'	4:4:311:G:H5'	2.12	0.49
4:4:1034:OMC:HM22	4:4:1035:B8T:C5'	2.42	0.49
13:AI:79:GLN:HB2	13:AI:81:PHE:CE1	2.47	0.49
3:1:122:G:H2'	3:1:123:C:C6	2.47	0.49
3:1:2185:C:H2'	3:1:2186:U:H6	1.77	0.49
3:1:2203:G:H2'	3:1:2204:C:C6	2.47	0.49
4:4:166:G:H4'	50:BJ:122:ASP:OD2	2.12	0.49
4:4:213:G:H2'	4:4:214:C:C6	2.46	0.49
4:4:1415:G:H1'	73:4:3227:HOH:O	2.09	0.49
6:AB:127:GLU:N	6:AB:127:GLU:OE1	2.45	0.49
8:AD:54:ARG:HA	8:AD:69:PRO:HA	1.94	0.49
14:AK:52:ILE:HB	21:AR:77:ARG:NH1	2.27	0.49
15:AL:91:LEU:HB3	15:AL:97:VAL:HG23	1.94	0.49
18:AO:155:LEU:HD21	18:AO:163:TYR:HA	1.92	0.49
32:Ac:84:ARG:HB2	32:Ac:84:ARG:NH1	2.26	0.49
34:Ae:53:LEU:O	34:Ae:57:LEU:HD23	2.11	0.49
37:Ah:89:GLU:O	37:Ah:91:VAL:HG23	2.12	0.49
40:Ak:19:ASN:CG	40:Ak:22:LYS:HB2	2.37	0.49
46:BF:11:PRO:HG3	46:BF:20:LYS:CD	2.42	0.49
47:BG:82:ALA:N	47:BG:97:LYS:O	2.44	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:BP:19:CYS:SG	56:BP:24:THR:HG22	2.52	0.49
68:Bb:39:LEU:HD21	68:Bb:55:LEU:HD22	1.94	0.49
2:3:488:GLY:HA3	2:3:593:VAL:HG23	1.93	0.49
3:1:613:G:H4'	3:1:614:U:O5'	2.12	0.49
3:1:623:G:O2'	3:1:624:G:H5'	2.12	0.49
3:1:684:A:H4'	3:1:685:G:H5'	1.94	0.49
3:1:1486:G:H2'	3:1:1487:G:H8	1.77	0.49
3:1:2011:A2M:H8	3:1:2011:A2M:O5'	2.12	0.49
3:1:2169:A:H2'	3:1:2170:C:C6	2.47	0.49
4:4:542:G:N1	4:4:720:A:OP2	2.26	0.49
4:4:584:C:H2'	4:4:585:C:C6	2.47	0.49
4:4:683:G:O2'	4:4:684:U:H5''	2.13	0.49
6:AB:207:THR:HG22	6:AB:303:PRO:HB3	1.93	0.49
10:AF:33:LYS:O	10:AF:37:ILE:HG13	2.12	0.49
13:AI:89:ARG:HD3	13:AI:103:GLU:O	2.12	0.49
14:AJ:10:VAL:HG13	14:AJ:86:MET:HE1	1.94	0.49
39:Aj:158:ARG:HD3	39:Aj:182:GLU:HG3	1.94	0.49
44:BD:118:ALA:HB1	44:BD:123:HIS:HD2	1.76	0.49
46:BF:105:GLU:OE1	46:BF:105:GLU:N	2.45	0.49
51:BK:36:VAL:CG1	51:BK:43:LEU:HD22	2.42	0.49
58:BR:18:LEU:H	58:BR:18:LEU:HD12	1.76	0.49
61:BU:15:GLU:CG	61:BU:138:ILE:HD11	2.43	0.49
62:BV:46:LEU:HD23	62:BV:57:ILE:HD13	1.94	0.49
67:Ba:17:THR:O	67:Ba:19:LYS:NZ	2.27	0.49
68:Bb:30:GLU:O	68:Bb:34:ILE:HG13	2.12	0.49
2:3:381:ARG:NH2	2:3:517:LEU:O	2.36	0.49
2:3:464:GLN:HG3	2:3:465:PRO:HD2	1.95	0.49
2:3:476:LYS:HZ3	2:3:479:LYS:HG2	1.76	0.49
3:1:220:U:H5'	73:1:5456:HOH:O	2.13	0.49
3:1:582:C:H2'	3:1:583:C:H6	1.78	0.49
3:1:925:U:H1'	3:1:2559:G:OP1	2.12	0.49
3:1:983:G:O2'	3:1:984:U:H5'	2.12	0.49
3:1:1481:A:H2'	3:1:1482:A:C8	2.47	0.49
4:4:174:C:H2'	4:4:175:U:C6	2.47	0.49
4:4:1182:C:H4'	4:4:1183:C:C5'	2.42	0.49
4:4:1324:U:OP2	4:4:1325:C:N4	2.45	0.49
8:AD:33:GLU:OE2	8:AD:33:GLU:N	2.43	0.49
12:AH:31:GLU:HG2	12:AH:56:VAL:HG13	1.94	0.49
18:AO:90:GLY:O	18:AO:94:ARG:HG3	2.12	0.49
19:AP:60:ASP:HA	19:AP:79:ARG:O	2.12	0.49
23:AT:142:ASN:HB3	23:AT:154:PHE:O	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:BE:39:PRO:HG2	45:BE:42:VAL:CG2	2.41	0.49
47:BG:43:LEU:HB3	47:BG:47:ILE:HG22	1.93	0.49
64:BX:42:TYR:HB3	64:BX:63:TYR:O	2.12	0.49
3:1:690:A:H2'	3:1:691:G:O4'	2.13	0.49
3:1:935:C:H2'	3:1:936:G:O4'	2.12	0.49
3:1:1577:C:H3'	73:1:7219:HOH:O	2.12	0.49
3:1:1600:A:H2'	3:1:1601:C:C6	2.47	0.49
3:1:1861:U:O2'	3:1:1862:U:H5'	2.13	0.49
3:1:2720:OMC:HM22	3:1:2721:G:H5'	1.94	0.49
4:4:475:OMG:CM2	67:Ba:18:PRO:HG2	2.43	0.49
4:4:1357:U:H5'	64:BX:84:PRO:HA	1.93	0.49
4:4:1492:C:OP2	64:BX:88:ARG:HG2	2.12	0.49
5:AA:58:MET:HE1	5:AA:80:VAL:HG21	1.93	0.49
7:AC:189:LEU:HG	7:AC:193:LEU:HD12	1.94	0.49
9:AE:6:ALA:HB3	9:AE:61:VAL:CG2	2.42	0.49
20:AQ:7:LEU:O	20:AQ:11:ILE:HG12	2.11	0.49
31:Ab:11:GLN:HB3	31:Ab:12:PRO:HD3	1.94	0.49
40:Ak:31:VAL:HG22	40:Ak:69:LEU:HG	1.95	0.49
42:BB:142:PRO:HA	42:BB:157:ASP:OD2	2.13	0.49
42:BB:175:TRP:CD2	42:BB:198:PRO:HG3	2.47	0.49
45:BE:100:ASP:HB2	45:BE:106:ASP:HB2	1.94	0.49
49:BI:57:ARG:NH2	57:BQ:16:ARG:O	2.45	0.49
49:BI:77:PRO:HD2	49:BI:79:PHE:CZ	2.47	0.49
53:BM:35:THR:HG22	53:BM:42:THR:HA	1.94	0.49
53:BM:82:ALA:HB2	53:BM:115:VAL:HB	1.93	0.49
2:3:633:ALA:O	2:3:637:VAL:HG23	2.12	0.49
3:1:1172:A:H1'	3:1:1237:A:N6	2.28	0.49
3:1:1754:C:O2	33:Ad:8:GLY:HA2	2.13	0.49
4:4:276:A:O2'	4:4:277:A:H5'	2.12	0.49
4:4:1081:U:O4	4:4:1082:A:N6	2.46	0.49
4:4:1087:C:O2'	4:4:1088:U:H5'	2.13	0.49
4:4:1102:G:H2'	4:4:1103:G:H8	1.78	0.49
4:4:1448:G:O2'	4:4:1449:U:OP1	2.30	0.49
4:4:1490:A:OP2	64:BX:4:LYS:NZ	2.45	0.49
16:AM:179:LEU:O	16:AM:183:LEU:HG	2.13	0.49
21:AR:15:MET:HE1	21:AR:41:HIS:CD2	2.48	0.49
25:AV:118:GLU:HA	25:AV:121:LYS:HE3	1.93	0.49
36:Ag:35:GLU:HG3	36:Ag:43:ARG:HE	1.77	0.49
51:BK:36:VAL:HG11	51:BK:43:LEU:HD22	1.95	0.49
58:BR:54:ILE:HD13	58:BR:128:ILE:HD11	1.95	0.49
61:BU:84:ILE:HG12	61:BU:94:ARG:HH11	1.78	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
62:BV:61:LYS:HZ3	62:BV:63:LYS:HB2	1.78	0.49
64:BX:20:TYR:HA	64:BX:31:PRO:HA	1.94	0.49
3:1:1657:C:H2'	3:1:1658:G:O4'	2.13	0.49
3:1:1807:C:O2'	3:1:2801:G:H4'	2.13	0.49
3:1:1816:OMC:HM22	3:1:1817:G:H5'	1.93	0.49
3:1:2135:A:H2'	3:1:2136:C:C6	2.48	0.49
3:1:2707:OMU:HM22	3:1:2708:C:H5'	1.93	0.49
4:4:111:A:OP1	58:BR:55:ARG:NH2	2.40	0.49
4:4:480:C:H2'	4:4:481:A:O4'	2.12	0.49
4:4:1014:A:O2'	43:BC:149:GLU:O	2.13	0.49
4:4:1049:U:O2'	4:4:1050:U:H5'	2.13	0.49
4:4:1070:A:C2'	4:4:1071:C:H5'	2.41	0.49
15:AL:115:LYS:HG3	15:AL:132:VAL:CG1	2.42	0.49
41:BA:120:THR:OG1	41:BA:124:TRP:HB2	2.13	0.49
49:BI:97:ARG:HG3	49:BI:98:GLN:HG3	1.95	0.49
50:BJ:39:PRO:CD	50:BJ:119:PRO:HB2	2.42	0.49
53:BM:25:SER:CB	53:BM:102:ALA:HB2	2.43	0.49
60:BT:80:LEU:HD23	60:BT:87:VAL:HB	1.95	0.49
1:2:35:C:O2'	1:2:36:C:H5'	2.11	0.49
2:3:328:VAL:HG23	2:3:330:GLY:H	1.78	0.49
2:3:334:ARG:HA	2:3:337:MET:CG	2.43	0.49
3:1:2:A:H2	3:1:3021:G:H1	1.54	0.49
3:1:12:G:H2'	3:1:13:C:H6	1.78	0.49
3:1:1525:U:C2'	3:1:1526:A:H5''	2.43	0.49
3:1:1542:G:H5''	73:1:7876:HOH:O	2.12	0.49
3:1:1946:A:C5	3:1:1947:OMG:H1'	2.48	0.49
3:1:2476:A:O2'	3:1:2506:G:H4'	2.12	0.49
3:1:2624:OMC:HM21	6:AB:225:PRO:HD2	1.94	0.49
73:1:4450:HOH:O	16:AM:84:LYS:HE2	2.12	0.49
4:4:1209:C:O2'	4:4:1210:OMG:H5'	2.13	0.49
11:AG:2:ILE:CD1	11:AG:133:LEU:HD23	2.43	0.49
44:BD:117:LEU:HD23	44:BD:157:ILE:HD13	1.94	0.49
48:BH:34:LEU:HD12	51:BK:104:LEU:HD13	1.93	0.49
50:BJ:117:SER:O	50:BJ:119:PRO:HD3	2.13	0.49
61:BU:2:THR:HG22	61:BU:153:VAL:CG1	2.41	0.49
3:1:626:G:H2'	3:1:627:G:H8	1.78	0.49
3:1:766:G:H2'	3:1:767:C:C6	2.47	0.49
3:1:1027:C:O2'	3:1:1028:A:H5'	2.13	0.49
3:1:1536:C:H2'	3:1:1537:G:H8	1.77	0.49
4:4:906:OMG:HM22	4:4:907:G:O4'	2.12	0.49
4:4:1420:G:H2'	4:4:1421:G:O4'	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:AD:26:ILE:CG1	8:AD:42:LEU:HD11	2.42	0.49
14:AJ:15:LEU:CD2	32:Ac:75:ALA:HB2	2.43	0.49
14:AK:6:ASP:OD2	14:AK:9:ARG:HB2	2.13	0.49
15:AL:82:GLY:HA3	15:AL:120:GLY:HA3	1.95	0.49
19:AP:10:ASN:O	19:AP:14:ARG:HG3	2.13	0.49
45:BE:96:ARG:O	45:BE:98:VAL:HG13	2.12	0.49
45:BE:97:VAL:HA	45:BE:106:ASP:O	2.13	0.49
45:BE:131:GLY:O	45:BE:147:PRO:HG3	2.13	0.49
46:BF:13:THR:HG23	46:BF:39:GLU:OE2	2.13	0.49
49:BI:40:VAL:HG22	49:BI:43:ARG:HH22	1.77	0.49
55:BO:55:LEU:HD22	55:BO:59:GLN:OE1	2.13	0.49
2:3:550:ARG:HD2	2:3:564:THR:OG1	2.11	0.49
3:1:535:G:H5''	3:1:538:C:H1'	1.93	0.49
3:1:611:G:OP2	3:1:612:A:O2'	2.25	0.49
3:1:1166:C:H2'	3:1:1167:G:H8	1.77	0.49
3:1:1328:G:H5'	7:AC:212:LYS:HE2	1.95	0.49
3:1:2532:G:H2'	3:1:2533:C:C6	2.48	0.49
3:1:2589:C:H4'	73:1:3853:HOH:O	2.13	0.49
3:1:2868:U:C1'	3:1:2869:A:H5''	2.43	0.49
3:1:2984:C:H4'	3:1:2985:C:O5'	2.13	0.49
4:4:68:G:H2'	4:4:69:G:H8	1.77	0.49
4:4:1404:C:OP1	50:BJ:62:ARG:NH1	2.45	0.49
8:AD:6:LEU:HD23	8:AD:173:LEU:HD12	1.95	0.49
15:AL:92:ARG:HE	15:AL:104:LEU:HD21	1.78	0.49
24:AU:72:MET:CE	24:AU:81:LEU:HD11	2.42	0.49
40:Ak:3:LEU:CD2	40:Ak:37:THR:HG21	2.43	0.49
45:BE:193:GLN:O	45:BE:210:LEU:HA	2.13	0.49
62:BV:43:ARG:NH1	62:BV:57:ILE:O	2.45	0.49
2:3:570:LEU:HD13	4:4:1366:C:C5	2.47	0.48
3:1:263:C:O2'	3:1:264:G:H5'	2.13	0.48
3:1:310:C:O2'	3:1:311:G:H5'	2.13	0.48
3:1:406:G:OP2	16:AM:48:ARG:NE	2.44	0.48
3:1:1603:G:H2'	3:1:1604:C:C6	2.48	0.48
3:1:1687:G:H2'	3:1:1688:U:O4'	2.12	0.48
3:1:2825:C:H5''	3:1:2827:G:H5''	1.95	0.48
73:1:7399:HOH:O	35:Af:50:LYS:HE2	2.13	0.48
4:4:278:G:H5''	58:BR:67:ARG:HG3	1.95	0.48
4:4:322:G:OP2	50:BJ:25:LYS:NZ	2.40	0.48
4:4:380:G:H2'	4:4:381:C:H6	1.77	0.48
4:4:769:G:OP1	57:BQ:107:LYS:HD3	2.13	0.48
4:4:1164:G:H4'	52:BL:61:GLN:HG3	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:1304:G:H2'	4:4:1305:A:C8	2.48	0.48
7:AC:177:ALA:O	7:AC:237:LEU:HD22	2.12	0.48
8:AD:105:GLY:HA3	8:AD:160:VAL:HG12	1.95	0.48
9:AE:82:MET:O	9:AE:86:VAL:HG22	2.13	0.48
10:AF:8:LYS:HB2	16:AM:18:GLU:HG3	1.94	0.48
12:AH:125:LYS:O	12:AH:129:GLU:HG3	2.13	0.48
39:Aj:136:PRO:HG3	39:Aj:166:LYS:CD	2.43	0.48
44:BD:131:GLY:O	44:BD:139:ARG:HD3	2.12	0.48
46:BF:133:VAL:HB	49:BI:95:PRO:HB3	1.94	0.48
55:BO:140:THR:CG2	55:BO:143:VAL:HG12	2.43	0.48
63:BW:97:ALA:HB3	63:BW:104:VAL:HB	1.95	0.48
64:BX:22:TYR:HA	64:BX:29:VAL:HG21	1.94	0.48
1:2:12:G:OP1	18:AO:24:ARG:NH1	2.46	0.48
2:3:488:GLY:CA	2:3:593:VAL:HG23	2.42	0.48
2:3:489:GLU:O	2:3:490:LEU:HD23	2.12	0.48
3:1:11:C:O2'	3:1:635:U:OP1	2.31	0.48
3:1:555:A:N1	3:1:2739:G:O2'	2.41	0.48
3:1:966:G:H2'	3:1:967:C:C6	2.48	0.48
3:1:1562:A:H3'	3:1:1563:G:C8	2.48	0.48
3:1:1944:U:H2'	3:1:1945:A:O4'	2.13	0.48
3:1:2315:C:H2'	3:1:2316:U:C6	2.48	0.48
4:4:847:C:OP2	54:BN:22:LYS:NZ	2.28	0.48
4:4:851:G:H4'	4:4:880:A2M:HM'3	1.94	0.48
4:4:1015:U:OP1	43:BC:150:ARG:HA	2.12	0.48
4:4:1060:A2M:H4'	4:4:1061:A:O5'	2.13	0.48
7:AC:32:LYS:HG2	7:AC:40:TYR:HE1	1.78	0.48
12:AH:67:TRP:O	12:AH:71:VAL:HG23	2.14	0.48
13:AI:94:ARG:HB3	13:AI:95:PRO:HD2	1.93	0.48
14:AK:72:GLU:OE2	14:AK:75:LYS:HE2	2.12	0.48
20:AQ:104:LYS:HD3	20:AQ:114:TRP:CG	2.47	0.48
20:AQ:106:GLN:CB	20:AQ:108:LYS:HE2	2.43	0.48
38:Ai:42:SER:OG	38:Ai:43:CYS:N	2.46	0.48
39:Aj:158:ARG:NH1	39:Aj:179:ALA:O	2.42	0.48
42:BB:110:PRO:HA	42:BB:115:TYR:CD2	2.48	0.48
46:BF:117:CYS:SG	49:BI:97:ARG:NH2	2.86	0.48
60:BT:108:HIS:CB	60:BT:115:TYR:HB3	2.42	0.48
2:3:440:THR:OG1	2:3:443:GLU:HG2	2.13	0.48
3:1:229:G:H5'	3:1:230:C:C5'	2.39	0.48
3:1:229:G:H5''	3:1:231:G:N7	2.27	0.48
3:1:1120:A:H2'	3:1:1121:A:C8	2.48	0.48
3:1:1419:C:H2'	3:1:1420:C:C6	2.48	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1:2703:A:H2'	3:1:2704:OMC:H6	1.79	0.48
4:4:364:G:H2'	4:4:365:C:C6	2.48	0.48
4:4:787:C:O2	49:BI:16:ASN:ND2	2.46	0.48
13:AI:135:THR:O	13:AI:139:LEU:HD12	2.13	0.48
18:AO:73:LYS:HE2	18:AO:73:LYS:HB2	1.56	0.48
41:BA:109:THR:HG21	41:BA:190:ARG:NH2	2.29	0.48
42:BB:83:PHE:HA	42:BB:99:THR:HG21	1.96	0.48
43:BC:137:GLY:HA3	43:BC:161:LEU:HB2	1.95	0.48
44:BD:134:LEU:HD12	44:BD:137:GLY:O	2.13	0.48
59:BS:10:LYS:O	59:BS:14:GLU:HG2	2.14	0.48
1:2:72:G:H2'	1:2:73:C:O4'	2.13	0.48
2:3:631:ASP:HA	2:3:634:ARG:NE	2.28	0.48
3:1:1:U:H5'	3:1:2743:U:C4	2.49	0.48
3:1:157:G:O2'	3:1:158:C:H5'	2.12	0.48
3:1:170:G:OP2	70:1:3102:SPM:N1	2.47	0.48
3:1:306:C:O2'	3:1:307:C:H5'	2.13	0.48
3:1:580:C:H2'	3:1:581:C:C6	2.47	0.48
3:1:650:A:O2'	3:1:1104:A:N1	2.43	0.48
3:1:1644:G:N7	73:1:3640:HOH:O	2.35	0.48
4:4:50:C:H4'	73:4:4034:HOH:O	2.13	0.48
4:4:66:C:O2'	4:4:67:C:H5'	2.14	0.48
4:4:278:G:H5''	58:BR:67:ARG:CG	2.43	0.48
4:4:1027:G:N7	4:4:1053:G:O2'	2.35	0.48
4:4:1189:C:O5'	4:4:1190:U:H5''	2.13	0.48
4:4:1219:G:H1'	4:4:1321:G:O2'	2.13	0.48
8:AD:122:TYR:CE2	8:AD:128:ILE:HD11	2.48	0.48
15:AL:49:MET:HA	15:AL:49:MET:HE3	1.95	0.48
15:AL:106:VAL:CG1	15:AL:128:VAL:HG22	2.44	0.48
34:Ae:9:GLU:OE1	34:Ae:9:GLU:N	2.46	0.48
41:BA:157:LYS:HE3	41:BA:169:GLU:CD	2.38	0.48
42:BB:10:LEU:HD13	42:BB:176:VAL:CG1	2.43	0.48
42:BB:81:TYR:HA	42:BB:203:THR:HG21	1.95	0.48
46:BF:18:MET:CB	46:BF:24:ILE:HD13	2.44	0.48
46:BF:184:LEU:HD23	46:BF:188:LEU:HD12	1.96	0.48
47:BG:54:LYS:O	47:BG:118:VAL:HB	2.13	0.48
53:BM:58:LYS:HB2	53:BM:59:PRO:HD3	1.95	0.48
59:BS:62:LYS:HA	59:BS:65:GLU:OE2	2.13	0.48
3:1:835:G:H2'	3:1:836:C:C6	2.48	0.48
3:1:1401:G:H1'	3:1:2825:C:C4	2.49	0.48
3:1:2421:A:O2'	3:1:2422:A:H5'	2.13	0.48
4:4:187:U:H2'	4:4:188:C:H6	1.79	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:1036:G:O2'	70:4:3017:SPM:H82	2.14	0.48
4:4:1098:U:O2'	4:4:1101:G:O6	2.31	0.48
4:4:1183:C:H2'	4:4:1184:OMC:H6	1.77	0.48
4:4:1377:C:H2'	4:4:1378:C:C6	2.48	0.48
47:BG:83:ASP:HB3	47:BG:96:ARG:HG2	1.94	0.48
47:BG:141:GLY:C	73:BG:216:HOH:O	2.57	0.48
49:BI:46:TYR:OH	69:Bc:2:SER:HA	2.13	0.48
62:BV:38:THR:O	62:BV:42:VAL:HG23	2.14	0.48
66:BZ:10:TYR:HE2	66:BZ:63:MET:HE3	1.78	0.48
2:3:476:LYS:HG3	2:3:480:GLU:OE1	2.12	0.48
3:1:75:U:H2'	25:AV:112:ALA:CB	2.44	0.48
3:1:1551:U:H2'	3:1:1552:G:H5'	1.95	0.48
3:1:1864:G:O2'	40:Ak:91:GLN:OE1	2.14	0.48
3:1:1922:A:H5'	73:1:3795:HOH:O	2.13	0.48
3:1:2492:A:H2'	3:1:2493:A:C8	2.48	0.48
3:1:2581:U:O2'	3:1:2582:G:H5'	2.13	0.48
3:1:2732:G:H2'	3:1:2733:U:C6	2.49	0.48
4:4:647:U:O2'	4:4:648:A:H5'	2.13	0.48
4:4:860:G:H2'	4:4:861:C:H6	1.78	0.48
4:4:1050:U:O2'	4:4:1051:A:O5'	2.30	0.48
4:4:1089:A:N6	73:4:3178:HOH:O	2.42	0.48
4:4:1451:A:H2'	4:4:1451:A:OP2	2.13	0.48
12:AH:31:GLU:CG	12:AH:56:VAL:HG13	2.44	0.48
22:AS:40:LYS:NZ	22:AS:99:GLY:O	2.46	0.48
27:AX:15:SER:OG	27:AX:18:GLU:HG3	2.14	0.48
31:Ab:9:LEU:HD12	31:Ab:13:LEU:CB	2.43	0.48
36:Ag:6:ASP:OD1	36:Ag:6:ASP:N	2.46	0.48
48:BH:138:THR:HG23	48:BH:208:ALA:HB1	1.94	0.48
55:BO:134:THR:OG1	55:BO:135:GLY:N	2.47	0.48
65:BY:38:VAL:HG12	65:BY:47:VAL:HG13	1.96	0.48
3:1:304:A:O2'	16:AM:170:LYS:HE2	2.14	0.48
3:1:835:G:H2'	3:1:836:C:H6	1.77	0.48
3:1:1479:C:H2'	3:1:1480:U:C6	2.49	0.48
3:1:1818:G:O2'	73:1:3401:HOH:O	2.20	0.48
3:1:1983:U:H2'	3:1:1984:A:O4'	2.13	0.48
3:1:2797:U:O2'	6:AB:53:HIS:ND1	2.37	0.48
4:4:68:G:H2'	4:4:69:G:C8	2.48	0.48
4:4:635:G:OP1	41:BA:198:LYS:NZ	2.29	0.48
4:4:828:G:H2'	4:4:830:A:OP2	2.13	0.48
4:4:1126:U:H5'	59:BS:5:LYS:HZ2	1.79	0.48
4:4:1338:U:O2'	48:BH:103:GLY:O	2.29	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AB:245:PRO:HD2	6:AB:248:MET:HE2	1.96	0.48
9:AE:132:VAL:HG13	9:AE:144:VAL:HG13	1.95	0.48
20:AQ:18:ARG:HD2	20:AQ:50:GLU:O	2.14	0.48
41:BA:68:ILE:O	41:BA:71:LEU:HD23	2.14	0.48
42:BB:117:GLU:OE2	46:BF:13:THR:HB	2.14	0.48
42:BB:146:LEU:HB3	42:BB:162:CYS:SG	2.54	0.48
49:BI:37:THR:HG23	49:BI:103:VAL:HG11	1.95	0.48
50:BJ:37:GLN:HB3	50:BJ:62:ARG:HH21	1.78	0.48
53:BM:85:ILE:CD1	53:BM:116:ILE:HD12	2.42	0.48
56:BP:25:ARG:HD3	73:BP:203:HOH:O	2.13	0.48
59:BS:5:LYS:HG2	59:BS:9:ILE:HG21	1.94	0.48
64:BX:30:VAL:HG21	64:BX:34:LYS:O	2.13	0.48
3:1:20:G:O2'	3:1:21:A:OP2	2.32	0.48
3:1:103:U:H2'	3:1:104:C:O4'	2.14	0.48
3:1:1746:C:O2'	3:1:1752:A:N1	2.35	0.48
3:1:1801:C:H5''	6:AB:233:GLY:CA	2.43	0.48
3:1:2318:A:N1	3:1:2337:C:N4	2.60	0.48
3:1:2419:A:H4'	3:1:2420:G:O5'	2.14	0.48
3:1:2462:G:N7	73:1:3652:HOH:O	2.35	0.48
70:1:3121:SPM:H81	73:1:6475:HOH:O	2.14	0.48
4:4:94:U:O2'	4:4:95:C:H5'	2.13	0.48
4:4:429:U:O2'	4:4:430:U:H5'	2.14	0.48
4:4:545:G:H2'	4:4:546:C:C6	2.49	0.48
4:4:1211:OMG:HM21	61:BU:54:ILE:HG21	1.94	0.48
7:AC:13:LEU:HD22	7:AC:26:ARG:NE	2.29	0.48
11:AG:43:GLU:OE1	11:AG:43:GLU:N	2.45	0.48
30:Aa:40:VAL:O	30:Aa:44:LEU:HB2	2.14	0.48
41:BA:42:ALA:CB	53:BM:37:LEU:HD12	2.43	0.48
41:BA:164:GLY:O	41:BA:168:LYS:HG2	2.14	0.48
47:BG:28:ARG:NE	73:BG:202:HOH:O	2.44	0.48
48:BH:78:ARG:HA	48:BH:78:ARG:HE	1.79	0.48
51:BK:49:GLU:O	51:BK:53:VAL:HG23	2.13	0.48
60:BT:63:LEU:HB2	60:BT:68:ARG:NH1	2.29	0.48
64:BX:52:GLU:HG3	64:BX:53:LEU:H	1.79	0.48
3:1:1265:A:OP2	73:1:3408:HOH:O	2.20	0.48
3:1:1279:C:H2'	3:1:1280:G:O4'	2.14	0.48
3:1:1350:G:N2	3:1:1353:A:OP2	2.34	0.48
3:1:1544:U:H2'	3:1:1545:A:H8	1.79	0.48
3:1:1547:G:H2'	3:1:1548:U:O4'	2.14	0.48
4:4:123:G:O2'	4:4:124:A:H5'	2.13	0.48
4:4:247:U:H4'	4:4:248:C:C5'	2.43	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:855:G:H1'	4:4:871:G:O6	2.14	0.48
4:4:887:G:H2'	4:4:888:G:C8	2.48	0.48
4:4:944:A:H5''	4:4:945:C:OP2	2.14	0.48
8:AD:26:ILE:HD11	8:AD:131:MET:CG	2.42	0.48
9:AE:175:GLY:N	9:AE:179:GLY:O	2.35	0.48
12:AH:90:LYS:O	12:AH:92:LYS:NZ	2.36	0.48
17:AN:145:HIS:O	17:AN:149:VAL:HG23	2.14	0.48
37:Ah:30:ARG:NH2	37:Ah:37:GLN:OE1	2.44	0.48
42:BB:37:PHE:CG	42:BB:161:PRO:HG3	2.49	0.48
43:BC:198:ARG:NH2	59:BS:40:ASP:OD2	2.46	0.48
44:BD:153:ASP:OD1	44:BD:154:LYS:NZ	2.44	0.48
45:BE:83:MET:SD	45:BE:119:PRO:HG2	2.53	0.48
46:BF:29:GLU:OE1	46:BF:29:GLU:N	2.46	0.48
48:BH:214:GLU:O	48:BH:218:ILE:HG13	2.13	0.48
54:BN:116:LEU:HG	54:BN:117:GLY:H	1.78	0.48
57:BQ:119:GLU:HA	57:BQ:122:ILE:HD12	1.96	0.48
60:BT:42:MET:HG3	60:BT:43:PRO:O	2.13	0.48
63:BW:92:ASP:O	63:BW:108:LYS:N	2.46	0.48
68:Bb:58:VAL:O	68:Bb:62:LEU:HD12	2.13	0.48
2:3:483:ARG:HD2	2:3:485:VAL:CG2	2.44	0.48
3:1:513:A:H5''	25:AV:88:ARG:HH12	1.79	0.48
3:1:733:C:H2'	3:1:734:G:C8	2.49	0.48
3:1:1084:C:H1'	3:1:2361:G:O6	2.13	0.48
3:1:1517:C:H2'	3:1:1518:G:H8	1.77	0.48
3:1:1989:A:H2'	3:1:1990:A2M:H8	1.96	0.48
3:1:2398:A:H2'	37:Ah:2:LYS:O	2.14	0.48
4:4:899:C:O2'	4:4:1310:C:OP2	2.29	0.48
5:AA:102:MET:SD	38:Ai:77:LEU:HD21	2.53	0.48
8:AD:26:ILE:HG13	8:AD:42:LEU:HD11	1.95	0.48
14:AK:10:VAL:HG22	14:AK:24:VAL:HG22	1.95	0.48
15:AL:48:VAL:HG22	15:AL:60:PHE:CG	2.48	0.48
18:AO:96:LYS:HB3	18:AO:96:LYS:HE3	1.64	0.48
19:AP:80:VAL:HG13	19:AP:82:VAL:HG13	1.96	0.48
24:AU:20:LYS:HE3	24:AU:64:LYS:HG3	1.96	0.48
31:Ab:9:LEU:CD1	31:Ab:13:LEU:HD23	2.44	0.48
48:BH:139:ALA:HB1	48:BH:165:ARG:HB3	1.95	0.48
52:BL:48:LYS:HE3	52:BL:50:LEU:HD11	1.96	0.48
60:BT:52:PRO:HG2	60:BT:55:GLN:OE1	2.14	0.48
66:BZ:69:ARG:HG3	66:BZ:69:ARG:O	2.14	0.48
2:3:476:LYS:HE2	2:3:476:LYS:HA	1.96	0.47
3:1:583:C:O2'	3:1:584:C:H5'	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1:738:C:H2'	3:1:739:A:O4'	2.13	0.47
3:1:1088:G:H2'	3:1:1089:C:C6	2.49	0.47
3:1:1535:C:H3'	73:1:3479:HOH:O	2.13	0.47
3:1:1771:G:H1'	73:1:5192:HOH:O	2.12	0.47
3:1:2951:U:O4	3:1:3010:A:H5''	2.14	0.47
3:1:2979:G:H2'	3:1:2980:G:C8	2.49	0.47
4:4:356:C:O2'	4:4:358:G:OP1	2.15	0.47
4:4:648:A:N1	4:4:661:G:O2'	2.34	0.47
4:4:775:A:H5'	4:4:1470:G:H4'	1.94	0.47
10:AF:82:PRO:O	10:AF:86:GLU:HG2	2.14	0.47
14:AK:18:GLU:HA	14:AK:21:ARG:HH11	1.77	0.47
19:AP:10:ASN:HB3	19:AP:13:LEU:HD12	1.95	0.47
30:Aa:40:VAL:HG21	30:Aa:87:VAL:CG2	2.39	0.47
34:Ae:20:VAL:CG2	34:Ae:63:LYS:HE3	2.44	0.47
40:Ak:3:LEU:HD21	40:Ak:37:THR:HG21	1.95	0.47
58:BR:24:VAL:CG1	58:BR:49:HIS:HB3	2.43	0.47
2:3:476:LYS:HD3	2:3:479:LYS:HB3	1.96	0.47
3:1:91:U:N3	25:AV:110:ASP:OD2	2.46	0.47
3:1:834:A:H2'	3:1:835:G:O4'	2.14	0.47
3:1:1665:G:N2	34:Ae:2:PRO:HG2	2.30	0.47
3:1:1957:OMG:HM22	3:1:1958:G:O4'	2.15	0.47
3:1:2314:G:O2'	3:1:2315:C:H5'	2.14	0.47
3:1:2848:G:O2'	3:1:2849:G:H5'	2.14	0.47
4:4:24:C:OP1	44:BD:9:LYS:NZ	2.33	0.47
4:4:454:G:H2'	4:4:456:A:H8	1.78	0.47
4:4:526:U:OP1	54:BN:8:TYR:OH	2.29	0.47
4:4:601:A:O2'	4:4:602:U:H5'	2.14	0.47
4:4:907:G:H2'	4:4:908:OMG:O4'	2.14	0.47
8:AD:84:PHE:O	8:AD:88:ALA:N	2.34	0.47
12:AH:146:LEU:O	12:AH:150:ARG:HG3	2.14	0.47
14:AK:47:ARG:NH2	14:AK:68:ALA:O	2.38	0.47
15:AL:106:VAL:CG1	15:AL:126:LEU:HD11	2.43	0.47
28:AY:111:ILE:O	39:Aj:138:THR:OG1	2.18	0.47
47:BG:15:LYS:NZ	47:BG:135:GLU:OE1	2.46	0.47
48:BH:121:TYR:CZ	63:BW:96:VAL:HG21	2.49	0.47
48:BH:190:GLU:OE1	63:BW:65:THR:HG21	2.14	0.47
51:BK:4:VAL:HG21	51:BK:97:ALA:CB	2.44	0.47
51:BK:20:LYS:HD3	51:BK:85:ILE:CG2	2.37	0.47
56:BP:24:THR:HG21	56:BP:37:CYS:HB2	1.97	0.47
62:BV:48:LYS:HE3	62:BV:48:LYS:HB3	1.53	0.47
66:BZ:43:ASP:CB	66:BZ:46:ARG:HG3	2.44	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:Bc:47:ARG:CD	73:Bc:202:HOH:O	2.58	0.47
2:3:636:TYR:CE1	2:3:640:ALA:HB3	2.49	0.47
3:1:271:A:H2'	3:1:272:A:C8	2.49	0.47
3:1:1025:G:O2'	3:1:1026:U:H5'	2.14	0.47
3:1:1077:G:N7	73:1:3655:HOH:O	2.36	0.47
3:1:1811:G:O2'	3:1:2112:U:O4	2.25	0.47
3:1:2431:U:O2	22:AS:23:ARG:NH1	2.36	0.47
3:1:2966:U:H2'	3:1:2967:G:O4'	2.13	0.47
4:4:213:G:H2'	4:4:214:C:H6	1.79	0.47
4:4:412:C:H2'	4:4:413:G:C8	2.50	0.47
4:4:1182:C:H4'	4:4:1183:C:H5'	1.96	0.47
4:4:1444:G:H5'	4:4:1444:G:H8	1.78	0.47
7:AC:237:LEU:O	7:AC:241:VAL:HG22	2.14	0.47
19:AP:50:ASN:HA	19:AP:71:LEU:O	2.14	0.47
26:AW:25:ASP:OD1	26:AW:25:ASP:N	2.30	0.47
39:Aj:59:LEU:HA	39:Aj:62:GLU:OE1	2.15	0.47
39:Aj:155:GLN:NE2	39:Aj:170:THR:HG23	2.29	0.47
44:BD:83:GLY:HA2	44:BD:149:ARG:NH2	2.29	0.47
51:BK:17:VAL:HA	51:BK:25:ALA:O	2.14	0.47
2:3:434:THR:HA	2:3:457:VAL:O	2.14	0.47
2:3:476:LYS:NZ	2:3:479:LYS:HG2	2.30	0.47
2:3:518:ASP:OD1	2:3:534:VAL:HG22	2.14	0.47
3:1:1073:G:H5''	3:1:1074:U:OP2	2.14	0.47
3:1:2995:A:H2'	3:1:2996:G:C8	2.49	0.47
4:4:1083:G:H4'	52:BL:43:ILE:HD11	1.96	0.47
4:4:1191:G:H5''	4:4:1192:C:OP2	2.14	0.47
4:4:1399:A:H2'	4:4:1400:G:O4'	2.13	0.47
6:AB:36:LEU:HD12	6:AB:40:THR:CG2	2.36	0.47
7:AC:69:ALA:HB2	7:AC:131:HIS:CE1	2.49	0.47
14:AJ:52:ILE:HD11	29:AZ:26:LYS:NZ	2.29	0.47
25:AV:83:THR:HG22	25:AV:93:TYR:CD1	2.50	0.47
31:Ab:36:TRP:CD1	31:Ab:37:ARG:HG3	2.48	0.47
38:Ai:62:CYS:SG	38:Ai:64:HIS:HB2	2.55	0.47
39:Aj:158:ARG:HD3	39:Aj:182:GLU:CG	2.44	0.47
42:BB:58:LEU:HD23	42:BB:160:ILE:HG21	1.97	0.47
44:BD:134:LEU:HD12	44:BD:137:GLY:C	2.40	0.47
46:BF:68:GLU:OE1	46:BF:68:GLU:N	2.40	0.47
52:BL:75:LYS:C	52:BL:76:ARG:HD2	2.39	0.47
55:BO:71:HIS:ND1	55:BO:72:GLU:HG3	2.30	0.47
69:Bc:57:CYS:HB3	69:Bc:60:CYS:O	2.14	0.47
2:3:628:ILE:HD12	2:3:629:VAL:N	2.29	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1:175:G:H2'	3:1:176:A:O4'	2.14	0.47
3:1:774:U:H2'	3:1:775:C:C6	2.49	0.47
3:1:1318:G:H2'	3:1:1319:G:H8	1.78	0.47
3:1:1340:A:OP1	73:1:3407:HOH:O	2.20	0.47
3:1:1385:C:OP1	7:AC:108:ARG:HA	2.14	0.47
3:1:1639:G:OP1	73:1:3404:HOH:O	2.20	0.47
3:1:2407:C:O2'	3:1:2408:OMU:H5''	2.15	0.47
73:1:3576:HOH:O	8:AD:75:THR:CG2	2.63	0.47
4:4:175:U:H2'	4:4:176:G:O4'	2.15	0.47
4:4:214:C:O2'	4:4:215:C:H5'	2.15	0.47
4:4:683:G:OP2	64:BX:37:ARG:NH2	2.46	0.47
4:4:942:A:H8	4:4:1324:U:H2'	1.79	0.47
70:4:3014:SPM:H31	73:4:3795:HOH:O	2.14	0.47
7:AC:34:TYR:OH	7:AC:167:PRO:HB2	2.14	0.47
12:AH:126:LYS:HA	12:AH:126:LYS:HD3	1.67	0.47
15:AL:106:VAL:HG13	15:AL:128:VAL:HA	1.96	0.47
37:Ah:5:LYS:HE2	37:Ah:91:VAL:CA	2.45	0.47
41:BA:98:ARG:HD3	73:BA:307:HOH:O	2.09	0.47
46:BF:59:LEU:HD23	46:BF:72:PHE:CE1	2.48	0.47
58:BR:33:TYR:HA	58:BR:135:VAL:HG13	1.95	0.47
1:2:50:C:H4'	18:AO:109:ARG:CD	2.45	0.47
2:3:598:LYS:CE	2:3:601:LEU:HD22	2.44	0.47
3:1:1645:G:H2'	3:1:1646:C:C6	2.49	0.47
3:1:1769:U:H2'	73:1:3406:HOH:O	2.13	0.47
3:1:2049:A:O2'	3:1:2050:G:H5'	2.14	0.47
3:1:2402:C:H2'	3:1:2403:U:C6	2.50	0.47
4:4:479:U:H5'	4:4:491:G:C4'	2.44	0.47
4:4:1389:G:O2'	4:4:1390:C:H5'	2.15	0.47
73:4:3428:HOH:O	48:BH:102:THR:HB	2.13	0.47
10:AF:137:ARG:NH1	10:AF:142:LEU:HD23	2.30	0.47
13:AI:110:VAL:HG23	13:AI:111:THR:O	2.15	0.47
21:AR:3:LYS:O	21:AR:22:VAL:HA	2.15	0.47
42:BB:16:TYR:CB	42:BB:51:ILE:HD11	2.45	0.47
44:BD:95:ILE:H	44:BD:95:ILE:HD12	1.79	0.47
47:BG:17:ARG:HA	47:BG:17:ARG:HD3	1.66	0.47
58:BR:16:VAL:CG1	58:BR:40:VAL:HG21	2.42	0.47
1:2:43:A:H2'	1:2:44:U:C6	2.50	0.47
1:2:105:G:O2'	3:1:1037:A:H5''	2.14	0.47
1:2:118:C:H2'	1:2:119:U:O4'	2.15	0.47
2:3:457:VAL:HA	2:3:468:VAL:HG23	1.97	0.47
2:3:591:ALA:O	2:3:612:VAL:HA	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:628:ILE:O	2:3:632:LEU:HD23	2.15	0.47
3:1:60:G:H2'	3:1:61:C:O4'	2.13	0.47
3:1:123:C:H2'	3:1:124:C:C6	2.50	0.47
3:1:626:G:H2'	3:1:627:G:C8	2.49	0.47
3:1:637:U:H2'	3:1:638:G:H8	1.79	0.47
3:1:858:U:H2'	3:1:859:C:C6	2.49	0.47
3:1:956:C:H2'	3:1:957:U:C6	2.49	0.47
3:1:1080:A:H2'	3:1:1081:A:C8	2.50	0.47
3:1:1299:C:OP2	19:AP:18:ARG:NH2	2.45	0.47
3:1:1401:G:H1'	3:1:2825:C:N4	2.30	0.47
3:1:1624:A:H2'	3:1:1625:G:O4'	2.15	0.47
3:1:1681:U:H4'	3:1:1682:C:H5'	1.96	0.47
3:1:2845:G:C2	6:AB:317:ARG:HG2	2.50	0.47
4:4:58:U:H2'	4:4:59:C:C6	2.50	0.47
4:4:103:C:OP1	4:4:316:G:H5'	2.14	0.47
4:4:182:C:O2'	45:BE:127:ALA:O	2.29	0.47
4:4:215:C:H2'	4:4:216:G:H8	1.79	0.47
4:4:325:A:H5'	50:BJ:3:LEU:CD2	2.45	0.47
4:4:460:G:H2'	4:4:461:C:C6	2.49	0.47
4:4:866:A:C5	4:4:867:G:H1'	2.49	0.47
4:4:877:OMU:HM22	4:4:878:A:O4'	2.15	0.47
4:4:1116:C:H2'	4:4:1117:U:C6	2.50	0.47
4:4:1164:G:C4'	52:BL:61:GLN:HG3	2.44	0.47
4:4:1168:G:C2	56:BP:39:ARG:HB3	2.50	0.47
6:AB:114:LEU:HD22	6:AB:118:LEU:CD1	2.45	0.47
6:AB:219:PHE:CG	6:AB:252:PRO:HB3	2.50	0.47
7:AC:63:TYR:CE1	7:AC:258:LEU:HD23	2.50	0.47
15:AL:85:ALA:HB2	15:AL:122:MET:HE3	1.97	0.47
20:AQ:70:GLY:HA2	20:AQ:73:ARG:HH12	1.78	0.47
25:AV:28:LEU:HD23	25:AV:98:PRO:HG2	1.97	0.47
30:Aa:67:GLU:HG2	30:Aa:68:LYS:HG3	1.95	0.47
39:Aj:44:TYR:HE2	39:Aj:47:ASP:HB2	1.79	0.47
39:Aj:104:PHE:CD1	39:Aj:109:LYS:HD3	2.50	0.47
43:BC:145:LYS:HB3	43:BC:148:THR:O	2.13	0.47
45:BE:111:PRO:HD2	45:BE:114:GLU:CD	2.39	0.47
46:BF:39:GLU:HB2	46:BF:42:ILE:HD13	1.96	0.47
53:BM:18:TRP:HA	53:BM:82:ALA:O	2.15	0.47
58:BR:43:ASP:OD2	58:BR:98:ARG:NH2	2.47	0.47
60:BT:42:MET:CG	60:BT:47:PHE:HB2	2.44	0.47
66:BZ:20:GLN:NE2	66:BZ:35:LYS:HG3	2.30	0.47
2:3:398:GLN:OE1	2:3:398:GLN:N	2.48	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:490:LEU:CD1	2:3:597:VAL:HG11	2.44	0.47
3:1:259:U:H2'	3:1:260:C:H6	1.79	0.47
3:1:444:A:H2'	3:1:445:C:C6	2.50	0.47
3:1:604:G:H2'	3:1:605:A:C8	2.50	0.47
3:1:957:U:H1'	3:1:1319:G:H1'	1.96	0.47
3:1:1291:C:O2'	3:1:1292:C:H5'	2.15	0.47
3:1:1395:A:H2'	3:1:1396:G:O4'	2.15	0.47
3:1:1427:G:H22	3:1:1783:A:H5''	1.79	0.47
3:1:2030:G:H3'	3:1:2031:G:H8	1.80	0.47
3:1:2403:U:H2'	3:1:2404:C:C6	2.49	0.47
3:1:2764:C:H2'	3:1:2765:C:H6	1.80	0.47
4:4:631:G:H2'	4:4:632:C:C6	2.50	0.47
11:AG:8:ASP:CB	11:AG:11:GLN:HB2	2.44	0.47
16:AM:30:LYS:O	16:AM:33:LYS:HG3	2.15	0.47
24:AU:21:ILE:CD1	24:AU:63:VAL:HB	2.45	0.47
43:BC:184:GLY:HA2	43:BC:186:TYR:CD1	2.49	0.47
49:BI:81:VAL:HG12	49:BI:123:GLY:O	2.15	0.47
58:BR:58:LEU:HD12	58:BR:112:ILE:CG2	2.44	0.47
66:BZ:10:TYR:CE2	66:BZ:63:MET:HE3	2.50	0.47
66:BZ:48:LEU:HD22	66:BZ:70:GLU:CG	2.44	0.47
69:Bc:14:PRO:HB2	69:Bc:23:LEU:HD22	1.97	0.47
2:3:387:ILE:CG2	2:3:543:GLU:HG3	2.45	0.47
3:1:1557:A:OP2	14:AJ:48:ARG:NH2	2.45	0.47
3:1:2859:G:O2'	9:AE:74:THR:HG23	2.15	0.47
4:4:183:C:OP2	73:4:3101:HOH:O	2.20	0.47
4:4:703:G:OP1	57:BQ:94:ARG:NH1	2.48	0.47
73:4:3573:HOH:O	45:BE:129:SER:HB3	2.14	0.47
6:AB:197:PRO:HB2	6:AB:327:GLU:HG2	1.97	0.47
8:AD:116:MET:HB3	8:AD:116:MET:HE3	1.63	0.47
9:AE:124:ILE:HG21	9:AE:162:ALA:HB1	1.97	0.47
29:AZ:15:GLY:HA3	29:AZ:88:ASP:O	2.15	0.47
41:BA:41:LEU:HD23	41:BA:59:VAL:HG11	1.95	0.47
41:BA:189:MET:HE3	41:BA:189:MET:HB3	1.70	0.47
48:BH:53:ARG:HB2	73:BH:301:HOH:O	2.15	0.47
48:BH:187:PRO:HD2	48:BH:190:GLU:HG3	1.97	0.47
1:2:17:U:OP2	1:2:73:C:O2'	2.31	0.47
3:1:670:U:H2'	3:1:671:C:H6	1.80	0.47
3:1:966:G:O2'	3:1:967:C:H5'	2.14	0.47
3:1:986:C:OP2	73:1:3409:HOH:O	2.20	0.47
3:1:3022:U:H2'	3:1:3023:G7M:C8	2.45	0.47
4:4:257:G:O2'	4:4:258:G:H5'	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:479:U:H2'	4:4:491:G:H1'	1.97	0.47
4:4:1030:C:H2'	4:4:1031:G:H8	1.79	0.47
4:4:1284:A:H5''	73:4:3526:HOH:O	2.15	0.47
8:AD:35:LEU:CD1	8:AD:72:VAL:HG23	2.45	0.47
9:AE:123:LYS:HE3	9:AE:123:LYS:HB3	1.68	0.47
14:AK:75:LYS:NZ	14:AK:76:ALA:HB2	2.30	0.47
17:AN:58:ARG:HB3	17:AN:132:PRO:HD3	1.96	0.47
21:AR:70:MET:HE3	21:AR:70:MET:HB3	1.83	0.47
23:AT:26:THR:OG1	23:AT:29:GLN:OE1	2.31	0.47
25:AV:51:ASP:OD1	25:AV:107:ASP:N	2.35	0.47
41:BA:156:LYS:O	41:BA:160:GLU:HG2	2.15	0.47
42:BB:16:TYR:CG	42:BB:51:ILE:HD11	2.49	0.47
42:BB:29:ASN:O	42:BB:33:GLU:HG2	2.15	0.47
45:BE:50:TYR:CG	62:BV:19:LEU:HD12	2.50	0.47
50:BJ:42:GLY:HA3	50:BJ:63:GLN:NE2	2.29	0.47
52:BL:44:PRO:HB3	52:BL:76:ARG:NH2	2.23	0.47
58:BR:64:GLU:OE1	58:BR:94:ARG:HD3	2.14	0.47
61:BU:75:ARG:NE	61:BU:96:ALA:O	2.47	0.47
68:Bb:15:ARG:HG2	68:Bb:34:ILE:CG2	2.45	0.47
68:Bb:17:ARG:NH1	73:Bb:103:HOH:O	2.47	0.47
1:2:44:U:N3	1:2:47:G:OP2	2.48	0.46
3:1:797:G:H2'	3:1:798:G:C8	2.50	0.46
3:1:2679:A:H2'	3:1:2680:A:O4'	2.15	0.46
3:1:2884:OMC:HM22	3:1:2885:OMC:O4'	2.15	0.46
4:4:102:A:N6	4:4:242:G:H1	2.08	0.46
4:4:678:C:H4'	4:4:679:A:O5'	2.15	0.46
4:4:1031:G:H2'	4:4:1032:U:C6	2.50	0.46
5:AA:119:SER:O	5:AA:122:THR:OG1	2.29	0.46
13:AI:52:VAL:HG22	13:AI:53:HIS:H	1.80	0.46
19:AP:31:ILE:O	19:AP:35:ILE:HG12	2.15	0.46
19:AP:83:ALA:HA	19:AP:103:LEU:O	2.15	0.46
20:AQ:97:ARG:HG2	20:AQ:118:TYR:CE1	2.50	0.46
25:AV:50:GLY:O	25:AV:66:LYS:NZ	2.48	0.46
28:AY:127:ARG:HG3	28:AY:128:GLU:H	1.79	0.46
29:AZ:86:VAL:HG11	29:AZ:94:ILE:HG21	1.96	0.46
38:Ai:84:GLU:OE2	38:Ai:84:GLU:N	2.42	0.46
39:Aj:78:VAL:CG1	39:Aj:143:ILE:HD13	2.44	0.46
43:BC:179:VAL:HG23	43:BC:181:LEU:CD1	2.46	0.46
47:BG:6:LEU:HD12	47:BG:21:ILE:CD1	2.43	0.46
48:BH:204:PRO:O	48:BH:210:ARG:HD3	2.15	0.46
49:BI:83:TYR:CZ	49:BI:120:LYS:HD3	2.50	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:BK:5:SER:HA	73:BK:308:HOH:O	2.14	0.46
51:BK:54:LYS:HD2	51:BK:81:MET:CE	2.45	0.46
57:BQ:83:GLU:O	57:BQ:84:LEU:HD23	2.15	0.46
59:BS:35:VAL:HG21	59:BS:51:ALA:HB2	1.97	0.46
62:BV:20:LEU:HD22	62:BV:87:ILE:HD13	1.97	0.46
2:3:379:THR:HG21	2:3:454:ASP:CG	2.41	0.46
2:3:478:TYR:O	2:3:482:GLY:N	2.34	0.46
2:3:602:ASP:O	2:3:605:VAL:HG22	2.15	0.46
3:1:120:C:H2'	3:1:121:U:C6	2.50	0.46
3:1:1498:G:O2'	3:1:1499:C:H5'	2.15	0.46
3:1:2692:G:H1'	6:AB:236:ARG:HH22	1.79	0.46
3:1:2845:G:H2'	3:1:2846:G:C8	2.49	0.46
4:4:519:U:OP2	4:4:520:G:O2'	2.20	0.46
4:4:686:G:O6	64:BX:15:LYS:HE3	2.14	0.46
4:4:873:A:H2'	4:4:874:A:H8	1.78	0.46
4:4:1017:G:H2'	4:4:1018:C:C6	2.49	0.46
6:AB:152:ARG:CZ	6:AB:159:LYS:HG2	2.45	0.46
7:AC:25:GLU:HG2	7:AC:26:ARG:O	2.16	0.46
7:AC:180:ILE:HB	7:AC:237:LEU:HD13	1.97	0.46
9:AE:48:VAL:HG13	9:AE:72:LEU:HD23	1.97	0.46
10:AF:40:ILE:O	10:AF:43:GLN:HG2	2.14	0.46
10:AF:49:LYS:HG3	10:AF:107:ILE:HD13	1.97	0.46
11:AG:1:MET:SD	11:AG:1:MET:N	2.74	0.46
11:AG:90:ARG:HG2	11:AG:92:ASP:OD1	2.16	0.46
23:AT:41:SER:O	23:AT:45:SER:OG	2.28	0.46
39:Aj:87:ILE:HD12	39:Aj:88:TRP:CD1	2.49	0.46
42:BB:139:MET:CE	46:BF:36:LEU:HD23	2.45	0.46
44:BD:109:GLN:CD	44:BD:125:ARG:HB2	2.39	0.46
45:BE:17:ARG:HD3	45:BE:17:ARG:HA	1.67	0.46
47:BG:106:ILE:HD13	47:BG:113:ILE:CD1	2.45	0.46
49:BI:71:ASP:HB3	49:BI:130:TYR:CE2	2.50	0.46
2:3:555:THR:CG2	4:4:891:G:H4'	2.45	0.46
2:3:636:TYR:CD1	2:3:640:ALA:HB3	2.50	0.46
3:1:496:G:H2'	3:1:497:A:C8	2.50	0.46
3:1:968:G:H5''	3:1:969:G:OP2	2.15	0.46
3:1:1448:G:H2'	3:1:1449:C:C6	2.50	0.46
3:1:2522:A:O4'	15:AL:72:ILE:HG21	2.15	0.46
3:1:2530:G:OP1	37:Ah:31:ARG:NH1	2.49	0.46
3:1:2555:OMC:HM22	3:1:2556:C:C5'	2.39	0.46
70:1:3126:SPM:H42	73:1:4560:HOH:O	2.15	0.46
4:4:437:G:N2	62:BV:35:SER:OG	2.41	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:1023:G:H4'	4:4:1024:U:H5'	1.95	0.46
6:AB:121:PRO:HD2	6:AB:124:PHE:CE2	2.50	0.46
8:AD:169:PHE:O	8:AD:174:GLY:N	2.49	0.46
9:AE:41:LYS:HG2	9:AE:43:PHE:CZ	2.50	0.46
14:AJ:75:LYS:HA	14:AJ:78:GLU:OE2	2.14	0.46
14:AJ:77:LEU:CD1	14:AJ:82:LEU:HB2	2.44	0.46
19:AP:90:LYS:HE3	19:AP:94:LYS:HE3	1.97	0.46
34:Ae:20:VAL:HG13	34:Ae:35:ARG:HB3	1.97	0.46
41:BA:51:LYS:O	41:BA:55:ARG:NE	2.48	0.46
42:BB:12:PRO:HB2	42:BB:14:GLU:OE2	2.14	0.46
49:BI:47:VAL:HG13	49:BI:63:VAL:HG13	1.97	0.46
50:BJ:70:TYR:CE1	50:BJ:75:ARG:HA	2.49	0.46
57:BQ:97:ARG:O	57:BQ:100:LYS:HG3	2.15	0.46
60:BT:15:TRP:HE1	60:BT:113:ILE:HD13	1.79	0.46
68:Bb:5:LEU:O	68:Bb:8:VAL:HG22	2.15	0.46
2:3:325:VAL:CB	2:3:635:VAL:HG22	2.43	0.46
2:3:329:THR:CG2	2:3:481:ARG:HE	2.29	0.46
2:3:337:MET:HE1	2:3:458:VAL:CG1	2.40	0.46
2:3:486:LYS:HA	2:3:595:ALA:O	2.15	0.46
3:1:467:U:H2'	3:1:468:C:H5'	1.97	0.46
3:1:745:C:H2'	3:1:746:G:O4'	2.15	0.46
3:1:1068:G:H5''	70:1:3125:SPM:H31	1.96	0.46
3:1:1770:G:OP2	73:1:3406:HOH:O	2.20	0.46
3:1:2429:C:H2'	3:1:2430:G:O4'	2.15	0.46
3:1:2969:A:C6	3:1:2996:G:H5'	2.51	0.46
4:4:29:G:H2'	4:4:30:C:H6	1.81	0.46
4:4:145:U:OP1	47:BG:89:ARG:N	2.41	0.46
4:4:767:C:O2'	4:4:768:C:H5'	2.15	0.46
4:4:1401:G:H22	4:4:1424:A:H2	1.63	0.46
4:4:1404:C:H2'	4:4:1405:C:C6	2.51	0.46
5:AA:31:PRO:HG2	5:AA:34:ILE:CG2	2.46	0.46
5:AA:31:PRO:HG2	5:AA:34:ILE:HG21	1.95	0.46
8:AD:89:LEU:O	8:AD:92:VAL:HG12	2.16	0.46
14:AJ:62:ILE:HD12	14:AJ:64:ILE:HG12	1.97	0.46
14:AK:40:LYS:C	14:AK:42:LEU:N	2.73	0.46
17:AN:29:ILE:HG13	17:AN:126:ARG:CD	2.46	0.46
21:AR:8:VAL:HG13	21:AR:18:VAL:HG22	1.97	0.46
21:AR:62:LYS:HD2	21:AR:62:LYS:O	2.15	0.46
23:AT:131:HIS:NE2	23:AT:162:GLU:OE1	2.44	0.46
40:Ak:8:GLU:HG2	40:Ak:64:PHE:HE2	1.79	0.46
41:BA:68:ILE:HA	41:BA:71:LEU:CD2	2.44	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:BB:74:LEU:HD23	42:BB:121:LEU:CD1	2.45	0.46
3:1:108:G:OP2	3:1:110:A:O2'	2.32	0.46
3:1:450:C:O2'	3:1:451:G:H5'	2.16	0.46
3:1:1649:G:O6	29:AZ:20:GLY:HA3	2.15	0.46
3:1:2104:OMG:HM22	3:1:2105:U:C5'	2.42	0.46
3:1:2594:C:C2'	3:1:2595:G:H5'	2.45	0.46
3:1:2721:G:H2'	3:1:2722:G:O4'	2.15	0.46
4:4:15:OMU:C2'	4:4:16:G:H5'	2.46	0.46
4:4:645:G:O2'	4:4:646:G:H5'	2.16	0.46
4:4:757:C:H2'	4:4:758:C:H6	1.80	0.46
4:4:912:A:H2'	4:4:913:G:H8	1.77	0.46
13:AI:127:MET:HG2	13:AI:143:VAL:HG12	1.98	0.46
16:AM:120:VAL:HG21	16:AM:130:GLU:HG3	1.97	0.46
29:AZ:64:PHE:CD1	29:AZ:65:PRO:HD2	2.50	0.46
46:BF:96:ARG:HG3	46:BF:100:GLU:OE2	2.16	0.46
47:BG:63:VAL:HA	47:BG:111:VAL:HG21	1.98	0.46
51:BK:44:GLU:O	61:BU:146:ARG:NH2	2.49	0.46
62:BV:31:HIS:O	62:BV:69:GLY:HA3	2.15	0.46
64:BX:36:ILE:O	64:BX:68:THR:HA	2.16	0.46
64:BX:53:LEU:H	64:BX:58:ALA:HB3	1.81	0.46
2:3:525:GLY:O	53:BM:53:ARG:NH2	2.48	0.46
3:1:82:A:OP2	73:1:3412:HOH:O	2.20	0.46
3:1:1430:A:H5'	3:1:1431:A:OP2	2.15	0.46
3:1:1578:G:H2'	3:1:1579:C:H6	1.80	0.46
3:1:1868:A:H4'	3:1:1869:U:OP1	2.15	0.46
3:1:2398:A:H4'	3:1:2399:A:O5'	2.16	0.46
4:4:93:C:H2'	4:4:94:U:C6	2.50	0.46
4:4:465:OMG:HM22	4:4:466:G:C5'	2.37	0.46
4:4:564:C:O2'	4:4:565:C:H5'	2.16	0.46
4:4:807:G:O2'	4:4:808:G:H2'	2.16	0.46
4:4:1089:A:C3'	4:4:1090:C:H5'	2.46	0.46
5:AA:30:TYR:OH	5:AA:155:THR:OG1	2.32	0.46
17:AN:102:ARG:HH12	17:AN:104:LEU:HD21	1.81	0.46
25:AV:117:ILE:O	25:AV:121:LYS:HE3	2.16	0.46
39:Aj:51:LEU:HD13	39:Aj:52:PRO:O	2.16	0.46
42:BB:140:GLY:HA3	69:Bc:28:ARG:NE	2.23	0.46
62:BV:31:HIS:HB2	62:BV:34:SER:OG	2.16	0.46
3:1:575:G:O2'	3:1:576:G:OP1	2.28	0.46
3:1:638:G:H2'	3:1:639:C:C6	2.49	0.46
3:1:872:OMC:HM22	3:1:873:G:O4'	2.15	0.46
3:1:1648:A:H4'	3:1:1649:G:OP2	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1:1808:A:H61	3:1:2117:C:H42	1.63	0.46
3:1:1861:U:H2'	3:1:1862:U:C6	2.51	0.46
3:1:2510:G:O3'	37:Ah:36:GLY:HA3	2.15	0.46
3:1:2795:C:O2'	3:1:2796:C:H5'	2.16	0.46
4:4:263:PSU:H5''	50:BJ:36:PRO:HA	1.98	0.46
4:4:391:C:OP1	62:BV:116:ARG:NH1	2.47	0.46
4:4:414:G:H2'	4:4:415:G:H8	1.81	0.46
4:4:420:G:H2'	4:4:421:A:C8	2.51	0.46
4:4:900:C:H1'	73:4:3208:HOH:O	2.15	0.46
4:4:1443:G:C3'	4:4:1444:G:H5''	2.46	0.46
9:AE:93:LYS:O	9:AE:189:VAL:HG22	2.16	0.46
10:AF:76:GLU:HG2	16:AM:11:TRP:CD1	2.51	0.46
14:AK:40:LYS:O	14:AK:42:LEU:N	2.49	0.46
21:AR:51:ARG:O	21:AR:52:GLU:HG2	2.16	0.46
23:AT:143:ILE:HD13	23:AT:151:ALA:HB1	1.97	0.46
30:Aa:56:ALA:HB3	30:Aa:91:GLN:HE22	1.81	0.46
43:BC:181:LEU:HD22	43:BC:186:TYR:CG	2.51	0.46
46:BF:129:SER:OG	46:BF:130:VAL:N	2.48	0.46
50:BJ:22:ARG:HG2	50:BJ:24:ARG:O	2.16	0.46
61:BU:155:PRO:HA	61:BU:156:PRO:HD3	1.84	0.46
3:1:452:G:O2'	3:1:453:C:H5'	2.16	0.46
3:1:585:U:HO2'	3:1:586:C:H5'	1.80	0.46
3:1:912:G:H2'	3:1:913:C:C6	2.50	0.46
3:1:914:C:H2'	3:1:915:C:C6	2.50	0.46
3:1:1838:C:H5''	38:Ai:9:VAL:CG1	2.34	0.46
3:1:2135:A:H5'	23:AT:152:THR:HB	1.97	0.46
3:1:2851:OMU:HM22	3:1:2852:A:C5'	2.41	0.46
4:4:138:G:N3	47:BG:112:GLN:NE2	2.63	0.46
4:4:622:G:N2	4:4:797:G:H4'	2.30	0.46
4:4:675:G:H2'	4:4:676:A:C8	2.51	0.46
4:4:702:A:O2'	4:4:703:G:H5'	2.15	0.46
4:4:1125:C:O2'	59:BS:52:GLY:HA3	2.16	0.46
4:4:1134:U:H2'	4:4:1135:A:H5'	1.97	0.46
4:4:1210:OMG:HM22	4:4:1211:OMG:O4'	2.15	0.46
7:AC:200:GLU:O	7:AC:204:GLU:HG2	2.16	0.46
8:AD:31:GLY:HA3	8:AD:34:ARG:HB2	1.98	0.46
8:AD:54:ARG:HH21	8:AD:67:GLY:HA2	1.80	0.46
17:AN:106:MET:HG3	17:AN:106:MET:O	2.16	0.46
22:AS:83:LYS:HZ2	22:AS:85:ILE:HD11	1.80	0.46
29:AZ:10:VAL:HB	29:AZ:92:SER:HB2	1.98	0.46
34:Ae:8:VAL:CG2	34:Ae:53:LEU:HD11	2.46	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:BB:16:TYR:HB3	42:BB:51:ILE:HD11	1.98	0.46
44:BD:61:LEU:HD13	46:BF:122:CYS:HA	1.97	0.46
45:BE:65:TYR:O	45:BE:89:VAL:HG23	2.15	0.46
45:BE:164:GLU:HG2	45:BE:165:ASN:CG	2.40	0.46
50:BJ:37:GLN:OE1	50:BJ:62:ARG:NH2	2.49	0.46
60:BT:55:GLN:HG3	60:BT:97:ILE:CD1	2.39	0.46
1:2:20:G:N7	73:2:208:HOH:O	2.35	0.46
2:3:604:LEU:CD2	2:3:625:LYS:HG2	2.46	0.46
3:1:596:A:OP1	73:1:3417:HOH:O	2.21	0.46
3:1:1919:A:H5'	3:1:2722:G:H4'	1.98	0.46
3:1:2186:U:O2'	3:1:2187:A:H5'	2.16	0.46
3:1:2562:A:N6	73:1:3734:HOH:O	2.39	0.46
4:4:147:G:H2'	4:4:148:G:C8	2.50	0.46
4:4:782:G:H2'	4:4:783:C:C6	2.50	0.46
4:4:1435:G:O2'	4:4:1436:C:O4'	2.30	0.46
4:4:1483:C:OP2	53:BM:136:ARG:HB3	2.15	0.46
8:AD:41:LEU:O	8:AD:45:LEU:HD23	2.15	0.46
10:AF:15:LEU:HB3	10:AF:16:PRO:HD2	1.98	0.46
10:AF:107:ILE:HG13	10:AF:109:VAL:O	2.16	0.46
13:AI:79:GLN:HB2	13:AI:81:PHE:HE1	1.80	0.46
18:AO:144:ARG:HA	18:AO:184:PHE:CD2	2.50	0.46
39:Aj:172:SER:OG	39:Aj:175:GLU:HG3	2.16	0.46
42:BB:89:PHE:HD2	42:BB:90:CYS:SG	2.39	0.46
43:BC:176:VAL:HG22	43:BC:189:GLU:HA	1.97	0.46
44:BD:80:TYR:CB	44:BD:88:PRO:HB3	2.45	0.46
48:BH:41:LEU:HB2	48:BH:47:PHE:CE1	2.51	0.46
48:BH:77:LYS:HE3	48:BH:77:LYS:HB3	1.56	0.46
48:BH:97:ARG:NH1	73:BH:308:HOH:O	2.49	0.46
50:BJ:70:TYR:OH	50:BJ:75:ARG:HD2	2.15	0.46
51:BK:9:GLU:HG2	51:BK:10:ASN:ND2	2.31	0.46
55:BO:120:HIS:CD2	55:BO:126:VAL:HG11	2.51	0.46
61:BU:37:LYS:HB3	73:BU:204:HOH:O	2.15	0.46
68:Bb:28:THR:O	68:Bb:32:LYS:HB2	2.16	0.46
2:3:481:ARG:NH2	2:3:482:GLY:HA2	2.31	0.46
3:1:69:C:OP1	27:AX:57:ARG:HD3	2.16	0.46
3:1:203:A:N6	3:1:213:G:H1'	2.31	0.46
3:1:513:A:H1'	3:1:528:G:N2	2.31	0.46
3:1:1715:A:H2'	3:1:1716:G:O4'	2.16	0.46
3:1:2208:U:H2'	3:1:2209:C:C6	2.50	0.46
4:4:201:G:O2'	4:4:202:G:H5'	2.16	0.46
4:4:233:G:H2'	4:4:234:G:O4'	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:382:G:N7	70:4:3014:SPM:N14	2.64	0.46
4:4:646:G:N3	53:BM:45:ARG:NH2	2.45	0.46
70:4:3005:SPM:H121	73:4:4062:HOH:O	2.15	0.46
5:AA:56:ILE:O	5:AA:63:GLU:HA	2.16	0.46
5:AA:80:VAL:HA	5:AA:91:VAL:O	2.16	0.46
8:AD:52:LEU:H	8:AD:52:LEU:HD12	1.81	0.46
13:AI:103:GLU:OE1	26:AW:23:ARG:HA	2.16	0.46
14:AJ:27:ASP:CB	14:AJ:35:VAL:HB	2.46	0.46
14:AK:5:ILE:CD1	14:AK:57:PRO:HG3	2.46	0.46
15:AL:139:GLU:OE2	15:AL:140:LYS:HG3	2.17	0.46
28:AY:72:ASP:O	28:AY:76:GLU:HG2	2.16	0.46
29:AZ:21:LEU:CD1	29:AZ:50:ILE:HD11	2.46	0.46
32:Ac:36:LYS:HD2	32:Ac:41:GLY:O	2.15	0.46
32:Ac:42:GLN:OE1	32:Ac:42:GLN:N	2.40	0.46
42:BB:21:VAL:CG1	42:BB:173:ILE:HD11	2.43	0.46
50:BJ:50:GLU:O	50:BJ:57:HIS:HA	2.16	0.46
55:BO:80:ASN:OD1	55:BO:92:HIS:HA	2.15	0.46
66:BZ:18:VAL:HG13	66:BZ:34:VAL:CG2	2.45	0.46
68:Bb:16:LEU:HD13	68:Bb:54:LEU:HB3	1.98	0.46
69:Bc:55:TYR:CE2	69:Bc:65:PRO:HD2	2.51	0.46
1:2:54:G:O2'	1:2:55:A:H5'	2.16	0.45
2:3:325:VAL:O	2:3:635:VAL:HG13	2.16	0.45
2:3:382:ASP:OD1	2:3:429:LYS:NZ	2.44	0.45
2:3:475:VAL:CG1	2:3:601:LEU:HG	2.45	0.45
3:1:140:C:H5'	24:AU:33:GLN:HE21	1.81	0.45
3:1:566:G:O2'	3:1:567:G:H5'	2.16	0.45
3:1:944:U:H5'	3:1:2544:A:O2'	2.16	0.45
3:1:1572:C:H2'	3:1:1573:C:H6	1.80	0.45
3:1:1636:G:H2'	3:1:1637:C:O4'	2.15	0.45
3:1:2512:U:H2'	3:1:2513:C:C6	2.51	0.45
4:4:5:4AC:O2	4:4:467:OMG:HM21	2.16	0.45
4:4:1289:OMG:HM21	4:4:1328:C:H1'	1.98	0.45
7:AC:41:MET:SD	7:AC:174:SER:HB2	2.56	0.45
8:AD:22:VAL:HG22	8:AD:135:VAL:CG2	2.40	0.45
8:AD:36:GLU:O	8:AD:40:ASN:ND2	2.49	0.45
43:BC:157:THR:OG1	43:BC:158:TYR:N	2.49	0.45
55:BO:22:VAL:HG23	55:BO:50:ALA:O	2.15	0.45
62:BV:108:ALA:HA	62:BV:111:ARG:HH21	1.81	0.45
63:BW:54:ILE:CG2	63:BW:69:ILE:HD12	2.46	0.45
66:BZ:43:ASP:OD1	66:BZ:46:ARG:NE	2.46	0.45
2:3:334:ARG:NH2	2:3:438:SER:HA	2.31	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1:326:A:O2'	3:1:327:A:H5'	2.15	0.45
3:1:492:OMC:HM22	3:1:493:OMC:H5''	1.97	0.45
3:1:950:C:H2'	3:1:951:C:C6	2.51	0.45
3:1:1123:G:O2'	3:1:1130:A:N1	2.47	0.45
3:1:1680:U:O2	20:AQ:36:ASP:HB3	2.15	0.45
3:1:2734:C:OP1	6:AB:16:TYR:OH	2.26	0.45
4:4:412:C:H2'	4:4:413:G:H8	1.81	0.45
4:4:572:OMC:HM22	4:4:573:C:C5'	2.44	0.45
4:4:779:G:O2'	4:4:780:A:H5'	2.16	0.45
4:4:1059:C:C4	4:4:1061:A:H5'	2.51	0.45
4:4:1210:OMG:OP1	61:BU:42:LYS:HG3	2.16	0.45
4:4:1223:U:H1'	4:4:1224:C:C5	2.50	0.45
9:AE:34:GLY:HA3	9:AE:86:VAL:HB	1.97	0.45
10:AF:64:LYS:NZ	10:AF:148:ARG:HB2	2.31	0.45
11:AG:7:LEU:CD1	11:AG:9:LEU:HD23	2.45	0.45
11:AG:17:GLU:HA	11:AG:45:ARG:O	2.16	0.45
12:AH:67:TRP:CH2	12:AH:71:VAL:HG21	2.51	0.45
13:AI:133:TRP:HB3	13:AI:136:ILE:HD13	1.98	0.45
16:AM:21:GLU:HG3	16:AM:25:ARG:HH12	1.81	0.45
18:AO:31:ARG:NH1	22:AS:34:GLU:OE2	2.49	0.45
18:AO:152:ALA:HB1	18:AO:163:TYR:CE1	2.50	0.45
28:AY:44:MET:HE1	28:AY:77:VAL:HG11	1.98	0.45
29:AZ:25:LYS:O	29:AZ:29:LEU:HB2	2.15	0.45
34:Ae:6:PHE:O	40:Ak:68:GLU:HG2	2.17	0.45
43:BC:170:ASN:CB	43:BC:171:ARG:HH11	2.30	0.45
45:BE:97:VAL:HG22	45:BE:107:LEU:CD2	2.45	0.45
45:BE:135:LEU:O	45:BE:142:ASN:HA	2.16	0.45
48:BH:99:GLY:HA2	48:BH:102:THR:HG23	1.98	0.45
50:BJ:102:LYS:HB2	50:BJ:117:SER:O	2.16	0.45
53:BM:107:ARG:CZ	53:BM:107:ARG:HB2	2.45	0.45
60:BT:32:ARG:CG	60:BT:50:LEU:HD22	2.42	0.45
62:BV:97:LEU:HD13	62:BV:100:GLU:OE1	2.17	0.45
64:BX:47:PRO:HA	64:BX:49:LEU:CD2	2.39	0.45
65:BY:48:LEU:O	65:BY:59:ALA:N	2.40	0.45
2:3:345:ASN:HA	2:3:368:VAL:O	2.16	0.45
2:3:571:ARG:NH1	2:3:573:SER:HB3	2.31	0.45
3:1:14:C:H2'	3:1:15:C:C6	2.51	0.45
3:1:305:A:H2'	3:1:306:C:O4'	2.16	0.45
3:1:662:C:H2'	3:1:663:G:H8	1.80	0.45
3:1:1518:G:H5'	3:1:1615:A:H1'	1.98	0.45
3:1:2667:OMG:H2'	3:1:2668:C:O4'	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:267:A:O2'	58:BR:118:PRO:O	2.33	0.45
4:4:675:G:H2'	4:4:676:A:H8	1.81	0.45
8:AD:10:LYS:HD2	8:AD:164:GLU:OE1	2.15	0.45
9:AE:5:TYR:HE1	9:AE:7:VAL:HB	1.80	0.45
9:AE:29:VAL:HG22	9:AE:42:GLU:HG3	1.99	0.45
17:AN:142:LYS:HB2	17:AN:144:GLU:OE2	2.17	0.45
25:AV:77:ILE:HG12	25:AV:96:ILE:O	2.16	0.45
28:AY:20:ARG:HB2	28:AY:63:TRP:CD1	2.51	0.45
42:BB:179:ARG:HB2	42:BB:194:LEU:HD11	1.98	0.45
45:BE:118:LYS:HE2	45:BE:120:LEU:CD2	2.45	0.45
46:BF:137:LYS:HB2	46:BF:142:GLU:OE2	2.16	0.45
51:BK:52:ARG:O	51:BK:56:GLN:HG3	2.16	0.45
1:2:34:C:OP2	18:AO:41:ASN:ND2	2.31	0.45
1:2:44:U:O2'	1:2:46:A:N7	2.36	0.45
3:1:44:A:H2'	3:1:45:A:C8	2.51	0.45
3:1:315:G:O2'	3:1:316:G:H5'	2.16	0.45
3:1:1077:G:OP1	73:1:3410:HOH:O	2.20	0.45
3:1:1595:G:H2'	3:1:1596:C:C6	2.51	0.45
3:1:1971:OMG:HM23	73:1:7037:HOH:O	2.16	0.45
3:1:2006:G:O2'	3:1:2007:G:H5'	2.17	0.45
4:4:506:C:O2'	4:4:510:U:OP1	2.33	0.45
4:4:1016:G:H5''	43:BC:143:SER:OG	2.16	0.45
4:4:1390:C:H2'	4:4:1391:C:H6	1.81	0.45
4:4:1390:C:O2'	4:4:1391:C:H5'	2.17	0.45
10:AF:10:PHE:CE2	10:AF:86:GLU:HG3	2.51	0.45
11:AG:105:LYS:O	11:AG:107:VAL:HG22	2.16	0.45
16:AM:30:LYS:H	16:AM:30:LYS:HG3	1.62	0.45
24:AU:6:VAL:HB	24:AU:22:THR:HB	1.98	0.45
30:Aa:54:GLY:HA3	30:Aa:88:GLU:CD	2.41	0.45
39:Aj:63:TYR:O	39:Aj:109:LYS:HE3	2.17	0.45
40:Ak:47:LEU:HD22	40:Ak:80:ILE:HG12	1.97	0.45
41:BA:63:ASP:OD1	41:BA:63:ASP:N	2.48	0.45
42:BB:11:VAL:HG13	42:BB:12:PRO:HD2	1.99	0.45
42:BB:11:VAL:HG21	42:BB:176:VAL:HG22	1.97	0.45
43:BC:194:PRO:HD2	43:BC:197:LEU:CD2	2.45	0.45
50:BJ:45:ASP:OD1	50:BJ:64:ALA:HA	2.16	0.45
53:BM:112:SER:OG	53:BM:114:LEU:HD23	2.17	0.45
57:BQ:64:LYS:HB3	57:BQ:65:PRO:HD3	1.97	0.45
3:1:349:U:H4'	7:AC:239:GLY:O	2.16	0.45
3:1:424:G:H2'	3:1:425:C:O4'	2.15	0.45
3:1:1022:C:H2'	3:1:1023:C:C6	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1:1318:G:H2'	3:1:1319:G:C8	2.51	0.45
3:1:1611:G:O2'	3:1:1612:C:H5'	2.16	0.45
3:1:1619:G:O2'	40:Ak:32:GLU:OE1	2.34	0.45
4:4:141:A:H2'	4:4:142:A:O4'	2.17	0.45
4:4:210:U:H5''	4:4:211:C:C5	2.51	0.45
4:4:270:C:H2'	4:4:271:C:C6	2.51	0.45
4:4:723:G:H2'	4:4:724:G:C8	2.51	0.45
4:4:1080:C:H2'	4:4:1081:U:H6	1.79	0.45
4:4:1080:C:O2'	4:4:1081:U:H5'	2.17	0.45
4:4:1206:U:OP2	48:BH:188:ILE:HG22	2.17	0.45
4:4:1434:G:H2'	4:4:1435:G:O4'	2.17	0.45
8:AD:113:GLU:HA	8:AD:129:TRP:O	2.17	0.45
10:AF:140:HIS:O	10:AF:142:LEU:HD13	2.17	0.45
13:AI:8:ARG:NH1	13:AI:113:GLU:HB3	2.32	0.45
14:AJ:15:LEU:HD21	32:Ac:75:ALA:HB2	1.98	0.45
14:AJ:73:VAL:O	14:AJ:77:LEU:HD23	2.16	0.45
17:AN:38:THR:HG23	17:AN:83:ASP:O	2.15	0.45
23:AT:57:LEU:HD21	23:AT:61:LYS:HZ3	1.81	0.45
26:AW:49:LYS:HD2	26:AW:49:LYS:HA	1.64	0.45
31:Ab:136:LYS:O	31:Ab:140:GLU:HG3	2.16	0.45
52:BL:54:VAL:CG2	56:BP:38:ARG:HG3	2.46	0.45
55:BO:24:TYR:CD2	55:BO:34:ILE:HD11	2.51	0.45
58:BR:43:ASP:OD1	58:BR:44:PRO:HD2	2.16	0.45
62:BV:80:ASP:OD1	62:BV:83:LEU:HB3	2.15	0.45
66:BZ:18:VAL:HG22	66:BZ:34:VAL:HG21	1.98	0.45
68:Bb:44:GLU:OE2	68:Bb:45:ARG:HG3	2.17	0.45
2:3:460:ASP:OD1	2:3:463:GLY:N	2.50	0.45
3:1:195:G:H2'	3:1:196:G:O4'	2.17	0.45
3:1:227:G:C2'	3:1:228:G:H5'	2.46	0.45
3:1:902:OMG:H3'	3:1:910:A:C2	2.52	0.45
3:1:1234:C:H2'	3:1:1235:C:H6	1.80	0.45
3:1:1424:G:OP1	3:1:2822:G:O2'	2.29	0.45
3:1:2110:A:H2'	3:1:2111:C:O4'	2.17	0.45
3:1:2771:U:O2'	73:1:3403:HOH:O	2.20	0.45
4:4:238:C:H1'	58:BR:115:GLU:OE1	2.17	0.45
4:4:927:U:H5'	4:4:950:C:H1'	1.98	0.45
4:4:928:G:H2'	4:4:929:G:O4'	2.17	0.45
4:4:1172:G:H4'	43:BC:183:PRO:HA	1.97	0.45
4:4:1386:G:H2'	4:4:1387:G:O4'	2.17	0.45
4:4:1447:G:O2'	4:4:1448:G:H5'	2.16	0.45
5:AA:58:MET:HE1	5:AA:80:VAL:CG2	2.47	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AB:202:ASP:HB2	6:AB:313:ARG:HG3	1.98	0.45
7:AC:52:GLU:HG3	7:AC:144:ARG:HB3	1.99	0.45
8:AD:99:SER:HA	8:AD:162:ARG:HH22	1.82	0.45
9:AE:105:VAL:HG22	9:AE:114:ILE:HG12	1.99	0.45
12:AH:35:VAL:O	16:AM:179:LEU:HD11	2.16	0.45
14:AJ:9:ARG:HE	14:AJ:61:LYS:HB2	1.81	0.45
28:AY:123:ASP:O	28:AY:125:LYS:HE3	2.16	0.45
41:BA:168:LYS:O	41:BA:172:GLU:HG2	2.16	0.45
48:BH:54:ASP:OD1	66:BZ:63:MET:HE1	2.17	0.45
51:BK:129:GLY:O	51:BK:130:ILE:HD13	2.17	0.45
55:BO:113:LYS:HG3	60:BT:19:THR:HG23	1.99	0.45
61:BU:103:LYS:O	61:BU:107:GLN:HG3	2.16	0.45
62:BV:117:GLU:OE1	62:BV:117:GLU:N	2.50	0.45
64:BX:30:VAL:CG1	64:BX:34:LYS:HD3	2.46	0.45
2:3:607:GLN:HG2	2:3:609:VAL:O	2.17	0.45
3:1:491:A:H2'	3:1:492:OMC:O4'	2.16	0.45
3:1:851:A:O2'	3:1:1778:A:H4'	2.17	0.45
3:1:1621:C:C2'	3:1:1622:G:H5'	2.46	0.45
3:1:1723:G:OP2	73:1:3420:HOH:O	2.21	0.45
3:1:2056:5MC:H2'	3:1:2057:A:H5''	1.98	0.45
3:1:2857:C:O2'	9:AE:153:SER:OG	2.33	0.45
3:1:2980:G:C6	3:1:2982:U:H4'	2.51	0.45
4:4:39:U:C2	4:4:312:C:H4'	2.52	0.45
4:4:885:U:H2'	4:4:886:U:C6	2.52	0.45
4:4:1492:C:C2	64:BX:5:ARG:HG2	2.51	0.45
5:AA:107:GLU:HG2	5:AA:114:GLY:N	2.32	0.45
8:AD:148:ARG:CD	18:AO:109:ARG:HE	2.29	0.45
14:AJ:24:VAL:HG23	14:AJ:86:MET:HE2	1.99	0.45
15:AL:81:VAL:HG11	15:AL:122:MET:HB2	1.98	0.45
16:AM:9:ALA:O	16:AM:13:ARG:HG2	2.16	0.45
18:AO:154:ARG:O	18:AO:157:GLU:HG3	2.17	0.45
29:AZ:25:LYS:HB2	29:AZ:25:LYS:HE2	1.57	0.45
32:Ac:63:ARG:HG2	32:Ac:64:PRO:HD2	1.98	0.45
41:BA:26:LYS:HB2	41:BA:26:LYS:HE2	1.62	0.45
42:BB:179:ARG:NH1	42:BB:193:ASP:OD1	2.49	0.45
43:BC:138:PHE:HA	43:BC:191:ARG:O	2.17	0.45
46:BF:47:LEU:HD23	46:BF:80:ASN:HB3	1.99	0.45
49:BI:98:GLN:HB3	69:Bc:4:ARG:O	2.17	0.45
51:BK:7:LEU:HD23	51:BK:7:LEU:HA	1.83	0.45
60:BT:57:ARG:O	60:BT:61:ARG:HG3	2.17	0.45
60:BT:77:ALA:HA	60:BT:87:VAL:HG11	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:BU:28:LYS:HA	61:BU:28:LYS:HD3	1.74	0.45
61:BU:146:ARG:HB3	61:BU:149:LEU:HG	1.98	0.45
62:BV:14:LEU:HD21	62:BV:23:LYS:HB2	1.98	0.45
62:BV:99:GLU:O	62:BV:102:LYS:HB2	2.17	0.45
2:3:351:SER:HB2	4:4:1195:G:H4'	1.99	0.45
2:3:481:ARG:CZ	2:3:482:GLY:HA2	2.47	0.45
3:1:294:G:H2'	3:1:295:G:O4'	2.16	0.45
3:1:472:A:O2'	3:1:473:G:H5'	2.17	0.45
3:1:582:C:O2'	3:1:583:C:H5'	2.16	0.45
3:1:636:C:H2'	3:1:637:U:C6	2.52	0.45
3:1:1504:G:H2'	3:1:1505:C:O4'	2.17	0.45
3:1:1631:G:H1'	3:1:1651:A:H61	1.81	0.45
3:1:2047:U:H2'	3:1:2048:A:N7	2.32	0.45
3:1:2193:C:OP1	5:AA:3:LYS:HD2	2.17	0.45
3:1:2617:A:H5''	73:1:4925:HOH:O	2.16	0.45
4:4:85:G:H2'	4:4:86:C:C6	2.51	0.45
7:AC:19:TYR:O	7:AC:20:ILE:HD13	2.17	0.45
8:AD:113:GLU:HB3	8:AD:128:ILE:CG2	2.47	0.45
18:AO:37:VAL:CG1	18:AO:116:VAL:HG12	2.47	0.45
19:AP:52:GLY:N	19:AP:73:GLY:O	2.50	0.45
30:Aa:76:VAL:CG2	30:Aa:90:LYS:HD2	2.47	0.45
39:Aj:159:SER:O	39:Aj:160:GLU:HG2	2.16	0.45
44:BD:98:LEU:HD23	44:BD:99:ASP:N	2.32	0.45
47:BG:6:LEU:HD23	47:BG:7:VAL:N	2.32	0.45
54:BN:49:MET:HE3	54:BN:104:ILE:HG21	1.98	0.45
60:BT:86:LYS:HD3	60:BT:87:VAL:N	2.32	0.45
68:Bb:17:ARG:CZ	68:Bb:54:LEU:HD21	2.47	0.45
2:3:332:ARG:NE	2:3:440:THR:HG22	2.32	0.45
2:3:600:VAL:O	2:3:604:LEU:HB2	2.17	0.45
3:1:894:G:H4'	3:1:895:G:O5'	2.16	0.45
3:1:1300:G:N1	7:AC:21:LYS:O	2.31	0.45
3:1:1638:C:H4'	3:1:1651:A:H4'	1.98	0.45
3:1:1906:C:OP2	73:1:3419:HOH:O	2.21	0.45
3:1:2022:A:O2'	3:1:2023:G:OP1	2.34	0.45
3:1:2045:C:H2'	3:1:2046:U:H5'	1.99	0.45
4:4:142:A:H2'	4:4:143:A:C8	2.52	0.45
4:4:144:C:H2'	4:4:145:U:O4'	2.17	0.45
4:4:210:U:H5''	4:4:211:C:H5	1.82	0.45
4:4:212:C:H5'	4:4:213:G:OP1	2.17	0.45
4:4:339:C:H2'	4:4:340:C:H6	1.81	0.45
11:AG:7:LEU:HD21	11:AG:12:ILE:CD1	2.47	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:AK:31:GLU:OE2	21:AR:75:VAL:HG13	2.17	0.45
15:AL:58:TRP:HB2	70:AL:201:SPM:H31	1.99	0.45
15:AL:97:VAL:HG11	15:AL:104:LEU:HG	1.98	0.45
17:AN:29:ILE:HG13	17:AN:126:ARG:HD3	1.98	0.45
19:AP:114:LYS:HE2	19:AP:114:LYS:HB3	1.58	0.45
23:AT:16:LEU:HD22	23:AT:130:ILE:HG23	1.99	0.45
41:BA:27:TRP:CZ3	53:BM:17:ARG:HD3	2.52	0.45
41:BA:149:ARG:HA	41:BA:152:GLU:CD	2.41	0.45
42:BB:175:TRP:CE3	42:BB:198:PRO:HG3	2.51	0.45
47:BG:69:HIS:HB3	47:BG:72:VAL:CG2	2.41	0.45
49:BI:6:LEU:HD22	49:BI:29:PRO:HD2	1.99	0.45
50:BJ:66:TYR:CG	50:BJ:79:LYS:HE2	2.52	0.45
52:BL:50:LEU:HD12	56:BP:32:TYR:OH	2.16	0.45
56:BP:28:VAL:O	56:BP:29:ILE:HG22	2.17	0.45
3:1:246:A:H4'	3:1:247:G:OP1	2.16	0.45
3:1:627:G:O2'	3:1:628:U:H5'	2.16	0.45
3:1:818:G:OP1	20:AQ:81:ARG:NH2	2.50	0.45
3:1:1265:A:O2'	3:1:1269:A:N1	2.42	0.45
3:1:1812:A:O2'	3:1:1818:G:N7	2.43	0.45
3:1:1954:U:O2'	5:AA:115:LYS:O	2.31	0.45
3:1:2154:G:O2'	3:1:2155:OMU:H5''	2.16	0.45
3:1:2327:A:H2'	3:1:2328:A:C8	2.52	0.45
3:1:2864:C:H2'	3:1:2865:A:O4'	2.16	0.45
4:4:130:A:O2'	4:4:131:C:H5'	2.17	0.45
4:4:1320:C:H2'	4:4:1321:G:H8	1.81	0.45
4:4:1435:G:H2'	4:4:1436:C:C6	2.51	0.45
4:4:1435:G:C3'	4:4:1436:C:H5''	2.47	0.45
8:AD:102:ASP:CG	8:AD:106:ASN:HB3	2.41	0.45
39:Aj:79:LEU:HD23	39:Aj:143:ILE:HD11	1.98	0.45
53:BM:32:ILE:O	53:BM:45:ARG:HA	2.17	0.45
53:BM:106:ILE:HD12	64:BX:45:VAL:HG23	1.99	0.45
69:Bc:45:SER:O	69:Bc:49:ARG:HG3	2.17	0.45
2:3:325:VAL:O	2:3:635:VAL:HA	2.17	0.44
2:3:329:THR:HG22	2:3:481:ARG:HE	1.82	0.44
2:3:506:MET:HA	2:3:506:MET:HE3	2.00	0.44
3:1:282:G:H5''	16:AM:56:PRO:HB2	1.99	0.44
3:1:593:G:OP2	28:AY:148:ARG:NH2	2.50	0.44
3:1:662:C:H2'	3:1:663:G:C8	2.52	0.44
3:1:1447:G:O2'	3:1:1448:G:H5'	2.17	0.44
3:1:1473:C:H5''	3:1:1474:C:OP2	2.18	0.44
3:1:1849:G:O2'	3:1:1850:U:H5'	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1:2554:C:OP2	73:1:3415:HOH:O	2.21	0.44
4:4:12:U:H2'	4:4:13:C:H6	1.80	0.44
4:4:215:C:H2'	4:4:216:G:C8	2.51	0.44
4:4:386:A:H2'	4:4:387:A:C8	2.52	0.44
4:4:389:C:H2'	4:4:390:G:C8	2.52	0.44
4:4:502:U:OP2	67:Ba:23:LYS:NZ	2.50	0.44
5:AA:48:GLY:O	5:AA:182:LYS:HE2	2.16	0.44
7:AC:27:PRO:HG2	7:AC:50:PHE:O	2.17	0.44
7:AC:68:SER:HA	7:AC:71:PHE:CE2	2.52	0.44
7:AC:279:ARG:HE	7:AC:279:ARG:HB2	1.55	0.44
8:AD:152:SER:OG	8:AD:153:LYS:N	2.50	0.44
8:AD:169:PHE:HA	8:AD:173:LEU:HB2	1.99	0.44
9:AE:103:MET:O	9:AE:105:VAL:HG23	2.18	0.44
13:AI:89:ARG:HH11	13:AI:104:ASP:HA	1.82	0.44
18:AO:25:ARG:O	18:AO:29:LEU:HG	2.17	0.44
38:AI:31:GLU:OE1	38:AI:35:ARG:NH2	2.50	0.44
38:AI:74:GLN:OE1	38:AI:79:LYS:HE2	2.17	0.44
40:AK:47:LEU:O	40:AK:51:GLU:HG3	2.17	0.44
42:BB:56:GLU:O	42:BB:60:ILE:HG13	2.18	0.44
43:BC:174:ARG:HA	43:BC:190:VAL:O	2.15	0.44
45:BE:177:GLY:N	45:BE:194:PHE:O	2.50	0.44
51:BK:103:GLU:HA	51:BK:106:LYS:CD	2.47	0.44
52:BL:54:VAL:HG12	52:BL:67:ASP:HB3	1.98	0.44
53:BM:107:ARG:O	53:BM:111:ARG:HG2	2.16	0.44
58:BR:33:TYR:HB3	58:BR:137:TRP:HB2	1.99	0.44
59:BS:26:GLU:HG3	59:BS:58:VAL:CG1	2.47	0.44
65:BY:42:LEU:HD23	65:BY:42:LEU:HA	1.83	0.44
69:Bc:23:LEU:HD12	69:Bc:45:SER:HB2	1.99	0.44
1:2:12:G:OP1	18:AO:24:ARG:HD2	2.18	0.44
3:1:379:C:H5	73:1:7147:HOH:O	1.98	0.44
3:1:1713:A:H2'	3:1:1714:A:C8	2.51	0.44
3:1:2643:G:O2'	73:1:3405:HOH:O	2.20	0.44
4:4:14:C:OP1	46:BF:140:SER:OG	2.16	0.44
4:4:344:C:O2'	4:4:345:C:H5'	2.17	0.44
4:4:1187:G:H4'	60:BT:135:THR:HG21	1.99	0.44
4:4:1210:OMG:HM23	4:4:1210:OMG:H1'	1.83	0.44
10:AF:6:ASP:HB3	10:AF:9:THR:HG23	1.99	0.44
15:AL:8:ALA:O	15:AL:12:ARG:HG3	2.17	0.44
22:AS:3:LYS:HE2	22:AS:3:LYS:HB2	1.70	0.44
28:AY:112:SER:O	39:Aj:142:LYS:NZ	2.43	0.44
28:AY:124:PHE:CZ	28:AY:126:ALA:HA	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:AZ:75:ALA:O	29:AZ:76:LYS:HG2	2.17	0.44
34:Ae:18:ALA:HB2	34:Ae:34:ALA:HB1	1.99	0.44
46:BF:143:VAL:HG22	46:BF:176:THR:HG23	1.98	0.44
47:BG:49:LEU:HB3	47:BG:53:VAL:CG1	2.46	0.44
59:BS:20:TYR:CD1	59:BS:38:LEU:HD13	2.51	0.44
62:BV:88:GLU:OE1	62:BV:89:PRO:HD2	2.17	0.44
2:3:434:THR:H	2:3:447:LYS:HE2	1.82	0.44
2:3:494:ALA:HB2	2:3:620:VAL:O	2.17	0.44
3:1:421:U:H5''	3:1:422:U:OP2	2.18	0.44
3:1:671:C:H2'	3:1:672:A:C8	2.51	0.44
3:1:902:OMG:H4'	3:1:903:A:OP1	2.18	0.44
3:1:1448:G:O2'	3:1:1449:C:H5'	2.17	0.44
3:1:1555:G:OP2	14:AJ:46:ARG:NH2	2.34	0.44
3:1:2743:U:H4'	3:1:2744:G:C5'	2.48	0.44
3:1:2988:A:H2'	3:1:2989:G:O4'	2.18	0.44
4:4:79:G:O2'	4:4:80:G:H5'	2.18	0.44
4:4:194:A:H5''	4:4:195:A:OP1	2.18	0.44
4:4:905:G:OP1	48:BH:171:ARG:NH2	2.51	0.44
4:4:943:A:N6	4:4:1190:U:OP1	2.51	0.44
5:AA:93:PRO:HA	5:AA:152:GLY:O	2.17	0.44
5:AA:195:SER:HB2	5:AA:197:TYR:CE1	2.52	0.44
8:AD:169:PHE:CD1	8:AD:173:LEU:HD22	2.52	0.44
16:AM:71:PRO:CB	16:AM:92:THR:HG22	2.41	0.44
28:AY:22:ILE:O	28:AY:25:THR:HG22	2.17	0.44
29:AZ:9:GLN:HB3	29:AZ:76:LYS:NZ	2.31	0.44
29:AZ:92:SER:HG	29:AZ:94:ILE:HB	1.83	0.44
41:BA:70:HIS:HA	41:BA:73:ILE:HD12	1.99	0.44
41:BA:179:LEU:CB	41:BA:192:VAL:HG11	2.47	0.44
47:BG:130:PRO:HG2	68:Bb:6:GLU:OE1	2.17	0.44
48:BH:211:LYS:O	48:BH:214:GLU:HG3	2.17	0.44
62:BV:46:LEU:HD23	62:BV:57:ILE:HG21	1.98	0.44
66:BZ:39:LEU:HD23	66:BZ:39:LEU:HA	1.67	0.44
1:2:54:G:H2'	1:2:55:A:C8	2.52	0.44
1:2:74:G:O2'	1:2:75:C:H5'	2.18	0.44
3:1:213:G:H3'	12:AH:25:ARG:HD2	2.00	0.44
3:1:567:G:H2'	3:1:568:C:C6	2.52	0.44
3:1:1244:G:O2'	3:1:1245:G:H5'	2.18	0.44
3:1:1978:G:O2'	5:AA:212:PRO:O	2.31	0.44
3:1:2701:A:N1	73:1:3669:HOH:O	2.36	0.44
70:1:3116:SPM:H132	23:AT:146:ARG:HA	1.99	0.44
4:4:218:C:H2'	4:4:219:A:H8	1.82	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:239:A:H2'	4:4:240:C:O4'	2.17	0.44
4:4:366:G:N2	4:4:368:A:H3'	2.32	0.44
4:4:440:C:H4'	62:BV:61:LYS:HE2	2.00	0.44
4:4:603:A:H2'	4:4:604:C:C6	2.51	0.44
4:4:699:G:O2'	4:4:700:C:H5'	2.17	0.44
4:4:1099:A:N1	61:BU:143:VAL:HG11	2.32	0.44
18:AO:153:LYS:O	18:AO:157:GLU:HG2	2.16	0.44
25:AV:52:THR:CB	25:AV:105:ASP:HB3	2.46	0.44
39:Aj:23:PHE:HB3	39:Aj:176:PHE:CD2	2.52	0.44
45:BE:126:THR:HB	45:BE:136:HIS:NE2	2.32	0.44
47:BG:5:LYS:HE2	47:BG:111:VAL:HG12	2.00	0.44
56:BP:24:THR:HG23	56:BP:26:GLU:H	1.81	0.44
58:BR:18:LEU:HD11	58:BR:24:VAL:CG2	2.48	0.44
63:BW:87:LEU:HA	63:BW:90:ARG:HB2	1.99	0.44
65:BY:37:MET:C	65:BY:51:PRO:HG3	2.42	0.44
68:Bb:17:ARG:CZ	68:Bb:54:LEU:HD11	2.48	0.44
2:3:334:ARG:HA	2:3:337:MET:HG2	2.00	0.44
2:3:571:ARG:HH11	2:3:573:SER:HB3	1.82	0.44
3:1:216:C:H2'	3:1:217:C:C6	2.52	0.44
3:1:394:C:O2'	3:1:395:G:H5'	2.18	0.44
3:1:1074:U:O5'	3:1:1075:G:H5'	2.17	0.44
3:1:1257:G:O6	3:1:2144:C:O2'	2.35	0.44
3:1:1428:G:C6	3:1:1777:A:H5'	2.52	0.44
3:1:1468:G:O2'	73:1:3423:HOH:O	2.21	0.44
3:1:2589:C:C5'	73:1:4650:HOH:O	2.64	0.44
4:4:35:G:H2'	4:4:36:G:H8	1.81	0.44
4:4:104:G:H2'	4:4:105:U:H6	1.83	0.44
4:4:119:U:H2'	4:4:120:C:H6	1.81	0.44
4:4:177:G:N2	58:BR:29:ILE:O	2.48	0.44
4:4:649:G:OP1	53:BM:50:MET:HG2	2.18	0.44
7:AC:219:ARG:HD2	7:AC:220:TYR:CZ	2.53	0.44
8:AD:166:VAL:HG11	8:AD:177:VAL:HG11	1.99	0.44
14:AJ:75:LYS:HA	14:AJ:78:GLU:HG2	1.99	0.44
15:AL:115:LYS:HE3	15:AL:132:VAL:CG1	2.46	0.44
20:AQ:32:VAL:HG22	20:AQ:37:ASP:HB3	2.00	0.44
23:AT:181:LEU:HA	23:AT:184:ARG:HB2	2.00	0.44
27:AX:9:LYS:HE2	27:AX:10:ALA:N	2.32	0.44
42:BB:37:PHE:CD1	42:BB:161:PRO:HG3	2.53	0.44
42:BB:110:PRO:HB3	46:BF:13:THR:HG22	2.00	0.44
51:BK:8:GLN:HE22	51:BK:11:PRO:HD2	1.83	0.44
62:BV:52:VAL:HG13	62:BV:53:GLU:O	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:BW:43:ILE:HD11	63:BW:86:ALA:HB2	2.00	0.44
65:BY:17:PHE:O	65:BY:66:LEU:N	2.50	0.44
68:Bb:17:ARG:HD2	73:Bb:103:HOH:O	2.16	0.44
69:Bc:56:ARG:HG3	69:Bc:63:VAL:CG1	2.44	0.44
3:1:579:G:O2'	73:1:3418:HOH:O	2.21	0.44
3:1:1290:C:H2'	3:1:1291:C:H6	1.83	0.44
3:1:1351:U:H1'	31:Ab:68:GLU:O	2.17	0.44
4:4:86:C:O2'	4:4:383:G:OP1	2.34	0.44
4:4:555:C:O2'	4:4:556:A:H5'	2.18	0.44
4:4:606:G:H2'	4:4:607:C:C6	2.52	0.44
4:4:606:G:H2'	4:4:607:C:H6	1.83	0.44
4:4:664:A:H4'	4:4:665:A:O5'	2.18	0.44
4:4:910:G:N1	4:4:1304:G:OP2	2.47	0.44
4:4:1173:C:C2'	4:4:1174:C:H5'	2.48	0.44
4:4:1253:A:N3	4:4:1319:G:O2'	2.35	0.44
6:AB:81:PRO:O	6:AB:150:GLN:HG3	2.18	0.44
6:AB:279:ILE:HD11	6:AB:333:VAL:HG11	1.99	0.44
9:AE:113:THR:HA	9:AE:124:ILE:O	2.18	0.44
14:AJ:4:VAL:CG2	29:AZ:56:LEU:HB3	2.48	0.44
27:AX:8:PRO:HG3	27:AX:57:ARG:HD2	2.00	0.44
29:AZ:12:ILE:HG12	29:AZ:17:VAL:HG21	1.98	0.44
39:Aj:177:LEU:HB3	39:Aj:181:ARG:NH2	2.33	0.44
41:BA:61:LEU:CD2	41:BA:171:LEU:HD23	2.47	0.44
41:BA:126:MET:HE1	41:BA:166:PHE:CD2	2.53	0.44
44:BD:53:ILE:CG2	44:BD:79:LEU:HD21	2.47	0.44
46:BF:201:LYS:NZ	49:BI:69:ILE:O	2.39	0.44
48:BH:143:GLU:HG3	48:BH:215:LEU:HD21	2.00	0.44
51:BK:75:VAL:HG11	51:BK:83:GLN:HB3	2.00	0.44
53:BM:106:ILE:HB	64:BX:45:VAL:CG2	2.47	0.44
55:BO:29:ILE:HG22	55:BO:31:GLY:H	1.83	0.44
55:BO:86:GLU:OE1	55:BO:86:GLU:N	2.50	0.44
58:BR:18:LEU:HD11	58:BR:24:VAL:HG23	1.99	0.44
62:BV:7:ALA:HB1	62:BV:9:PHE:CZ	2.52	0.44
64:BX:49:LEU:HD23	64:BX:49:LEU:H	1.81	0.44
2:3:375:VAL:O	2:3:430:SER:HA	2.18	0.44
3:1:728:C:H2'	3:1:729:G:O4'	2.17	0.44
3:1:938:A:O2'	73:1:3421:HOH:O	2.21	0.44
3:1:994:G:O2'	3:1:995:G:H5'	2.17	0.44
3:1:1327:G:O2'	7:AC:212:LYS:NZ	2.46	0.44
3:1:1339:G:H1'	3:1:1364:A:N6	2.33	0.44
3:1:2455:C:O2'	3:1:2456:U:H5'	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1:2885:OMC:HM22	3:1:2886:C:C5'	2.45	0.44
4:4:188:C:H2'	4:4:189:C:H6	1.82	0.44
4:4:593:C:H4'	4:4:594:G:OP2	2.18	0.44
4:4:740:C:H2'	4:4:741:A:O4'	2.18	0.44
4:4:1309:C:H2'	4:4:1310:C:C6	2.52	0.44
6:AB:26:PRO:HG2	6:AB:311:VAL:CG2	2.47	0.44
7:AC:188:LYS:NZ	7:AC:192:VAL:HB	2.32	0.44
12:AH:7:VAL:HG13	12:AH:24:GLY:HA3	1.99	0.44
14:AJ:13:LYS:O	14:AJ:20:GLY:N	2.43	0.44
18:AO:170:TYR:HD1	18:AO:175:LEU:HD23	1.82	0.44
29:AZ:37:ILE:HD12	29:AZ:84:LEU:HD11	2.00	0.44
32:Ac:37:CYS:HB3	32:Ac:42:GLN:OE1	2.18	0.44
45:BE:125:LYS:HD3	45:BE:153:ILE:O	2.17	0.44
46:BF:61:GLN:HG2	46:BF:68:GLU:HG3	2.00	0.44
46:BF:114:ARG:HH11	69:Bc:8:ILE:HG22	1.81	0.44
46:BF:118:GLY:O	49:BI:97:ARG:N	2.51	0.44
47:BG:8:LEU:HD11	47:BG:117:LEU:CD2	2.47	0.44
47:BG:8:LEU:HD11	47:BG:117:LEU:HD23	2.00	0.44
50:BJ:110:VAL:HG23	50:BJ:129:LEU:HD12	1.98	0.44
56:BP:19:CYS:SG	56:BP:37:CYS:HB3	2.57	0.44
58:BR:130:LYS:HB2	58:BR:133:ASP:OD1	2.18	0.44
61:BU:10:ASP:OD1	61:BU:11:LEU:HD12	2.18	0.44
61:BU:24:VAL:HG21	61:BU:113:PHE:HE2	1.82	0.44
62:BV:31:HIS:CD2	62:BV:37:PRO:HD3	2.52	0.44
1:2:95:C:H2'	1:2:96:G:O4'	2.18	0.44
2:3:475:VAL:HG22	2:3:628:ILE:CD1	2.44	0.44
2:3:550:ARG:HE	2:3:550:ARG:HB3	1.44	0.44
3:1:44:A:OP2	3:1:108:G:N1	2.47	0.44
3:1:139:C:H2'	3:1:140:C:C6	2.52	0.44
3:1:336:G:H2'	3:1:337:A:O4'	2.18	0.44
3:1:576:G:H2'	3:1:577:A:O4'	2.18	0.44
3:1:637:U:H2'	3:1:638:G:C8	2.52	0.44
3:1:919:G:H4'	70:1:3134:SPM:H21	2.00	0.44
3:1:1162:C:H1'	73:1:3717:HOH:O	2.17	0.44
3:1:1669:U:OP1	34:Ae:24:LYS:NZ	2.41	0.44
3:1:2063:C:OP2	3:1:2064:U:O2'	2.33	0.44
3:1:2088:OMU:HM22	3:1:2089:G:C5'	2.43	0.44
3:1:2119:G:H2'	3:1:2120:C:C6	2.53	0.44
4:4:524:A:H5''	4:4:525:C:OP1	2.17	0.44
4:4:639:U:H2'	4:4:640:C:H6	1.83	0.44
4:4:1479:C:H2'	4:4:1480:C:C6	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AB:148:ALA:HA	6:AB:162:GLU:O	2.18	0.44
6:AB:175:ASP:OD2	6:AB:175:ASP:N	2.51	0.44
12:AH:72:LEU:HB2	16:AM:180:LEU:HD13	1.99	0.44
48:BH:114:ARG:O	48:BH:118:ILE:HG13	2.18	0.44
55:BO:6:ARG:HH11	55:BO:9:VAL:HG22	1.83	0.44
60:BT:64:LYS:H	60:BT:64:LYS:HG2	1.64	0.44
64:BX:87:GLU:HA	64:BX:90:LYS:HZ1	1.81	0.44
2:3:604:LEU:HG	2:3:610:VAL:CG2	2.47	0.44
3:1:90:U:OP2	27:AX:4:ARG:NH2	2.51	0.44
3:1:212:G:H5'	12:AH:7:VAL:HB	2.00	0.44
3:1:660:G:H2'	3:1:661:C:C6	2.53	0.44
3:1:682:C:H5'	73:1:5284:HOH:O	2.17	0.44
3:1:1110:G:OP1	73:1:3411:HOH:O	2.20	0.44
3:1:1678:G:H2'	3:1:1679:U:O4'	2.18	0.44
3:1:1889:G:H2'	3:1:1891:A:OP2	2.18	0.44
3:1:2053:A:H2'	3:1:2054:G:O4'	2.18	0.44
3:1:2331:C:O2'	3:1:2332:G:H5'	2.18	0.44
70:1:3120:SPM:H132	73:1:5008:HOH:O	2.18	0.44
4:4:75:C:H6	4:4:212:C:H2'	1.82	0.44
4:4:183:C:O2'	45:BE:131:GLY:HA2	2.18	0.44
4:4:328:G:N1	4:4:331:A:OP2	2.51	0.44
4:4:1007:G:H4'	4:4:1008:A:OP1	2.18	0.44
4:4:1156:C:H5'	43:BC:164:ILE:HG22	1.99	0.44
4:4:1260:G:OP2	63:BW:98:LYS:NZ	2.50	0.44
6:AB:109:GLU:OE2	6:AB:123:LYS:HG2	2.17	0.44
8:AD:49:GLU:HG3	8:AD:50:PRO:HD2	2.00	0.44
10:AF:11:TYR:O	16:AM:22:ARG:NH2	2.26	0.44
12:AH:87:VAL:CG2	16:AM:160:LEU:HD11	2.48	0.44
13:AI:74:PRO:HA	13:AI:77:ARG:CZ	2.48	0.44
18:AO:11:PHE:O	18:AO:15:ARG:HG2	2.18	0.44
18:AO:88:ILE:O	18:AO:92:LYS:HG3	2.18	0.44
31:Ab:108:ILE:HG21	31:Ab:117:ARG:HG2	1.99	0.44
40:Ak:8:GLU:OE2	40:Ak:56:TYR:OH	2.23	0.44
45:BE:98:VAL:HG21	45:BE:236:ILE:O	2.17	0.44
45:BE:198:VAL:HA	58:BR:140:LYS:O	2.18	0.44
46:BF:10:GLU:OE2	46:BF:12:LYS:HB2	2.17	0.44
47:BG:19:PHE:HB3	47:BG:46:LEU:HD23	2.00	0.44
50:BJ:65:ARG:HG2	50:BJ:66:TYR:CD1	2.52	0.44
54:BN:97:ILE:CD1	54:BN:129:VAL:HG21	2.47	0.44
61:BU:83:LYS:NZ	61:BU:87:LYS:O	2.45	0.44
1:2:56:A:H2'	1:2:57:G:O4'	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:435:VAL:HG21	2:3:444:VAL:CG2	2.39	0.43
2:3:572:TYR:HB3	2:3:575:VAL:HG11	1.99	0.43
3:1:5:C:H4'	3:1:6:A:H5'	2.00	0.43
3:1:136:G:H2'	3:1:137:G:O4'	2.18	0.43
3:1:325:G:H5''	3:1:326:A:OP1	2.18	0.43
3:1:1496:A:O4'	33:Ad:42:SER:HB2	2.18	0.43
4:4:52:U:H2'	4:4:53:G:H8	1.83	0.43
4:4:188:C:H2'	4:4:189:C:C6	2.53	0.43
4:4:479:U:H5'	4:4:491:G:H4'	2.00	0.43
4:4:669:C:O2'	4:4:670:C:H5'	2.18	0.43
4:4:1094:U:H2'	4:4:1095:C:C6	2.52	0.43
4:4:1371:G:O4'	4:4:1478:MA6:H4'	2.18	0.43
4:4:1472:A:H2'	4:4:1473:G:C8	2.53	0.43
9:AE:9:GLU:HB3	9:AE:56:LYS:HE2	2.00	0.43
9:AE:13:PRO:HG2	9:AE:16:VAL:HG21	1.98	0.43
14:AK:32:ASN:O	14:AK:52:ILE:HG13	2.18	0.43
16:AM:112:LEU:HD22	16:AM:135:ASP:HA	2.00	0.43
20:AQ:94:ARG:O	20:AQ:98:ARG:HG2	2.18	0.43
24:AU:80:VAL:CG1	27:AX:32:LYS:HG3	2.47	0.43
28:AY:66:TRP:CZ2	28:AY:166:TYR:HB2	2.53	0.43
47:BG:38:ILE:HG12	47:BG:55:ILE:HG13	1.98	0.43
47:BG:126:PRO:HA	68:Bb:14:THR:OG1	2.18	0.43
48:BH:181:SER:OG	48:BH:188:ILE:HA	2.18	0.43
57:BQ:23:PRO:HB3	57:BQ:25:TRP:CH2	2.53	0.43
3:1:356:U:O4	70:1:3108:SPM:N1	2.50	0.43
3:1:1077:G:O6	73:1:3414:HOH:O	2.20	0.43
3:1:1173:G:H5'	3:1:1236:G:N1	2.33	0.43
3:1:1638:C:H5''	73:1:5307:HOH:O	2.16	0.43
3:1:2104:OMG:HM22	3:1:2105:U:C4'	2.48	0.43
3:1:2179:A:N6	73:1:4048:HOH:O	2.50	0.43
3:1:2212:U:H4'	3:1:2213:G:C5'	2.48	0.43
3:1:2516:G:O2'	3:1:2517:C:H5''	2.18	0.43
3:1:2589:C:H5'	73:1:4650:HOH:O	2.17	0.43
3:1:2703:A:H2'	3:1:2704:OMC:C6	2.53	0.43
3:1:2898:G:O2'	6:AB:121:PRO:HD3	2.17	0.43
4:4:806:A:H4'	4:4:807:G:O5'	2.17	0.43
4:4:1117:U:O2	52:BL:44:PRO:HG2	2.18	0.43
4:4:1126:U:OP1	59:BS:5:LYS:HD2	2.18	0.43
4:4:1372:U:H5'	73:4:4265:HOH:O	2.18	0.43
8:AD:3:TRP:HB2	8:AD:78:ARG:O	2.17	0.43
12:AH:126:LYS:HG3	12:AH:130:ARG:NH1	2.32	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:AI:91:PRO:HA	13:AI:100:VAL:O	2.17	0.43
17:AN:52:LYS:HD2	17:AN:135:VAL:CG2	2.45	0.43
20:AQ:31:GLU:O	20:AQ:31:GLU:HG2	2.18	0.43
37:Ah:3:PHE:O	37:Ah:91:VAL:N	2.38	0.43
39:Aj:61:GLU:OE1	39:Aj:61:GLU:N	2.51	0.43
45:BE:194:PHE:CE1	45:BE:208:VAL:HB	2.53	0.43
47:BG:41:THR:O	47:BG:44:LYS:HB2	2.17	0.43
51:BK:3:TRP:CE3	51:BK:93:ARG:HD3	2.54	0.43
63:BW:72:LYS:HG2	63:BW:73:TYR:CE1	2.53	0.43
66:BZ:26:GLY:HA2	66:BZ:74:ILE:CG2	2.48	0.43
69:Bc:55:TYR:OH	69:Bc:65:PRO:HD2	2.19	0.43
3:1:63:A:OP2	3:1:103:U:O2'	2.13	0.43
3:1:236:A:H5'	12:AH:125:LYS:HZ1	1.82	0.43
3:1:777:C:OP1	7:AC:133:GLU:HG3	2.19	0.43
3:1:1314:G:H2'	3:1:1315:G:O4'	2.19	0.43
3:1:1853:C:O2'	3:1:1854:U:H5'	2.18	0.43
4:4:84:G:O2'	4:4:85:G:H5'	2.18	0.43
4:4:130:A:H2'	4:4:131:C:C6	2.53	0.43
4:4:324:C:OP1	4:4:1425:C:O2'	2.36	0.43
4:4:757:C:H2'	4:4:758:C:C6	2.53	0.43
4:4:1278:G:OP1	60:BT:56:ARG:NH2	2.38	0.43
4:4:1433:G:H2'	4:4:1434:G:H8	1.82	0.43
4:4:1465:U:O2	53:BM:141:VAL:HA	2.19	0.43
5:AA:98:PRO:O	5:AA:101:THR:OG1	2.31	0.43
10:AF:65:LEU:HB2	10:AF:126:LEU:HD21	2.00	0.43
31:Ab:20:ARG:HG3	31:Ab:73:LYS:HD3	1.99	0.43
40:Ak:37:THR:O	40:Ak:41:LYS:HG2	2.18	0.43
46:BF:27:ILE:HG12	46:BF:47:LEU:HD11	2.00	0.43
53:BM:46:VAL:HG23	53:BM:71:ALA:HB2	2.00	0.43
62:BV:25:VAL:CG1	62:BV:75:VAL:HB	2.43	0.43
62:BV:60:ARG:HD3	62:BV:92:ILE:HD11	1.99	0.43
62:BV:100:GLU:O	62:BV:104:LEU:HG	2.19	0.43
69:Bc:44:ARG:NH1	69:Bc:53:VAL:O	2.51	0.43
2:3:343:MET:HA	2:3:366:ALA:O	2.17	0.43
3:1:814:G:H2'	3:1:815:C:C6	2.54	0.43
3:1:1307:C:H2'	3:1:1308:G:H8	1.83	0.43
3:1:1633:A:O2'	3:1:1634:G:H5'	2.18	0.43
3:1:1913:U:O2'	3:1:1914:U:H5'	2.19	0.43
3:1:2440:A:H2'	3:1:2441:G:H8	1.82	0.43
3:1:2749:C:H4'	6:AB:146:LEU:HD11	1.99	0.43
4:4:152:A:H2'	4:4:153:A:C8	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:380:G:H5'	45:BE:25:VAL:CG2	2.46	0.43
4:4:624:A:O2'	4:4:625:G:H5'	2.19	0.43
4:4:1124:A:H4'	4:4:1125:C:O5'	2.18	0.43
4:4:1138:C:OP1	59:BS:3:ARG:HD3	2.19	0.43
4:4:1204:A:OP1	4:4:1301:G:O2'	2.29	0.43
4:4:1387:G:O2'	4:4:1388:A:H5'	2.18	0.43
4:4:1434:G:H5''	4:4:1435:G:OP2	2.18	0.43
7:AC:67:LEU:O	7:AC:70:ARG:HG2	2.17	0.43
8:AD:89:LEU:HA	8:AD:92:VAL:HG12	1.99	0.43
13:AI:127:MET:HG3	13:AI:144:VAL:O	2.18	0.43
24:AU:29:ALA:HA	24:AU:33:GLN:OE1	2.19	0.43
28:AY:59:ARG:HD2	28:AY:59:ARG:HA	1.82	0.43
28:AY:148:ARG:HD2	28:AY:177:ARG:O	2.19	0.43
31:Ab:59:LYS:NZ	31:Ab:68:GLU:OE2	2.49	0.43
41:BA:41:LEU:HD23	41:BA:64:ILE:HD11	2.01	0.43
41:BA:44:VAL:HG11	53:BM:38:THR:HG23	2.00	0.43
42:BB:146:LEU:O	42:BB:164:ASN:ND2	2.51	0.43
48:BH:132:ILE:HD13	48:BH:132:ILE:HA	1.85	0.43
54:BN:91:ASP:O	54:BN:138:TRP:NE1	2.30	0.43
58:BR:17:THR:HA	58:BR:22:LYS:O	2.18	0.43
58:BR:24:VAL:HG11	58:BR:49:HIS:HB3	2.00	0.43
62:BV:26:LEU:HD11	62:BV:72:LYS:HG2	2.00	0.43
64:BX:38:LEU:HD12	64:BX:96:GLN:O	2.18	0.43
66:BZ:35:LYS:HE3	66:BZ:35:LYS:HA	1.99	0.43
1:2:42:C:O2'	1:2:43:A:H5'	2.18	0.43
1:2:95:C:H1'	3:1:1153:A:H4'	2.01	0.43
3:1:244:A:H2'	3:1:245:U:O4'	2.18	0.43
3:1:507:G:N1	3:1:510:A:OP2	2.43	0.43
3:1:1571:C:H2'	3:1:1572:C:C6	2.54	0.43
3:1:1584:G:O2'	3:1:1585:G:H5'	2.18	0.43
3:1:2011:A2M:HM'3	3:1:2011:A2M:H1'	1.69	0.43
3:1:2777:A:H2'	3:1:2778:G:O4'	2.19	0.43
3:1:2781:A:H2'	3:1:2782:C:H6	1.82	0.43
3:1:2835:G:OP1	6:AB:306:ARG:NH1	2.39	0.43
3:1:2962:G:H2'	3:1:2963:C:C6	2.53	0.43
4:4:186:U:O2'	4:4:187:U:H5'	2.19	0.43
4:4:475:OMG:HM21	67:Ba:18:PRO:HG2	2.00	0.43
4:4:780:A:OP2	64:BX:8:ARG:NE	2.39	0.43
4:4:1108:G:O2'	4:4:1109:G:H5'	2.19	0.43
9:AE:8:GLU:HG3	9:AE:72:LEU:HB3	1.99	0.43
14:AJ:6:ASP:HB3	14:AJ:61:LYS:HZ1	1.84	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:AM:166:GLU:O	16:AM:170:LYS:HG3	2.18	0.43
23:AT:16:LEU:HD21	23:AT:20:LYS:HE2	2.00	0.43
28:AY:151:LEU:HB3	28:AY:163:ASP:OD1	2.18	0.43
58:BR:34:VAL:HG11	58:BR:128:ILE:CG2	2.48	0.43
68:Bb:36:LYS:HE3	68:Bb:40:LYS:NZ	2.33	0.43
2:3:337:MET:HE1	2:3:458:VAL:CG2	2.45	0.43
2:3:573:SER:OG	2:3:574:LYS:N	2.51	0.43
3:1:83:G:C8	35:Af:32:LYS:HG3	2.53	0.43
3:1:339:U:O2	3:1:359:U:H3'	2.19	0.43
3:1:820:U:C2'	3:1:821:G:H5'	2.48	0.43
3:1:1247:C:H2'	3:1:1248:C:C6	2.53	0.43
3:1:1297:G:H2'	3:1:1298:C:H6	1.84	0.43
3:1:2123:G:OP1	30:Aa:24:SER:HA	2.19	0.43
3:1:2206:U:H2'	3:1:2207:G:C8	2.54	0.43
3:1:2494:C:H2'	3:1:2495:C:C6	2.54	0.43
4:4:205:G:H2'	4:4:206:C:H6	1.83	0.43
4:4:365:C:H2'	4:4:366:G:O4'	2.18	0.43
4:4:1021:U:H3	4:4:1160:G:H1	1.65	0.43
4:4:1295:G:H4'	55:BO:31:GLY:O	2.19	0.43
7:AC:212:LYS:HE2	7:AC:212:LYS:HB2	1.68	0.43
10:AF:11:TYR:CE1	10:AF:21:TYR:HA	2.53	0.43
12:AH:7:VAL:CG1	12:AH:24:GLY:HA3	2.49	0.43
13:AI:93:ARG:CZ	13:AI:97:GLY:HA2	2.49	0.43
24:AU:39:GLN:OE1	24:AU:45:LYS:HD3	2.19	0.43
26:AW:50:LEU:HD13	26:AW:52:TRP:NE1	2.34	0.43
30:Aa:19:ARG:O	30:Aa:19:ARG:HG3	2.19	0.43
39:Aj:87:ILE:H	39:Aj:87:ILE:HG13	1.59	0.43
46:BF:112:PRO:HB2	46:BF:198:TYR:OH	2.18	0.43
53:BM:76:LEU:HD23	53:BM:80:ILE:O	2.19	0.43
55:BO:10:ARG:HA	55:BO:14:THR:O	2.18	0.43
68:Bb:8:VAL:HG11	68:Bb:45:ARG:NH1	2.34	0.43
3:1:253:A:OP1	16:AM:3:SER:HB3	2.19	0.43
3:1:510:A:H5'	73:1:7865:HOH:O	2.18	0.43
3:1:1526:A:H4'	3:1:1527:U:OP2	2.16	0.43
3:1:1552:G:C5'	73:1:5162:HOH:O	2.46	0.43
3:1:1806:C:O2'	3:1:2802:U:OP1	2.32	0.43
3:1:1855:G:O2'	3:1:1856:C:H5'	2.19	0.43
3:1:2151:A:N3	3:1:2569:G:O2'	2.42	0.43
3:1:2463:G:H2'	3:1:2464:C:C6	2.53	0.43
4:4:13:C:OP1	46:BF:182:THR:HG23	2.18	0.43
4:4:190:C:H2'	4:4:191:C:H6	1.84	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:746:G:O2'	4:4:747:G:H5'	2.19	0.43
4:4:791:C:H2'	4:4:792:U:O4'	2.18	0.43
4:4:1089:A:C2'	4:4:1090:C:H5'	2.49	0.43
4:4:1292:C:O2'	4:4:1293:U:H5'	2.19	0.43
4:4:1321:G:H2'	4:4:1322:U:O4'	2.18	0.43
8:AD:89:LEU:CD1	8:AD:173:LEU:HD23	2.49	0.43
16:AM:180:LEU:HB3	16:AM:181:PRO:HD3	2.01	0.43
20:AQ:135:TYR:CE1	20:AQ:141:LEU:HD11	2.53	0.43
31:Ab:20:ARG:HD3	31:Ab:77:VAL:HG23	2.00	0.43
37:Ah:5:LYS:HE2	37:Ah:91:VAL:HA	2.01	0.43
39:Aj:96:ARG:HE	39:Aj:96:ARG:HB2	1.63	0.43
41:BA:22:TRP:CZ3	41:BA:25:LYS:HD2	2.54	0.43
42:BB:84:LYS:HA	42:BB:84:LYS:HD2	1.86	0.43
42:BB:179:ARG:O	42:BB:183:ARG:HG3	2.18	0.43
43:BC:163:LYS:HA	43:BC:191:ARG:HH12	1.84	0.43
53:BM:104:ALA:HA	53:BM:107:ARG:NH1	2.33	0.43
60:BT:127:HIS:CD2	73:BT:209:HOH:O	2.72	0.43
63:BW:79:LEU:O	63:BW:79:LEU:HD22	2.19	0.43
2:3:391:SER:HB2	2:3:547:ARG:NH1	2.34	0.43
3:1:268:G:N1	3:1:271:A:OP2	2.52	0.43
3:1:696:U:O4	7:AC:251:PRO:HD3	2.19	0.43
3:1:706:A:H2'	3:1:707:G:O4'	2.18	0.43
3:1:715:G:N7	73:1:3672:HOH:O	2.37	0.43
3:1:833:A:H2'	3:1:834:A:O4'	2.18	0.43
3:1:1094:A:H5'	3:1:1316:U:H1'	2.00	0.43
3:1:1456:A:H2'	3:1:1457:A:C8	2.54	0.43
3:1:1840:G:H1'	73:1:6925:HOH:O	2.17	0.43
3:1:2781:A:H2'	3:1:2782:C:C6	2.54	0.43
73:1:3579:HOH:O	27:AX:53:ARG:NE	2.43	0.43
4:4:393:A:H3'	4:4:394:C:C6	2.53	0.43
4:4:504:C:H2'	4:4:505:G:H8	1.84	0.43
4:4:713:G:OP2	57:BQ:70:LYS:HE3	2.19	0.43
4:4:1011:U:H2'	4:4:1014:A:OP1	2.18	0.43
4:4:1085:U:O2'	4:4:1246:A:H2'	2.19	0.43
4:4:1428:G:H2'	4:4:1429:C:C6	2.53	0.43
4:4:1484:G:OP1	53:BM:131:ARG:NH2	2.52	0.43
7:AC:46:THR:HG22	7:AC:47:PRO:O	2.19	0.43
10:AF:45:GLY:HA3	10:AF:118:GLU:O	2.19	0.43
15:AL:78:PRO:HB2	15:AL:117:LEU:CD1	2.49	0.43
15:AL:94:ARG:HH21	15:AL:96:GLU:HG3	1.83	0.43
20:AQ:106:GLN:HB2	20:AQ:108:LYS:HE2	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:BB:34:GLU:OE2	42:BB:35:ARG:HD2	2.19	0.43
42:BB:88:MET:HE3	42:BB:88:MET:HB3	1.63	0.43
43:BC:184:GLY:O	43:BC:185:ILE:HG12	2.19	0.43
45:BE:121:ARG:NH1	45:BE:222:ASP:O	2.35	0.43
46:BF:70:ASN:OD1	46:BF:70:ASN:N	2.51	0.43
46:BF:186:PHE:O	46:BF:190:VAL:HG23	2.19	0.43
51:BK:54:LYS:HD3	51:BK:85:ILE:CG1	2.48	0.43
65:BY:21:ARG:HA	65:BY:27:ASN:O	2.18	0.43
2:3:367:VAL:HG11	2:3:428:ALA:CB	2.48	0.43
3:1:6:A:C6	23:AT:183:LYS:HG2	2.54	0.43
3:1:494:G:N2	3:1:497:A:OP2	2.35	0.43
3:1:613:G:H1'	3:1:614:U:OP2	2.18	0.43
3:1:661:C:H2'	3:1:662:C:C6	2.53	0.43
3:1:724:A:H1'	3:1:725:G:OP2	2.18	0.43
3:1:776:A:H2'	3:1:777:C:H6	1.83	0.43
3:1:1028:A:H2'	3:1:1031:C:C5	2.53	0.43
3:1:1909:A:H61	38:AI:19:TYR:HA	1.82	0.43
3:1:2197:A:H2'	3:1:2198:C:C6	2.54	0.43
4:4:140:G:N2	4:4:143:A:OP2	2.52	0.43
4:4:160:A:H2'	4:4:161:U:C6	2.54	0.43
4:4:184:C:O2'	4:4:185:C:H5'	2.18	0.43
4:4:332:C:OP2	73:4:3102:HOH:O	2.21	0.43
4:4:440:C:C5'	62:BV:61:LYS:HG2	2.44	0.43
4:4:651:G:O2'	4:4:652:G:H5'	2.18	0.43
4:4:730:G:H4'	4:4:1472:A:H4'	2.00	0.43
4:4:764:G:H2'	4:4:765:U:O4'	2.19	0.43
4:4:1272:A:N1	55:BO:143:VAL:HG11	2.34	0.43
4:4:1400:G:H2'	4:4:1401:G:C8	2.54	0.43
5:AA:40:VAL:CG2	5:AA:72:LEU:HD11	2.45	0.43
8:AD:167:GLU:HG3	8:AD:171:LYS:HE2	2.01	0.43
9:AE:41:LYS:HG3	9:AE:42:GLU:N	2.34	0.43
44:BD:14:GLY:HA3	44:BD:47:ARG:HB3	2.00	0.43
44:BD:92:LEU:HA	44:BD:95:ILE:CD1	2.48	0.43
51:BK:36:VAL:HG22	51:BK:71:ILE:HB	2.00	0.43
53:BM:84:HIS:C	53:BM:85:ILE:HD12	2.43	0.43
54:BN:24:ARG:HE	54:BN:24:ARG:HB3	1.45	0.43
57:BQ:16:ARG:HD3	57:BQ:62:LEU:HD11	2.01	0.43
57:BQ:102:LEU:HD23	57:BQ:102:LEU:HA	1.76	0.43
64:BX:21:VAL:O	64:BX:29:VAL:HG21	2.19	0.43
3:1:84:G:N7	35:AF:30:LYS:HD2	2.34	0.43
3:1:476:C:H2'	3:1:477:G:O4'	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1:766:G:H2'	3:1:767:C:H6	1.83	0.43
3:1:781:C:H2'	3:1:782:G:H8	1.83	0.43
3:1:1739:G:H5''	3:1:1740:C:H5'	2.01	0.43
3:1:1782:C:H5''	73:1:3448:HOH:O	2.18	0.43
3:1:1870:A:C4	20:AQ:102:THR:HG21	2.54	0.43
3:1:2129:C:OP1	23:AT:97:LYS:NZ	2.46	0.43
3:1:2365:C:H2'	3:1:2366:OMG:O4'	2.19	0.43
70:1:3106:SPM:H82	73:1:7526:HOH:O	2.18	0.43
4:4:542:G:P	57:BQ:124:ARG:HH21	2.42	0.43
4:4:855:G:H4'	4:4:856:U:O5'	2.19	0.43
4:4:1217:G:C5'	51:BK:22:THR:HG21	2.49	0.43
4:4:1337:G:O3'	51:BK:79:GLY:HA3	2.18	0.43
4:4:1479:C:H2'	4:4:1480:C:H6	1.84	0.43
8:AD:13:PRO:O	8:AD:16:ARG:NH1	2.52	0.43
8:AD:171:LYS:HZ3	8:AD:171:LYS:HG3	1.71	0.43
13:AI:116:PRO:HG2	13:AI:139:LEU:CD1	2.48	0.43
17:AN:83:ASP:HA	17:AN:86:TYR:CE1	2.54	0.43
39:Aj:80:GLN:OE1	39:Aj:80:GLN:HA	2.19	0.43
39:Aj:168:ILE:HD12	39:Aj:168:ILE:HA	1.94	0.43
42:BB:67:ARG:NH2	69:Bc:35:PRO:HA	2.28	0.43
51:BK:64:ASP:O	51:BK:67:LYS:HG3	2.18	0.43
59:BS:20:TYR:CZ	59:BS:38:LEU:HD22	2.54	0.43
61:BU:29:PRO:HA	61:BU:30:PRO:HD3	1.90	0.43
67:Ba:19:LYS:HA	67:Ba:19:LYS:HD3	1.77	0.43
1:2:34:C:C2'	1:2:35:C:H5'	2.47	0.42
1:2:38:G:O2'	1:2:47:G:N7	2.47	0.42
2:3:327:HIS:N	2:3:483:ARG:HH22	2.15	0.42
2:3:637:VAL:HG22	2:3:641:MET:HE3	2.01	0.42
3:1:50:G:H2'	3:1:51:U:C6	2.54	0.42
3:1:111:U:H5'	73:1:6918:HOH:O	2.18	0.42
3:1:333:C:O2'	3:1:334:U:H5'	2.18	0.42
3:1:2003:C:H5''	37:Ah:32:SER:OG	2.18	0.42
3:1:2022:A:H5''	5:AA:231:THR:HB	2.00	0.42
3:1:2184:C:H2'	3:1:2185:C:H6	1.83	0.42
4:4:125:G:O2'	4:4:126:G:H5'	2.19	0.42
4:4:300:G:N2	4:4:303:A:OP2	2.44	0.42
4:4:414:G:H2'	4:4:415:G:C8	2.53	0.42
4:4:442:A:H5''	62:BV:91:TYR:CE2	2.54	0.42
4:4:461:C:H2'	4:4:462:OMG:O4'	2.19	0.42
4:4:822:C:H2'	4:4:823:G:O4'	2.19	0.42
4:4:1171:U:H4'	43:BC:180:LEU:HD12	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:1183:C:H2'	4:4:1184:OMC:C6	2.54	0.42
4:4:1388:A:H2'	4:4:1389:G:H8	1.84	0.42
5:AA:130:ARG:HG3	5:AA:137:ILE:HD11	2.01	0.42
6:AB:46:ALA:O	6:AB:309:LEU:HD12	2.19	0.42
6:AB:243:GLN:NE2	73:AB:401:HOH:O	2.27	0.42
9:AE:91:ARG:HB3	9:AE:192:GLU:HG3	2.01	0.42
11:AG:79:ASN:HB3	11:AG:82:LYS:HB3	2.01	0.42
11:AG:173:LYS:O	11:AG:177:ALA:HB2	2.19	0.42
13:AI:73:LYS:HB3	13:AI:75:GLU:CD	2.44	0.42
17:AN:103:MET:HG3	17:AN:114:GLU:HG2	2.01	0.42
30:Aa:67:GLU:HG2	30:Aa:68:LYS:HE3	2.01	0.42
31:Ab:133:ASN:OD1	31:Ab:133:ASN:N	2.51	0.42
33:Ad:4:THR:HB	33:Ad:5:PRO:HD3	2.01	0.42
44:BD:50:LEU:HD22	44:BD:100:VAL:HB	2.00	0.42
45:BE:104:TYR:CE1	45:BE:188:ILE:HD13	2.54	0.42
45:BE:157:ASP:OD2	45:BE:171:HIS:NE2	2.51	0.42
48:BH:160:VAL:CG2	48:BH:165:ARG:HG2	2.49	0.42
49:BI:106:THR:HG22	49:BI:122:GLY:O	2.19	0.42
50:BJ:104:ALA:O	50:BJ:115:VAL:HG23	2.19	0.42
55:BO:107:ASP:OD1	55:BO:107:ASP:N	2.50	0.42
59:BS:5:LYS:CG	59:BS:9:ILE:HG21	2.48	0.42
62:BV:99:GLU:O	62:BV:103:LYS:HE2	2.19	0.42
66:BZ:22:LEU:HD21	66:BZ:35:LYS:CG	2.49	0.42
2:3:379:THR:HG21	2:3:454:ASP:HB2	2.01	0.42
2:3:580:ALA:O	2:3:584:SER:HB3	2.19	0.42
3:1:626:G:O2'	3:1:627:G:H5'	2.18	0.42
3:1:1022:C:H2'	3:1:1023:C:H6	1.84	0.42
3:1:1039:C:O2'	3:1:2381:A:N7	2.53	0.42
3:1:1161:U:H2'	3:1:1162:C:C6	2.54	0.42
3:1:2212:U:H4'	3:1:2213:G:O5'	2.20	0.42
3:1:2575:C:H2'	3:1:2576:G:C8	2.54	0.42
3:1:2832:G:H5'	3:1:2966:U:OP1	2.19	0.42
4:4:570:A:O3'	45:BE:18:LYS:HE3	2.18	0.42
4:4:619:G:H2'	4:4:620:C:C6	2.54	0.42
4:4:790:G:H5''	42:BB:30:LYS:HD2	2.01	0.42
4:4:1047:G:H2'	4:4:1048:G:C8	2.53	0.42
4:4:1102:G:O2'	4:4:1103:G:H5'	2.20	0.42
4:4:1153:G:O2'	4:4:1154:G:H5'	2.19	0.42
4:4:1417:U:H2'	4:4:1418:G:H8	1.84	0.42
8:AD:2:LYS:O	8:AD:6:LEU:HD12	2.19	0.42
8:AD:98:ARG:HG2	8:AD:178:ASP:C	2.44	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:AQ:23:PRO:O	20:AQ:26:VAL:HG13	2.19	0.42
20:AQ:110:ASP:OD2	20:AQ:110:ASP:N	2.52	0.42
24:AU:80:VAL:HG12	27:AX:32:LYS:HA	2.01	0.42
29:AZ:71:LEU:HD23	29:AZ:81:ILE:O	2.18	0.42
38:AI:37:LYS:HB3	38:AI:46:LEU:CD2	2.49	0.42
39:AJ:182:GLU:OE1	39:AJ:183:LYS:N	2.52	0.42
41:BA:59:VAL:HG22	41:BA:75:LEU:O	2.19	0.42
45:BE:11:TYR:HA	45:BE:17:ARG:NH2	2.31	0.42
50:BJ:113:ALA:CB	50:BJ:127:ALA:HB1	2.49	0.42
56:BP:40:CYS:HA	56:BP:43:GLU:OE1	2.19	0.42
58:BR:54:ILE:CD1	58:BR:128:ILE:HD11	2.49	0.42
64:BX:8:ARG:NH1	73:BX:203:HOH:O	2.53	0.42
65:BY:19:ARG:HA	65:BY:29:GLN:O	2.19	0.42
65:BY:29:GLN:NE2	65:BY:42:LEU:HG	2.34	0.42
2:3:491:MET:CE	2:3:620:VAL:HG12	2.44	0.42
3:1:76:A:H5'	25:AV:25:ARG:NH1	2.34	0.42
3:1:382:G:H2'	3:1:383:U:C6	2.54	0.42
3:1:530:G:N1	3:1:533:A:OP2	2.42	0.42
3:1:1537:G:H2'	3:1:1538:C:C6	2.54	0.42
3:1:1570:U:H2'	3:1:1571:C:H6	1.83	0.42
3:1:1882:G:N7	20:AQ:73:ARG:NH2	2.67	0.42
4:4:176:G:N1	4:4:179:A:OP2	2.51	0.42
4:4:220:G:H2'	4:4:221:U:O4'	2.20	0.42
4:4:425:C:H2'	4:4:426:G:C8	2.54	0.42
4:4:534:A:H2'	4:4:535:A:C8	2.54	0.42
4:4:697:C:H2'	4:4:698:G:O4'	2.19	0.42
4:4:927:U:OP1	4:4:927:U:H2'	2.19	0.42
4:4:1335:C:H2'	4:4:1336:G:C8	2.54	0.42
4:4:1369:C:O5'	4:4:1369:C:H6	2.02	0.42
5:AA:58:MET:HB2	5:AA:62:VAL:O	2.18	0.42
6:AB:174:ILE:HG23	6:AB:175:ASP:OD2	2.19	0.42
7:AC:176:ASP:OD1	7:AC:176:ASP:N	2.51	0.42
7:AC:190:PHE:HD2	7:AC:199:VAL:HG21	1.84	0.42
8:AD:137:LEU:HD11	8:AD:169:PHE:CE2	2.54	0.42
10:AF:8:LYS:HA	10:AF:8:LYS:HD2	1.64	0.42
11:AG:14:GLU:HB3	11:AG:15:LYS:NZ	2.33	0.42
17:AN:76:TYR:CD2	17:AN:152:ALA:HB2	2.52	0.42
18:AO:64:THR:HA	18:AO:85:LEU:HD13	2.01	0.42
29:AZ:8:LEU:HD22	29:AZ:12:ILE:CD1	2.48	0.42
30:Aa:77:VAL:HG22	30:Aa:87:VAL:HG22	2.02	0.42
31:Ab:7:ARG:HB2	31:Ab:85:PHE:CZ	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:Ae:29:PHE:CD2	34:Ae:44:ARG:HG2	2.53	0.42
34:Ae:33:LYS:HA	34:Ae:41:TYR:O	2.20	0.42
39:Aj:142:LYS:HA	39:Aj:142:LYS:HD3	1.80	0.42
41:BA:46:ALA:HB2	41:BA:52:LEU:HG	2.01	0.42
46:BF:13:THR:OG1	46:BF:14:ALA:N	2.51	0.42
46:BF:71:GLN:HG2	46:BF:92:SER:O	2.19	0.42
51:BK:58:PRO:HB2	51:BK:91:ILE:CG2	2.47	0.42
57:BQ:25:TRP:NE1	65:BY:30:VAL:HG11	2.34	0.42
65:BY:33:SER:OG	65:BY:34:HIS:ND1	2.51	0.42
66:BZ:34:VAL:O	66:BZ:49:THR:HA	2.19	0.42
66:BZ:39:LEU:HA	66:BZ:44:LYS:NZ	2.34	0.42
2:3:483:ARG:HG3	2:3:485:VAL:HG23	2.01	0.42
3:1:132:A:N1	3:1:1540:G:O2'	2.39	0.42
3:1:1926:U:O2'	5:AA:172:ALA:HB2	2.19	0.42
3:1:1990:A2M:H2	3:1:2208:U:O4'	2.18	0.42
4:4:13:C:H5''	46:BF:182:THR:HG21	2.01	0.42
4:4:1173:C:O2'	4:4:1174:C:H5'	2.19	0.42
4:4:1435:G:C2'	4:4:1436:C:H5''	2.49	0.42
7:AC:238:ILE:HG12	7:AC:249:VAL:HG22	2.01	0.42
9:AE:96:VAL:HG13	9:AE:103:MET:HE2	2.01	0.42
12:AH:38:ASN:OD1	12:AH:41:GLN:NE2	2.28	0.42
17:AN:38:THR:HG21	17:AN:84:ALA:HA	2.02	0.42
25:AV:111:LYS:H	25:AV:111:LYS:HG3	1.62	0.42
27:AX:33:LEU:HB3	27:AX:48:ILE:HG12	2.01	0.42
27:AX:39:ARG:HE	27:AX:39:ARG:HB3	1.58	0.42
39:Aj:8:VAL:HA	39:Aj:69:ALA:HB3	2.00	0.42
47:BG:10:ASP:OD1	47:BG:13:SER:N	2.53	0.42
54:BN:40:LYS:HD2	54:BN:41:TYR:CZ	2.53	0.42
55:BO:30:ARG:O	55:BO:98:LEU:HD23	2.20	0.42
59:BS:57:LEU:H	59:BS:57:LEU:HD22	1.84	0.42
60:BT:121:SER:HB2	60:BT:122:PRO:HD2	2.00	0.42
63:BW:62:LYS:HB3	63:BW:62:LYS:HE2	1.57	0.42
2:3:337:MET:O	2:3:338:LEU:HD23	2.20	0.42
2:3:459:ILE:HD13	2:3:459:ILE:HA	1.86	0.42
3:1:71:G:H2'	3:1:72:G:H8	1.85	0.42
3:1:378:G:C4'	73:1:6172:HOH:O	2.54	0.42
3:1:543:A:O2'	3:1:544:A:H5'	2.18	0.42
3:1:1834:A:H2'	3:1:1835:C:O4'	2.19	0.42
3:1:1867:U:H2'	3:1:1868:A:C8	2.54	0.42
3:1:2354:U:H2'	3:1:2355:U:C6	2.54	0.42
3:1:2649:G:H2'	3:1:2650:C:C6	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1:2967:G:OP2	73:1:3424:HOH:O	2.21	0.42
73:1:5274:HOH:O	22:AS:18:LYS:HB2	2.19	0.42
4:4:672:G:O2'	4:4:673:A:H5'	2.19	0.42
4:4:829:A:H2'	4:4:830:A:C8	2.54	0.42
4:4:1074:C:O2'	4:4:1075:C:H5'	2.19	0.42
4:4:1090:C:H3'	4:4:1090:C:OP2	2.20	0.42
8:AD:148:ARG:NE	18:AO:107:LEU:O	2.41	0.42
14:AJ:69:SER:O	14:AJ:73:VAL:HG13	2.19	0.42
18:AO:84:LEU:HG	18:AO:184:PHE:HE1	1.84	0.42
18:AO:152:ALA:HB1	18:AO:163:TYR:HE1	1.84	0.42
25:AV:118:GLU:O	25:AV:122:ARG:HB2	2.18	0.42
38:AI:52:LEU:HD12	38:AI:56:ILE:HG22	2.01	0.42
40:AK:39:THR:O	40:AK:43:LYS:HD3	2.20	0.42
42:BB:126:PRO:HG2	42:BB:151:THR:CG2	2.49	0.42
43:BC:171:ARG:CG	73:BC:310:HOH:O	2.32	0.42
44:BD:117:LEU:HD23	44:BD:157:ILE:CD1	2.50	0.42
46:BF:27:ILE:HG13	46:BF:31:PHE:CE2	2.53	0.42
46:BF:38:LYS:HA	46:BF:38:LYS:HD2	1.83	0.42
50:BJ:45:ASP:HA	50:BJ:63:GLN:O	2.20	0.42
53:BM:37:LEU:HD23	53:BM:37:LEU:HA	1.73	0.42
62:BV:26:LEU:HD11	62:BV:72:LYS:CG	2.49	0.42
62:BV:90:LEU:HD23	62:BV:90:LEU:HA	1.68	0.42
63:BW:98:LYS:HE2	63:BW:103:GLU:OE2	2.19	0.42
65:BY:16:ARG:O	65:BY:33:SER:HB3	2.19	0.42
66:BZ:30:GLU:OE1	66:BZ:30:GLU:N	2.42	0.42
68:Bb:25:GLU:HB2	68:Bb:27:LYS:HZ2	1.85	0.42
3:1:915:C:O2'	33:Ad:50:TRP:O	2.31	0.42
3:1:1102:A:O2'	3:1:2156:C:O2'	2.28	0.42
3:1:1297:G:H2'	3:1:1298:C:C6	2.55	0.42
3:1:2028:G:H2'	3:1:2029:G:C8	2.55	0.42
3:1:2030:G:H2'	3:1:2031:G:C1'	2.50	0.42
3:1:2037:C:H2'	3:1:2038:U:C6	2.54	0.42
4:4:650:G:OP1	53:BM:47:SER:OG	2.25	0.42
4:4:1083:G:C4'	52:BL:43:ILE:HD11	2.50	0.42
4:4:1433:G:H2'	4:4:1434:G:C8	2.55	0.42
4:4:1480:C:H2'	4:4:1481:U:C6	2.55	0.42
7:AC:180:ILE:CG2	7:AC:185:GLU:HB3	2.49	0.42
9:AE:50:MET:HE2	9:AE:50:MET:HB3	1.84	0.42
12:AH:145:VAL:HG22	15:AL:37:MET:HE3	2.02	0.42
18:AO:73:LYS:HG2	18:AO:175:LEU:HB3	2.00	0.42
20:AQ:128:ASP:OD2	20:AQ:128:ASP:N	2.52	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:AT:64:LEU:HD23	23:AT:64:LEU:HA	1.79	0.42
24:AU:74:LEU:O	24:AU:78:LEU:HG	2.19	0.42
30:Aa:80:LEU:HD11	30:Aa:86:ARG:HD3	2.01	0.42
39:Aj:66:PHE:O	39:Aj:111:LEU:HA	2.20	0.42
48:BH:13:SER:O	48:BH:14:ARG:HG3	2.19	0.42
49:BI:53:ILE:CD1	49:BI:62:VAL:HG23	2.50	0.42
50:BJ:78:VAL:HG11	50:BJ:110:VAL:HG11	2.00	0.42
57:BQ:85:PRO:HG3	57:BQ:134:LYS:HG2	2.02	0.42
61:BU:47:MET:HE2	61:BU:47:MET:HB2	1.75	0.42
62:BV:46:LEU:HD23	62:BV:57:ILE:HG23	2.01	0.42
1:2:33:A:H2'	1:2:34:C:C6	2.54	0.42
1:2:104:G:H5''	73:2:244:HOH:O	2.19	0.42
3:1:53:G:O2'	3:1:54:C:H5'	2.20	0.42
3:1:146:C:H2'	3:1:147:C:C6	2.55	0.42
3:1:383:U:O2'	3:1:384:G:H5'	2.20	0.42
3:1:1866:G:H3'	3:1:1867:U:H5''	2.02	0.42
3:1:2702:G:OP1	73:1:3428:HOH:O	2.22	0.42
3:1:2839:C:N4	73:1:3664:HOH:O	2.36	0.42
4:4:92:G:N2	4:4:358:G:H5'	2.34	0.42
4:4:303:A:H2'	4:4:525:C:H42	1.84	0.42
4:4:1120:G:H2'	4:4:1121:G:O4'	2.19	0.42
4:4:1126:U:H5'	59:BS:5:LYS:NZ	2.35	0.42
4:4:1194:C:OP1	55:BO:136:ARG:HG3	2.19	0.42
4:4:1273:U:H4'	55:BO:137:PHE:HE2	1.83	0.42
6:AB:208:LYS:HB3	6:AB:208:LYS:HE3	1.90	0.42
6:AB:258:GLY:O	6:AB:260:HIS:N	2.53	0.42
7:AC:58:LEU:HD21	7:AC:141:LEU:HG	2.02	0.42
8:AD:19:ILE:HA	8:AD:137:LEU:HD23	2.02	0.42
9:AE:181:GLY:O	36:Ag:3:ILE:HG21	2.19	0.42
10:AF:29:ASP:HA	10:AF:32:GLU:CG	2.50	0.42
14:AK:23:ALA:CB	14:AK:36:ILE:HD12	2.50	0.42
14:AK:42:LEU:HD12	14:AK:87:LYS:HG3	2.00	0.42
16:AM:14:LYS:HA	16:AM:14:LYS:HE2	2.02	0.42
20:AQ:78:ARG:HG2	20:AQ:82:ARG:CZ	2.50	0.42
31:Ab:81:HIS:HB2	31:Ab:87:GLU:HG2	2.01	0.42
41:BA:52:LEU:HA	41:BA:55:ARG:CD	2.38	0.42
42:BB:126:PRO:HG2	42:BB:151:THR:HG21	2.00	0.42
45:BE:47:VAL:CG1	45:BE:107:LEU:HD12	2.50	0.42
49:BI:5:ASP:OD2	49:BI:8:SER:OG	2.26	0.42
49:BI:108:GLN:HG3	49:BI:121:ILE:HD13	2.00	0.42
54:BN:71:LYS:HG2	67:Ba:7:LEU:HD23	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:BN:96:TYR:HE2	54:BN:138:TRP:HD1	1.67	0.42
55:BO:88:GLY:HA2	60:BT:32:ARG:HD2	2.02	0.42
58:BR:18:LEU:HD12	58:BR:22:LYS:O	2.20	0.42
60:BT:80:LEU:CD1	60:BT:84:GLY:HA3	2.39	0.42
64:BX:81:LYS:HA	64:BX:81:LYS:HD3	1.90	0.42
2:3:481:ARG:NH1	2:3:481:ARG:O	2.53	0.42
3:1:364:C:O2'	3:1:365:C:H5'	2.20	0.42
3:1:920:A:H2'	3:1:921:U:C6	2.55	0.42
3:1:1125:C:H1'	3:1:1132:U:N3	2.34	0.42
3:1:1439:G:C2'	3:1:1440:G:H5'	2.50	0.42
3:1:1769:U:C2'	73:1:3406:HOH:O	2.67	0.42
3:1:1925:A:O3'	5:AA:187:PRO:HB2	2.20	0.42
3:1:2412:G:O2'	3:1:2413:C:H5'	2.20	0.42
3:1:2910:G:O2'	3:1:2911:G:H5'	2.20	0.42
4:4:188:C:O2'	4:4:189:C:H5'	2.20	0.42
4:4:202:G:O2'	4:4:203:C:H5'	2.20	0.42
4:4:206:C:H2'	4:4:207:C:O4'	2.19	0.42
4:4:656:A:H2'	4:4:657:A:C8	2.55	0.42
4:4:1318:4AC:H2'	4:4:1319:G:C8	2.54	0.42
4:4:1360:A:N1	4:4:1459:6MZ:O2'	2.47	0.42
6:AB:47:TYR:CE1	6:AB:309:LEU:HD13	2.54	0.42
10:AF:64:LYS:HG2	10:AF:116:VAL:O	2.20	0.42
14:AJ:58:THR:HG23	14:AJ:60:LYS:N	2.19	0.42
14:AJ:91:LYS:HB3	14:AJ:91:LYS:HE3	1.72	0.42
30:Aa:15:ILE:HG12	30:Aa:39:PHE:CE1	2.54	0.42
44:BD:118:ALA:HB1	44:BD:123:HIS:CD2	2.54	0.42
46:BF:125:ASP:N	46:BF:125:ASP:OD1	2.53	0.42
50:BJ:44:GLU:O	50:BJ:63:GLN:HG2	2.20	0.42
50:BJ:73:LYS:HE2	50:BJ:73:LYS:HB2	1.73	0.42
53:BM:24:TYR:OH	53:BM:90:PRO:HB3	2.20	0.42
54:BN:51:ARG:CD	54:BN:102:GLU:HG3	2.49	0.42
54:BN:139:ARG:HA	54:BN:139:ARG:HD3	1.82	0.42
55:BO:118:ILE:HD12	60:BT:134:LEU:HD11	2.02	0.42
57:BQ:84:LEU:HD23	57:BQ:84:LEU:HA	1.83	0.42
61:BU:138:ILE:O	61:BU:142:LEU:HB2	2.20	0.42
69:Bc:14:PRO:O	69:Bc:23:LEU:HD13	2.20	0.42
3:1:30:C:H2'	3:1:31:U:H6	1.84	0.42
3:1:139:C:H2'	3:1:140:C:H6	1.84	0.42
3:1:376:C:H2'	3:1:377:C:O4'	2.20	0.42
3:1:396:G:O2'	3:1:397:G:H5'	2.20	0.42
3:1:1623:A:H2'	3:1:1624:A:O4'	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:542:G:O6	4:4:719:G:H3'	2.20	0.42
4:4:879:A2M:H1'	4:4:879:A2M:HM'3	1.58	0.42
4:4:1008:A:H4'	4:4:1009:G:O5'	2.20	0.42
4:4:1464:G:C8	4:4:1464:G:H5''	2.55	0.42
73:4:3577:HOH:O	62:BV:119:ARG:HG2	2.18	0.42
11:AG:23:GLU:HG3	11:AG:53:LYS:HD2	2.02	0.42
15:AL:117:LEU:C	15:AL:137:ALA:HB2	2.44	0.42
17:AN:35:ASP:HB3	17:AN:39:THR:CG2	2.49	0.42
25:AV:2:PRO:HA	25:AV:23:LEU:CD1	2.47	0.42
26:AW:1:MET:HE1	26:AW:15:PRO:HG2	2.02	0.42
38:Ai:55:GLY:O	38:Ai:67:ALA:HA	2.20	0.42
43:BC:153:PHE:CE2	43:BC:155:LYS:HE3	2.55	0.42
53:BM:55:ASP:O	53:BM:58:LYS:HG3	2.20	0.42
59:BS:34:ALA:O	59:BS:38:LEU:HB2	2.20	0.42
2:3:366:ALA:HB2	2:3:377:PHE:CE1	2.54	0.42
3:1:2361:G:OP1	3:1:2387:C:O2'	2.31	0.42
3:1:2993:A:H2'	3:1:2994:G:O4'	2.19	0.42
4:4:134:C:O2	68:Bb:52:ARG:NH2	2.52	0.42
4:4:216:G:O2'	4:4:217:C:H5'	2.20	0.42
4:4:561:G:O2'	4:4:562:C:H5'	2.20	0.42
4:4:781:U:H4'	4:4:782:G:OP2	2.19	0.42
4:4:824:A:O3'	69:Bc:50:LYS:NZ	2.52	0.42
4:4:1369:C:H1'	4:4:1459:6MZ:N1	2.35	0.42
9:AE:155:PHE:CE2	9:AE:159:ILE:HD11	2.55	0.42
11:AG:1:MET:SD	11:AG:132:ARG:HG3	2.60	0.42
13:AI:117:LYS:HD3	13:AI:117:LYS:HA	1.93	0.42
17:AN:44:ARG:HA	17:AN:47:PHE:CD2	2.55	0.42
20:AQ:4:VAL:HG21	20:AQ:29:LEU:HD22	2.02	0.42
20:AQ:12:LEU:HD13	20:AQ:49:ALA:HB2	2.01	0.42
25:AV:116:LEU:HD13	25:AV:119:ARG:NH2	2.34	0.42
27:AX:5:LYS:HG2	27:AX:54:MET:CE	2.50	0.42
27:AX:61:ILE:O	27:AX:65:LEU:HD13	2.19	0.42
30:Aa:15:ILE:HB	30:Aa:73:VAL:HG23	2.01	0.42
38:Ai:6:THR:OG1	38:Ai:10:GLY:HA2	2.20	0.42
41:BA:119:LYS:NZ	41:BA:120:THR:O	2.37	0.42
41:BA:149:ARG:HA	41:BA:152:GLU:CG	2.49	0.42
42:BB:89:PHE:CD2	42:BB:90:CYS:SG	3.13	0.42
46:BF:72:PHE:O	46:BF:91:LYS:HA	2.20	0.42
47:BG:6:LEU:O	47:BG:18:GLN:HA	2.19	0.42
48:BH:69:PRO:O	48:BH:89:GLU:HG3	2.20	0.42
48:BH:145:THR:OG1	48:BH:156:VAL:HG13	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:BO:76:ALA:HB1	55:BO:90:ASP:OD2	2.20	0.42
58:BR:6:LEU:HG	58:BR:39:ALA:HA	2.02	0.42
2:3:442:GLU:HB3	2:3:636:TYR:CB	2.41	0.41
3:1:236:A:H5'	12:AH:125:LYS:NZ	2.35	0.41
3:1:340:G:H5'	3:1:359:U:HO2'	1.84	0.41
3:1:603:U:H2'	3:1:604:G:O4'	2.20	0.41
3:1:735:G:O2'	3:1:736:G:H5'	2.20	0.41
3:1:1083:C:O2'	73:1:3430:HOH:O	2.22	0.41
3:1:1164:C:O2'	21:AR:16:LYS:O	2.38	0.41
3:1:1391:U:OP2	3:1:1392:A:O2'	2.37	0.41
3:1:1683:C:O2'	3:1:1684:C:H5'	2.20	0.41
3:1:2070:G:H5''	73:4:4180:HOH:O	2.19	0.41
3:1:2095:A:H2'	3:1:2096:U:O4'	2.19	0.41
3:1:2697:G:H2'	3:1:2698:UR3:O4'	2.19	0.41
4:4:367:A:H2'	4:4:368:A:C8	2.55	0.41
4:4:1046:C:H2'	4:4:1047:G:C8	2.55	0.41
4:4:1447:G:H2'	4:4:1448:G:O4'	2.20	0.41
73:4:3573:HOH:O	45:BE:129:SER:CB	2.67	0.41
5:AA:31:PRO:HG3	5:AA:64:PHE:HB3	2.01	0.41
5:AA:37:ARG:HG2	5:AA:59:GLU:HB2	2.02	0.41
9:AE:102:PRO:HB2	9:AE:139:LYS:NZ	2.35	0.41
11:AG:178:LYS:HE3	11:AG:179:LYS:HG2	2.02	0.41
19:AP:76:LEU:HD12	19:AP:76:LEU:HA	1.87	0.41
21:AR:49:ARG:HE	21:AR:49:ARG:HB2	1.79	0.41
22:AS:73:TYR:CE2	22:AS:90:PRO:HG3	2.53	0.41
41:BA:122:ASP:OD1	41:BA:122:ASP:N	2.51	0.41
45:BE:161:TYR:CD1	45:BE:163:LEU:HD23	2.55	0.41
49:BI:103:VAL:O	49:BI:126:LEU:HB2	2.19	0.41
51:BK:12:ARG:NH2	51:BK:14:ILE:HD11	2.35	0.41
51:BK:54:LYS:HD3	51:BK:85:ILE:HG12	2.02	0.41
54:BN:71:LYS:HB3	54:BN:94:LEU:HD13	2.02	0.41
62:BV:11:ILE:HG13	62:BV:45:TRP:HH2	1.85	0.41
1:2:86:U:H2'	1:2:87:G:C8	2.55	0.41
3:1:215:C:H2'	3:1:216:C:H6	1.85	0.41
3:1:956:C:H2'	3:1:957:U:H6	1.84	0.41
3:1:1535:C:O2'	3:1:1536:C:H5'	2.18	0.41
3:1:1819:C:O2	6:AB:228:HIS:NE2	2.33	0.41
3:1:2783:G:O4'	9:AE:122:SER:HB3	2.20	0.41
3:1:2836:C:H2'	3:1:2837:C:O4'	2.20	0.41
4:4:485:G:C5'	54:BN:116:LEU:HD11	2.51	0.41
4:4:584:C:H2'	4:4:585:C:H6	1.83	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:783:C:O2'	57:BQ:4:ARG:HD2	2.20	0.41
4:4:1006:G:H1'	4:4:1181:C:OP2	2.20	0.41
4:4:1178:A:H4'	4:4:1179:A:C5'	2.48	0.41
4:4:1242:G:H2'	4:4:1243:G:O4'	2.20	0.41
4:4:1289:OMG:OP1	55:BO:128:GLY:HA3	2.20	0.41
4:4:1399:A:H3'	4:4:1400:G:H8	1.85	0.41
4:4:1446:G:H2'	4:4:1447:G:C5'	2.50	0.41
5:AA:73:TYR:HA	38:Ai:66:PHE:HA	2.00	0.41
6:AB:51:MET:CE	6:AB:73:ALA:HB1	2.50	0.41
14:AJ:9:ARG:HD3	14:AJ:10:VAL:N	2.35	0.41
15:AL:12:ARG:HD3	15:AL:18:HIS:HA	2.01	0.41
16:AM:28:LEU:HD23	16:AM:28:LEU:HA	1.83	0.41
20:AQ:147:LYS:HE2	20:AQ:147:LYS:HB2	1.70	0.41
42:BB:190:PRO:HD3	73:BB:311:HOH:O	2.20	0.41
47:BG:63:VAL:HG12	47:BG:109:SER:HB2	2.02	0.41
48:BH:24:ILE:O	48:BH:59:ARG:HG3	2.19	0.41
51:BK:10:ASN:CB	51:BK:11:PRO:CD	2.95	0.41
63:BW:57:GLU:OE1	63:BW:57:GLU:N	2.54	0.41
68:Bb:34:ILE:O	68:Bb:38:VAL:HG23	2.20	0.41
1:2:52:C:H4'	18:AO:142:ARG:NH2	2.34	0.41
1:2:64:C:O2'	1:2:65:C:H5'	2.20	0.41
1:2:65:C:O2'	1:2:66:G:H5'	2.20	0.41
2:3:434:THR:N	2:3:447:LYS:HE2	2.36	0.41
3:1:265:C:C1'	73:1:4001:HOH:O	2.66	0.41
3:1:917:G:OP2	3:1:918:U:O2'	2.28	0.41
3:1:957:U:H2'	3:1:958:C:C6	2.55	0.41
3:1:1500:A:O4'	3:1:1948:G:H5'	2.19	0.41
3:1:1555:G:H3'	14:AJ:48:ARG:HH21	1.86	0.41
3:1:1638:C:C4'	3:1:1651:A:H4'	2.50	0.41
3:1:1794:G:OP1	30:Aa:30:LYS:NZ	2.38	0.41
3:1:2398:A:H4'	3:1:2399:A:O4'	2.20	0.41
3:1:2457:G:N3	3:1:2496:G:H2'	2.35	0.41
3:1:2627:U:H2'	3:1:2628:OMU:C6	2.51	0.41
4:4:73:C:H2'	4:4:74:G:C8	2.56	0.41
4:4:529:G:O2'	4:4:530:C:H5'	2.20	0.41
4:4:701:C:C2'	4:4:702:A:H5'	2.50	0.41
4:4:876:U:H2'	4:4:877:OMU:O4'	2.20	0.41
4:4:1177:G:O2'	4:4:1178:A:OP2	2.24	0.41
4:4:1380:C:H2'	4:4:1381:C:H6	1.86	0.41
5:AA:167:LYS:HB2	38:Ai:71:TYR:CE2	2.55	0.41
8:AD:58:SER:CB	8:AD:65:ARG:HA	2.40	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:AE:102:PRO:O	9:AE:116:ASN:HB3	2.20	0.41
10:AF:137:ARG:O	10:AF:142:LEU:HB2	2.20	0.41
11:AG:15:LYS:HD3	11:AG:15:LYS:HA	1.87	0.41
12:AH:2:ILE:HD12	12:AH:2:ILE:HA	1.86	0.41
13:AI:100:VAL:HG22	26:AW:20:MET:CE	2.50	0.41
18:AO:80:SER:OG	18:AO:143:ILE:O	2.33	0.41
23:AT:59:GLN:HB3	23:AT:177:TYR:CE1	2.55	0.41
27:AX:14:MET:HE2	27:AX:19:ARG:HG2	2.02	0.41
28:AY:71:ALA:HA	28:AY:111:ILE:HG13	2.02	0.41
38:AI:39:ARG:CZ	38:AI:46:LEU:HB2	2.51	0.41
39:AJ:51:LEU:HD22	39:AJ:52:PRO:CD	2.49	0.41
59:BS:5:LYS:O	59:BS:10:LYS:HE3	2.20	0.41
60:BT:10:LYS:O	60:BT:13:GLN:NE2	2.53	0.41
60:BT:94:ARG:O	60:BT:130:GLY:N	2.53	0.41
1:2:68:C:H2'	1:2:69:G:H8	1.84	0.41
2:3:529:MET:HE2	2:3:529:MET:HB3	1.74	0.41
2:3:550:ARG:HH22	2:3:562:LYS:HG2	1.86	0.41
3:1:421:U:P	37:Ah:38:ARG:HH21	2.43	0.41
3:1:902:OMG:H3'	3:1:910:A:H2	1.85	0.41
3:1:1612:C:O2'	3:1:1688:U:O2'	2.32	0.41
3:1:1755:G:H5'	70:1:3114:SPM:H61	2.02	0.41
3:1:1990:A2M:HM'3	3:1:1990:A2M:H1'	1.89	0.41
3:1:2645:A:C8	9:AE:176:ARG:HG3	2.56	0.41
3:1:2803:G:N1	3:1:2833:C:OP2	2.27	0.41
4:4:242:G:P	58:BR:91:ARG:HH12	2.44	0.41
4:4:709:G:H4'	4:4:710:C:OP1	2.20	0.41
4:4:728:A:H2'	4:4:729:A:O4'	2.20	0.41
4:4:833:C:H2'	4:4:834:G:O4'	2.20	0.41
4:4:926:U:O2	4:4:1188:G:O2'	2.30	0.41
4:4:1230:C:P	61:BU:121:ARG:HH22	2.42	0.41
4:4:1377:C:H2'	4:4:1378:C:H6	1.84	0.41
6:AB:196:THR:O	6:AB:199:GLN:HG2	2.20	0.41
10:AF:76:GLU:OE2	16:AM:20:HIS:ND1	2.49	0.41
12:AH:9:VAL:HG21	12:AH:20:LYS:CE	2.50	0.41
14:AK:69:SER:OG	14:AK:72:GLU:HB2	2.19	0.41
14:AK:86:MET:HE3	14:AK:86:MET:HB3	1.74	0.41
37:Ah:65:VAL:O	37:Ah:81:SER:HA	2.20	0.41
41:BA:72:PRO:HB3	41:BA:100:TYR:HB2	2.03	0.41
45:BE:54:LEU:O	45:BE:54:LEU:HD22	2.21	0.41
55:BO:29:ILE:HG21	55:BO:32:ILE:HD13	2.02	0.41
64:BX:19:PRO:HG2	64:BX:32:ARG:NH1	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:446:TYR:CZ	2:3:641:MET:HE1	2.56	0.41
2:3:471:LYS:HZ3	2:3:626:MET:HB2	1.85	0.41
3:1:684:A:H4'	3:1:685:G:C5'	2.49	0.41
3:1:746:G:O2'	73:1:3413:HOH:O	2.20	0.41
3:1:987:U:H2'	3:1:988:G:O4'	2.21	0.41
3:1:1410:U:H2'	3:1:1411:G:O4'	2.21	0.41
3:1:1781:C:O2	3:1:2813:U:O2'	2.37	0.41
3:1:2349:G:H2'	3:1:2349:G:N3	2.34	0.41
4:4:85:G:H2'	4:4:86:C:H6	1.86	0.41
4:4:900:C:C1'	73:4:3208:HOH:O	2.68	0.41
4:4:1137:G:H2'	4:4:1138:C:C6	2.55	0.41
70:4:3012:SPM:H91	57:BQ:11:ARG:HG2	2.02	0.41
5:AA:182:LYS:HD2	5:AA:184:TRP:CZ2	2.55	0.41
7:AC:231:SER:HB2	7:AC:279:ARG:NH2	2.35	0.41
8:AD:24:VAL:O	8:AD:73:ALA:HA	2.20	0.41
12:AH:29:LEU:HD23	12:AH:29:LEU:HA	1.89	0.41
13:AI:12:VAL:HB	13:AI:14:TYR:CE2	2.56	0.41
21:AR:32:LYS:HE2	21:AR:32:LYS:HB2	1.79	0.41
24:AU:45:LYS:HB3	24:AU:66:ALA:HB3	2.02	0.41
34:Ae:5:ILE:HG23	34:Ae:10:LEU:HD23	2.02	0.41
41:BA:41:LEU:HD22	41:BA:59:VAL:HG11	2.02	0.41
41:BA:191:LYS:HE3	41:BA:193:GLU:OE2	2.20	0.41
42:BB:23:LEU:O	42:BB:163:ASN:HB2	2.21	0.41
50:BJ:65:ARG:HD3	50:BJ:81:LYS:CE	2.41	0.41
62:BV:14:LEU:HG	62:BV:25:VAL:HG23	2.01	0.41
67:Ba:34:ASN:OD1	67:Ba:34:ASN:N	2.52	0.41
68:Bb:15:ARG:O	68:Bb:18:GLU:HG2	2.20	0.41
3:1:1401:G:H4'	3:1:1402:A:OP1	2.20	0.41
3:1:1556:C:H1'	14:AJ:51:ASN:HB2	2.01	0.41
4:4:571:U:O2'	44:BD:5:LYS:HD3	2.21	0.41
4:4:775:A:H2'	4:4:777:A:H5''	2.01	0.41
4:4:915:U:H2'	4:4:916:U:O4'	2.20	0.41
4:4:1287:U:H4'	55:BO:115:TRP:CE2	2.55	0.41
4:4:1299:A:H2'	4:4:1300:C:O4'	2.21	0.41
4:4:1357:U:OP1	64:BX:85:ARG:HG3	2.21	0.41
4:4:1376:A:O2'	4:4:1377:C:H5'	2.20	0.41
73:4:3469:HOH:O	58:BR:57:LYS:CG	2.55	0.41
6:AB:4:LYS:HA	6:AB:4:LYS:HD2	1.87	0.41
6:AB:202:ASP:OD1	6:AB:265:TYR:HA	2.21	0.41
7:AC:16:LEU:HD12	19:AP:19:PHE:HB2	2.02	0.41
7:AC:98:ILE:H	7:AC:98:ILE:HG13	1.64	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:AD:88:ALA:HA	8:AD:117:LEU:CD1	2.42	0.41
8:AD:145:GLN:CD	8:AD:154:VAL:HG23	2.45	0.41
8:AD:165:ALA:O	8:AD:168:PHE:HB3	2.19	0.41
12:AH:150:ARG:O	12:AH:154:GLU:HB2	2.21	0.41
14:AK:15:LEU:HD12	14:AK:54:HIS:CD2	2.55	0.41
16:AM:2:PRO:HA	16:AM:6:GLN:OE1	2.20	0.41
20:AQ:117:LEU:HD21	20:AQ:135:TYR:CE1	2.56	0.41
24:AU:1:MET:HE3	24:AU:1:MET:HB2	1.95	0.41
25:AV:113:ARG:O	25:AV:117:ILE:HG13	2.21	0.41
29:AZ:12:ILE:CG1	29:AZ:17:VAL:HG21	2.50	0.41
39:Aj:55:LYS:HD3	39:Aj:55:LYS:HA	1.68	0.41
41:BA:57:LEU:O	41:BA:76:ARG:HA	2.21	0.41
48:BH:94:LEU:CD1	48:BH:170:LEU:HB3	2.51	0.41
48:BH:155:SER:OG	48:BH:156:VAL:N	2.53	0.41
51:BK:19:LYS:HB3	51:BK:19:LYS:HE2	1.87	0.41
62:BV:47:ALA:HB1	62:BV:52:VAL:O	2.21	0.41
62:BV:78:TYR:CE1	62:BV:88:GLU:HG2	2.56	0.41
68:Bb:35:LEU:HD13	68:Bb:35:LEU:O	2.19	0.41
2:3:479:LYS:O	2:3:479:LYS:HD3	2.21	0.41
3:1:66:A:H4'	3:1:67:G:O5'	2.20	0.41
3:1:301:G:O2'	3:1:302:G:H5'	2.21	0.41
3:1:410:C:H2'	3:1:411:U:C6	2.56	0.41
3:1:445:C:O2'	3:1:446:U:H5'	2.19	0.41
3:1:1674:G:O2'	3:1:1675:G:H5'	2.21	0.41
3:1:2177:A:H2'	3:1:2178:G:O4'	2.20	0.41
3:1:2403:U:H1'	3:1:2489:G:H1'	2.03	0.41
3:1:2445:A:H1'	73:1:6917:HOH:O	2.20	0.41
4:4:282:A:C5'	4:4:283:A:H3'	2.48	0.41
4:4:636:U:O2'	53:BM:125:ILE:O	2.27	0.41
4:4:751:A:H2'	4:4:752:G:O4'	2.20	0.41
7:AC:87:GLU:HG2	7:AC:102:LYS:HE2	2.03	0.41
9:AE:103:MET:HA	9:AE:115:GLU:O	2.21	0.41
9:AE:115:GLU:OE1	9:AE:123:LYS:HD2	2.21	0.41
13:AI:75:GLU:HG2	13:AI:76:LEU:HD13	2.02	0.41
17:AN:38:THR:CG2	17:AN:84:ALA:HA	2.50	0.41
17:AN:76:TYR:O	17:AN:80:TYR:HB2	2.21	0.41
41:BA:157:LYS:HE2	41:BA:175:LEU:HA	2.03	0.41
42:BB:72:ARG:NH2	42:BB:119:ASP:OD1	2.46	0.41
42:BB:77:THR:HA	42:BB:129:ASP:OD2	2.20	0.41
43:BC:176:VAL:HG22	43:BC:189:GLU:HB2	2.02	0.41
44:BD:63:MET:HE1	44:BD:71:LEU:HD12	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:BE:179:LEU:HB2	45:BE:229:THR:O	2.21	0.41
50:BJ:105:ILE:CD1	50:BJ:114:VAL:HG13	2.49	0.41
51:BK:46:TRP:HB3	51:BK:52:ARG:HG3	2.01	0.41
53:BM:65:MET:HG2	53:BM:108:ALA:HB2	2.03	0.41
55:BO:11:ILE:O	55:BO:29:ILE:HD11	2.20	0.41
55:BO:79:LEU:HD22	55:BO:92:HIS:HB2	2.03	0.41
55:BO:100:LEU:HD23	55:BO:100:LEU:HA	1.91	0.41
57:BQ:75:LEU:HD23	57:BQ:75:LEU:HA	1.87	0.41
62:BV:13:SER:HB2	62:BV:26:LEU:HD23	2.01	0.41
2:3:491:MET:HE1	2:3:620:VAL:CG1	2.46	0.41
3:1:29:G:N3	3:1:481:G:O2'	2.54	0.41
3:1:674:G:H2'	3:1:675:G:H8	1.85	0.41
3:1:901:A:H4'	3:1:2702:G:H4'	2.03	0.41
3:1:1643:U:H2'	3:1:1644:G:H5'	2.02	0.41
3:1:1979:G:H2'	3:1:1980:C:O4'	2.21	0.41
3:1:2200:G:O2'	3:1:2201:C:H5'	2.20	0.41
3:1:2469:G:O6	3:1:2475:A:H5''	2.21	0.41
3:1:2621:C:H2'	3:1:2622:G:O4'	2.21	0.41
3:1:2711:G:H2'	3:1:2712:A:C8	2.55	0.41
4:4:6:G:O2'	4:4:7:OMG:H5'	2.20	0.41
4:4:118:C:O2'	45:BE:31:PRO:HB3	2.21	0.41
4:4:270:C:H2'	4:4:271:C:H6	1.85	0.41
4:4:1102:G:H2'	4:4:1103:G:C8	2.56	0.41
4:4:1139:C:H2'	4:4:1140:G:H8	1.86	0.41
4:4:1218:C:H2'	4:4:1219:G:H5'	2.03	0.41
4:4:1487:U:OP2	64:BX:10:ARG:NE	2.52	0.41
5:AA:88:VAL:HG21	38:AI:81:ILE:HG13	2.03	0.41
6:AB:202:ASP:OD2	6:AB:315:PRO:HA	2.20	0.41
10:AF:5:ILE:HG13	10:AF:87:GLU:OE2	2.21	0.41
18:AO:47:GLN:HG2	18:AO:61:GLY:CA	2.51	0.41
22:AS:10:TYR:O	22:AS:11:LYS:HG2	2.21	0.41
29:AZ:28:LEU:HD21	29:AZ:54:ALA:HB2	2.03	0.41
36:Ag:49:LYS:HE2	36:Ag:49:LYS:HB3	1.88	0.41
41:BA:81:ARG:HB2	41:BA:88:SER:OG	2.20	0.41
42:BB:159:MET:HE2	42:BB:159:MET:HB3	1.86	0.41
46:BF:130:VAL:O	46:BF:147:PRO:HB3	2.20	0.41
47:BG:106:ILE:HG13	47:BG:106:ILE:H	1.65	0.41
48:BH:184:ASN:HB2	48:BH:185:PRO:HD2	2.02	0.41
53:BM:23:ILE:HD12	53:BM:87:VAL:HG12	2.03	0.41
55:BO:105:ASP:O	55:BO:109:MET:HE3	2.21	0.41
60:BT:73:LYS:NZ	73:BT:204:HOH:O	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
62:BV:33:LYS:HA	62:BV:33:LYS:HD2	1.86	0.41
63:BW:41:ARG:CA	63:BW:48:GLU:HG2	2.46	0.41
64:BX:40:VAL:HG12	64:BX:41:PRO:CD	2.50	0.41
68:Bb:36:LYS:O	68:Bb:39:LEU:HB2	2.20	0.41
2:3:348:ASP:O	2:3:424:ALA:N	2.54	0.41
2:3:487:VAL:HA	2:3:597:VAL:HG12	2.02	0.41
2:3:589:HIS:O	2:3:611:PRO:HD2	2.21	0.41
3:1:86:A:H2'	3:1:87:G:O4'	2.21	0.41
3:1:209:C:H4'	3:1:210:A:C8	2.56	0.41
3:1:316:G:O2'	3:1:317:C:H5'	2.21	0.41
3:1:411:U:H2'	3:1:412:C:C6	2.56	0.41
3:1:631:A:H4'	31:Ab:25:ARG:NH1	2.36	0.41
3:1:784:G:H2'	3:1:785:A:O4'	2.20	0.41
3:1:844:A:O2'	3:1:845:G:H5'	2.21	0.41
3:1:874:U:H2'	3:1:875:OMU:O4'	2.20	0.41
3:1:939:G:H2'	3:1:1067:G:H5''	2.03	0.41
3:1:1355:G:H2'	3:1:1356:U:O4'	2.21	0.41
3:1:1401:G:H22	3:1:2825:C:P	2.44	0.41
3:1:1676:G:H8	73:1:6725:HOH:O	2.03	0.41
3:1:1757:C:H2'	3:1:1759:C:C5	2.56	0.41
3:1:1857:G:H5''	73:1:6913:HOH:O	2.20	0.41
3:1:1886:G:H2'	3:1:1887:U:O4'	2.21	0.41
3:1:2382:G:H4'	22:AS:57:ARG:HG2	2.02	0.41
3:1:2640:G:OP1	9:AE:170:LYS:NZ	2.51	0.41
3:1:2805:A:O2'	30:Aa:71:ARG:NH1	2.45	0.41
3:1:2969:A:P	3:1:2994:G:H1	2.43	0.41
4:4:139:G:H5''	47:BG:5:LYS:CE	2.51	0.41
4:4:428:C:O2'	4:4:429:U:H5'	2.21	0.41
4:4:527:G:H5''	73:4:4242:HOH:O	2.20	0.41
4:4:646:G:N1	4:4:665:A:OP2	2.51	0.41
4:4:886:U:H2'	4:4:887:G:O4'	2.21	0.41
4:4:1052:A:H2'	4:4:1054:U:H5'	2.03	0.41
4:4:1091:C:H3'	4:4:1092:C:H6	1.85	0.41
4:4:1253:A:H2'	4:4:1254:A:C8	2.56	0.41
4:4:1435:G:H3'	4:4:1436:C:C5'	2.51	0.41
73:4:3844:HOH:O	64:BX:14:ASP:HB3	2.20	0.41
6:AB:51:MET:HE2	6:AB:73:ALA:HB1	2.03	0.41
8:AD:10:LYS:HG3	8:AD:15:LYS:O	2.20	0.41
8:AD:58:SER:HB2	8:AD:65:ARG:CD	2.48	0.41
14:AK:9:ARG:HD2	14:AK:10:VAL:H	1.85	0.41
15:AL:35:LYS:HB3	15:AL:35:LYS:HE3	1.81	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:AL:81:VAL:HA	15:AL:84:LEU:HB3	2.03	0.41
16:AM:170:LYS:HE2	16:AM:170:LYS:HB3	1.72	0.41
20:AQ:92:LYS:O	20:AQ:96:MET:HG3	2.20	0.41
22:AS:19:ALA:HB3	22:AS:22:GLU:HG2	2.03	0.41
33:Ad:16:HIS:HA	33:Ad:27:TYR:O	2.21	0.41
39:Aj:36:GLY:HA2	39:Aj:49:MET:HG2	2.02	0.41
39:Aj:68:LEU:CD2	39:Aj:97:LEU:HD11	2.45	0.41
41:BA:120:THR:HA	41:BA:158:ALA:O	2.20	0.41
41:BA:167:LEU:HA	41:BA:167:LEU:HD23	1.63	0.41
42:BB:182:LEU:HD23	42:BB:187:GLU:OE2	2.21	0.41
43:BC:170:ASN:CB	43:BC:171:ARG:HD2	2.50	0.41
44:BD:63:MET:HE2	44:BD:68:ARG:HA	2.01	0.41
44:BD:65:ALA:HA	44:BD:68:ARG:NH1	2.36	0.41
44:BD:98:LEU:HD23	44:BD:99:ASP:H	1.85	0.41
48:BH:75:TYR:CD2	48:BH:84:HIS:HB2	2.55	0.41
56:BP:37:CYS:O	56:BP:38:ARG:HB3	2.21	0.41
59:BS:25:THR:CG2	59:BS:30:GLU:HB3	2.51	0.41
60:BT:74:ILE:HG23	60:BT:105:LEU:CD1	2.50	0.41
61:BU:113:PHE:C	61:BU:124:THR:HG23	2.45	0.41
62:BV:102:LYS:HB3	62:BV:102:LYS:HE3	1.58	0.41
66:BZ:25:THR:O	66:BZ:29:GLY:HA2	2.21	0.41
2:3:523:VAL:HA	2:3:527:ASN:O	2.21	0.41
3:1:795:C:H2'	3:1:796:C:C6	2.55	0.41
3:1:837:C:O2'	3:1:838:C:H5'	2.21	0.41
3:1:874:U:H2'	3:1:875:OMU:C6	2.51	0.41
3:1:1166:C:H2'	3:1:1167:G:C8	2.55	0.41
3:1:1552:G:C4'	73:1:5162:HOH:O	2.67	0.41
3:1:2352:U:O2'	3:1:2353:G:H5'	2.21	0.41
3:1:2417:U:H1'	8:AD:112:LYS:CD	2.44	0.41
3:1:2647:C:OP1	3:1:2780:A:O2'	2.38	0.41
3:1:2802:U:H2'	3:1:2803:G:O4'	2.21	0.41
3:1:2965:G:H2'	3:1:2966:U:C6	2.55	0.41
3:1:3012:C:H2'	3:1:3013:G:O4'	2.21	0.41
70:1:3107:SPM:H41	73:1:4169:HOH:O	2.20	0.41
4:4:14:C:OP2	46:BF:182:THR:OG1	2.31	0.41
4:4:58:U:H5''	4:4:389:C:H1'	2.03	0.41
4:4:883:A:H2'	4:4:884:A:C8	2.56	0.41
4:4:888:G:H2'	4:4:889:C:O4'	2.21	0.41
4:4:1054:U:H2'	4:4:1055:C:O4'	2.21	0.41
4:4:1097:C:H4'	61:BU:132:ASP:HB3	2.03	0.41
4:4:1111:G:N2	4:4:1113:A:H62	2.18	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:1323:G:H2'	4:4:1324:U:O4'	2.21	0.41
8:AD:111:ILE:CD1	8:AD:117:LEU:HD21	2.51	0.41
13:AI:24:MET:HE2	13:AI:24:MET:HA	2.02	0.41
14:AJ:60:LYS:NZ	14:AJ:82:LEU:HD22	2.35	0.41
14:AJ:96:GLU:OE2	14:AJ:96:GLU:N	2.54	0.41
17:AN:5:PRO:HB2	17:AN:7:ARG:HG2	2.03	0.41
20:AQ:10:GLU:OE1	20:AQ:11:ILE:HD13	2.20	0.41
24:AU:37:GLU:O	24:AU:41:LEU:HB2	2.21	0.41
39:AJ:53:SER:HA	39:AJ:56:LEU:HD13	2.03	0.41
39:AJ:183:LYS:HA	39:AJ:183:LYS:HD2	1.99	0.41
42:BB:121:LEU:CD2	42:BB:123:VAL:HG13	2.51	0.41
44:BD:50:LEU:HB2	44:BD:103:ILE:HD12	2.03	0.41
45:BE:170:THR:HG22	45:BE:172:LEU:CD1	2.51	0.41
47:BG:127:PRO:HG2	68:Bb:13:ILE:HB	2.02	0.41
49:BI:75:ILE:HG12	49:BI:93:TYR:CZ	2.56	0.41
50:BJ:105:ILE:HD12	50:BJ:130:ILE:HD11	2.03	0.41
51:BK:68:LYS:HE3	51:BK:68:LYS:HB3	1.92	0.41
53:BM:136:ARG:O	64:BX:28:LYS:HA	2.20	0.41
54:BN:144:LYS:HA	54:BN:145:PRO:HD3	1.94	0.41
55:BO:56:PRO:HB2	55:BO:58:ASP:OD2	2.21	0.41
61:BU:4:VAL:HG22	61:BU:131:VAL:HG12	2.02	0.41
61:BU:78:TYR:O	61:BU:96:ALA:HB2	2.20	0.41
62:BV:60:ARG:HA	62:BV:92:ILE:CD1	2.51	0.41
66:BZ:16:GLY:N	66:BZ:62:VAL:O	2.51	0.41
1:2:55:A:OP1	18:AO:169:ARG:HB2	2.21	0.40
1:2:84:A:H2'	1:2:85:C:O4'	2.21	0.40
2:3:459:ILE:HG22	2:3:460:ASP:O	2.21	0.40
3:1:1:U:C2'	3:1:2:A:C8	3.02	0.40
3:1:140:C:H5'	24:AU:33:GLN:NE2	2.36	0.40
3:1:502:A:H2'	3:1:503:A:O4'	2.21	0.40
3:1:716:A:H2'	3:1:717:A:O4'	2.21	0.40
3:1:748:G:OP2	73:1:3429:HOH:O	2.22	0.40
3:1:1882:G:OP2	73:1:3427:HOH:O	2.22	0.40
3:1:2491:A:H2'	3:1:2492:A:O4'	2.22	0.40
4:4:140:G:H5''	47:BG:63:VAL:O	2.21	0.40
4:4:205:G:H2'	4:4:206:C:C6	2.55	0.40
4:4:798:U:H2'	4:4:799:C:C6	2.56	0.40
4:4:1389:G:H2'	4:4:1390:C:C6	2.56	0.40
4:4:1417:U:OP1	4:4:1417:U:H4'	2.20	0.40
4:4:1444:G:HO2'	4:4:1445:G:H8	1.70	0.40
6:AB:55:VAL:HG21	26:AW:1:MET:CE	2.51	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AB:185:LEU:HA	6:AB:185:LEU:HD12	1.76	0.40
8:AD:3:TRP:CD2	8:AD:78:ARG:HB3	2.56	0.40
14:AK:11:VAL:HG12	14:AK:57:PRO:HA	2.04	0.40
21:AR:4:ILE:HG12	21:AR:22:VAL:HG22	2.03	0.40
30:Aa:82:ASP:OD1	30:Aa:84:THR:HG23	2.20	0.40
39:Aj:74:ILE:HD13	39:Aj:74:ILE:HA	1.84	0.40
41:BA:106:ARG:HA	41:BA:106:ARG:HD3	1.92	0.40
42:BB:106:MET:HE3	42:BB:116:LEU:CG	2.49	0.40
42:BB:181:VAL:O	42:BB:185:ARG:HD3	2.21	0.40
43:BC:178:HIS:HB2	43:BC:185:ILE:HG22	2.03	0.40
53:BM:111:ARG:HH12	64:BX:51:ARG:CD	2.34	0.40
60:BT:96:MET:O	60:BT:128:TYR:HA	2.21	0.40
1:2:8:A:H5''	1:2:9:C:OP2	2.21	0.40
2:3:501:PRO:O	2:3:579:THR:HB	2.21	0.40
2:3:540:ARG:HA	2:3:541:PRO:HD3	1.91	0.40
2:3:602:ASP:OD1	2:3:602:ASP:N	2.52	0.40
3:1:632:G:O2'	3:1:1347:G:OP1	2.28	0.40
3:1:1469:U:O4	24:AU:55:PRO:HG3	2.20	0.40
3:1:1747:C:H2'	3:1:1748:G:O4'	2.21	0.40
3:1:2147:G:H5'	73:1:6530:HOH:O	2.20	0.40
3:1:2388:OMG:HM22	3:1:2389:G:H5'	2.03	0.40
3:1:2447:A:H5''	18:AO:22:ARG:HD3	2.03	0.40
3:1:2567:C:N3	73:1:3679:HOH:O	2.37	0.40
3:1:2599:C:O2'	3:1:2600:C:H5'	2.21	0.40
4:4:97:G:N2	50:BJ:23:VAL:O	2.34	0.40
4:4:658:U:H2'	4:4:659:C:H5'	2.03	0.40
4:4:1016:G:H1'	43:BC:185:ILE:CG2	2.45	0.40
4:4:1118:A:H2'	4:4:1119:G:H8	1.86	0.40
4:4:1211:OMG:CM2	61:BU:54:ILE:HG21	2.51	0.40
4:4:1244:C:O5'	4:4:1245:A:H5'	2.22	0.40
4:4:1273:U:H1'	55:BO:141:ALA:O	2.21	0.40
6:AB:30:THR:O	6:AB:313:ARG:NH1	2.54	0.40
6:AB:32:PRO:HG3	6:AB:314:TYR:O	2.21	0.40
9:AE:99:THR:HG21	36:Ag:3:ILE:HG23	2.03	0.40
14:AJ:72:GLU:HA	14:AJ:75:LYS:CE	2.42	0.40
15:AL:86:GLU:HG2	19:AP:75:GLU:OE1	2.20	0.40
16:AM:39:ARG:CZ	16:AM:61:VAL:HG22	2.52	0.40
18:AO:23:LYS:HB3	18:AO:23:LYS:HE2	1.83	0.40
18:AO:39:LYS:HG3	18:AO:44:LEU:CD2	2.52	0.40
34:Ae:27:GLU:OE2	34:Ae:27:GLU:HA	2.21	0.40
47:BG:6:LEU:HG	47:BG:113:ILE:HG23	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:BG:136:LEU:HD11	47:BG:140:LYS:CE	2.51	0.40
51:BK:95:LEU:HB3	51:BK:104:LEU:HD21	2.03	0.40
53:BM:72:ALA:HB1	53:BM:114:LEU:HD23	2.02	0.40
60:BT:104:GLY:C	60:BT:105:LEU:HD23	2.46	0.40
62:BV:9:PHE:HB2	62:BV:45:TRP:CE2	2.56	0.40
68:Bb:27:LYS:HB3	68:Bb:30:GLU:OE1	2.21	0.40
68:Bb:39:LEU:HD23	68:Bb:39:LEU:HA	1.84	0.40
1:2:92:C:H2'	1:2:93:C:C6	2.57	0.40
2:3:479:LYS:HE2	2:3:479:LYS:HA	2.02	0.40
2:3:492:THR:HG22	2:3:493:PRO:HD2	2.03	0.40
3:1:830:C:H2'	3:1:831:G:O4'	2.22	0.40
3:1:1436:C:OP1	35:Af:3:ARG:HG2	2.21	0.40
3:1:1885:G:H5'	50:BJ:96:ARG:HH11	1.86	0.40
3:1:2028:G:H2'	3:1:2029:G:H8	1.87	0.40
3:1:2118:G:OP2	6:AB:222:THR:OG1	2.32	0.40
3:1:2736:G:OP1	6:AB:19:LYS:HB2	2.21	0.40
4:4:108:C:O2'	58:BR:55:ARG:HD2	2.21	0.40
4:4:190:C:H2'	4:4:191:C:C6	2.57	0.40
4:4:415:G:H2'	4:4:416:C:C6	2.55	0.40
4:4:1128:C:O2'	4:4:1129:C:H5'	2.20	0.40
4:4:1348:C:H1'	66:BZ:27:VAL:HG13	2.03	0.40
4:4:1428:G:O2'	4:4:1429:C:H5'	2.22	0.40
5:AA:41:VAL:HG11	5:AA:57:ARG:HG3	2.03	0.40
9:AE:87:THR:CG2	9:AE:88:LYS:HD2	2.51	0.40
11:AG:91:PRO:HD3	11:AG:158:TRP:CG	2.57	0.40
11:AG:177:ALA:HA	11:AG:180:ILE:HD12	2.04	0.40
12:AH:126:LYS:O	12:AH:130:ARG:HG3	2.22	0.40
22:AS:58:TYR:CE1	22:AS:86:ILE:HD11	2.56	0.40
23:AT:66:ASP:CB	23:AT:72:ARG:HG3	2.42	0.40
31:Ab:15:ARG:HG3	31:Ab:18:ARG:NH1	2.34	0.40
35:Af:37:ARG:HG2	35:Af:38:SER:N	2.35	0.40
38:Ai:8:ILE:HG13	38:Ai:9:VAL:HG13	2.03	0.40
42:BB:121:LEU:HD21	42:BB:123:VAL:HG13	2.03	0.40
42:BB:129:ASP:OD1	42:BB:129:ASP:N	2.53	0.40
54:BN:6:SER:HB3	54:BN:7:PRO:CD	2.51	0.40
57:BQ:43:ARG:HD3	57:BQ:43:ARG:HA	1.81	0.40
59:BS:11:SER:O	59:BS:15:LYS:HG2	2.21	0.40
68:Bb:39:LEU:O	68:Bb:43:ARG:HG3	2.21	0.40
3:1:159:G:OP1	33:Ad:43:LYS:HE2	2.20	0.40
3:1:649:U:H3'	73:1:4903:HOH:O	2.21	0.40
3:1:823:A:H5'	38:Ai:10:GLY:C	2.46	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1:1033:C:H2'	3:1:1034:C:H5'	2.03	0.40
3:1:1145:U:H5''	3:1:1146:C:OP1	2.22	0.40
3:1:1289:G:N7	73:1:3670:HOH:O	2.36	0.40
3:1:1484:G:H2'	3:1:1485:C:C6	2.57	0.40
3:1:1568:C:H2'	3:1:1569:G:H8	1.87	0.40
3:1:1681:U:O4	20:AQ:40:ALA:HB2	2.21	0.40
3:1:2071:OMG:HM22	3:1:2072:U:H5'	2.04	0.40
3:1:2090:A:H5'	3:1:2092:U:O4	2.21	0.40
4:4:339:C:H2'	4:4:340:C:C6	2.56	0.40
4:4:482:G:H1'	4:4:497:C:O2'	2.21	0.40
4:4:631:G:H2'	4:4:632:C:H6	1.86	0.40
4:4:942:A:C8	4:4:1324:U:H2'	2.56	0.40
4:4:1302:U:O2'	73:4:3104:HOH:O	2.22	0.40
4:4:1320:C:H2'	4:4:1321:G:C8	2.57	0.40
4:4:1363:C:O2'	4:4:1364:A:OP1	2.36	0.40
4:4:1388:A:H2'	4:4:1389:G:C8	2.57	0.40
5:AA:125:LEU:CD2	5:AA:139:ARG:HH12	2.35	0.40
7:AC:190:PHE:CD2	7:AC:199:VAL:HG21	2.56	0.40
18:AO:153:LYS:HE3	18:AO:153:LYS:HB3	1.79	0.40
21:AR:48:ILE:HG22	21:AR:50:ILE:HD12	2.03	0.40
23:AT:57:LEU:HD21	23:AT:61:LYS:NZ	2.36	0.40
29:AZ:8:LEU:HD22	29:AZ:12:ILE:HD11	2.04	0.40
37:Ah:1:MET:HE2	37:Ah:1:MET:HB3	1.82	0.40
39:Aj:77:HIS:O	39:Aj:80:GLN:NE2	2.55	0.40
40:Ak:38:ALA:O	40:Ak:42:VAL:HG23	2.21	0.40
42:BB:7:TYR:OH	42:BB:55:ASP:HB3	2.22	0.40
44:BD:92:LEU:HA	44:BD:95:ILE:HD13	2.04	0.40
46:BF:16:GLY:CA	46:BF:42:ILE:HD11	2.51	0.40
46:BF:137:LYS:HB2	46:BF:142:GLU:CD	2.46	0.40
48:BH:54:ASP:HB3	48:BH:57:LEU:HB2	2.03	0.40
62:BV:23:LYS:HG3	62:BV:77:VAL:HB	2.03	0.40
64:BX:7:ASN:O	64:BX:8:ARG:HB2	2.21	0.40
66:BZ:24:ARG:HA	66:BZ:32:THR:HA	2.04	0.40
2:3:379:THR:HG21	2:3:454:ASP:CB	2.51	0.40
3:1:171:A:H2'	3:1:172:A:O4'	2.22	0.40
3:1:262:U:H2'	3:1:263:C:C6	2.57	0.40
3:1:740:A:H5''	3:1:741:C:OP2	2.22	0.40
3:1:810:C:O2'	3:1:1481:A:N3	2.48	0.40
3:1:859:C:H5''	3:1:860:U:O5'	2.22	0.40
3:1:1285:C:OP1	28:AY:143:ARG:HB3	2.21	0.40
3:1:1302:U:H4'	3:1:1303:G:OP2	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1:2051:G:N2	3:1:2089:G:H2'	2.37	0.40
3:1:2163:C:H2'	3:1:2164:C:H6	1.87	0.40
3:1:2846:G:H2'	3:1:2847:G:O4'	2.22	0.40
70:1:3139:SPM:H131	73:1:5715:HOH:O	2.21	0.40
4:4:170:G:O2'	4:4:171:G:H5'	2.21	0.40
4:4:304:G:H2'	4:4:305:C:C6	2.56	0.40
4:4:824:A:H5'	4:4:825:A:OP2	2.21	0.40
4:4:1052:A:O3'	4:4:1053:G:H3'	2.21	0.40
5:AA:69:ALA:HB2	5:AA:104:PHE:CE1	2.57	0.40
6:AB:44:PHE:HD1	6:AB:194:VAL:HG21	1.87	0.40
7:AC:133:GLU:HG3	7:AC:133:GLU:H	1.68	0.40
8:AD:59:ILE:H	8:AD:64:ILE:HG13	1.85	0.40
8:AD:77:ARG:HE	8:AD:77:ARG:HB2	1.70	0.40
16:AM:98:ARG:O	16:AM:102:GLU:HG3	2.21	0.40
28:AY:97:LYS:HE3	28:AY:97:LYS:HB3	1.73	0.40
34:Ae:12:LYS:HE3	34:Ae:16:GLU:OE2	2.22	0.40
39:Aj:152:VAL:HG12	39:Aj:154:LYS:H	1.87	0.40
40:Ak:69:LEU:HD22	40:Ak:73:ILE:HD11	2.03	0.40
51:BK:14:ILE:CD1	51:BK:98:TYR:HA	2.51	0.40
55:BO:132:VAL:CG1	55:BO:133:THR:HG23	2.52	0.40
57:BQ:84:LEU:HD13	57:BQ:88:LEU:HD23	2.03	0.40
57:BQ:134:LYS:HE3	57:BQ:134:LYS:HB2	1.98	0.40
60:BT:74:ILE:HD12	60:BT:102:MET:CE	2.51	0.40
63:BW:66:PRO:HG2	63:BW:81:PHE:CZ	2.56	0.40
64:BX:52:GLU:HG3	64:BX:58:ALA:CB	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	3	291/655 (44%)	268 (92%)	22 (8%)	1 (0%)	36 53

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	AA	237/244 (97%)	229 (97%)	8 (3%)	0	100	100
6	AB	334/338 (99%)	324 (97%)	10 (3%)	0	100	100
7	AC	276/285 (97%)	269 (98%)	7 (2%)	0	100	100
8	AD	176/178 (99%)	167 (95%)	9 (5%)	0	100	100
9	AE	193/196 (98%)	187 (97%)	6 (3%)	0	100	100
10	AF	143/149 (96%)	140 (98%)	3 (2%)	0	100	100
11	AG	181/186 (97%)	179 (99%)	2 (1%)	0	100	100
12	AH	153/157 (98%)	151 (99%)	2 (1%)	0	100	100
13	AI	136/144 (94%)	134 (98%)	2 (2%)	0	100	100
14	AJ	99/103 (96%)	95 (96%)	4 (4%)	0	100	100
14	AK	88/103 (85%)	81 (92%)	5 (6%)	2 (2%)	5	7
15	AL	150/156 (96%)	144 (96%)	6 (4%)	0	100	100
16	AM	182/189 (96%)	179 (98%)	3 (2%)	0	100	100
17	AN	167/178 (94%)	161 (96%)	6 (4%)	0	100	100
18	AO	198/205 (97%)	193 (98%)	5 (2%)	0	100	100
19	AP	119/122 (98%)	118 (99%)	1 (1%)	0	100	100
20	AQ	144/147 (98%)	143 (99%)	1 (1%)	0	100	100
21	AR	74/78 (95%)	74 (100%)	0	0	100	100
22	AS	96/99 (97%)	91 (95%)	5 (5%)	0	100	100
23	AT	181/184 (98%)	176 (97%)	5 (3%)	0	100	100
24	AU	79/81 (98%)	75 (95%)	4 (5%)	0	100	100
25	AV	119/128 (93%)	117 (98%)	1 (1%)	1 (1%)	16	29
26	AW	54/62 (87%)	52 (96%)	2 (4%)	0	100	100
27	AX	65/79 (82%)	65 (100%)	0	0	100	100
28	AY	170/179 (95%)	163 (96%)	6 (4%)	1 (1%)	21	36
29	AZ	96/101 (95%)	92 (96%)	4 (4%)	0	100	100
30	Aa	86/91 (94%)	84 (98%)	2 (2%)	0	100	100
31	Ab	138/153 (90%)	137 (99%)	1 (1%)	0	100	100
32	Ac	81/84 (96%)	80 (99%)	1 (1%)	0	100	100
33	Ad	50/52 (96%)	47 (94%)	3 (6%)	0	100	100
34	Ae	64/67 (96%)	63 (98%)	1 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	Af	48/51 (94%)	47 (98%)	1 (2%)	0	100	100
36	Ag	48/53 (91%)	46 (96%)	2 (4%)	0	100	100
37	Ah	89/91 (98%)	89 (100%)	0	0	100	100
38	Ai	97/102 (95%)	90 (93%)	7 (7%)	0	100	100
39	Aj	181/184 (98%)	172 (95%)	9 (5%)	0	100	100
40	Ak	88/93 (95%)	87 (99%)	1 (1%)	0	100	100
41	BA	185/222 (83%)	181 (98%)	4 (2%)	0	100	100
42	BB	196/208 (94%)	188 (96%)	8 (4%)	0	100	100
43	BC	75/216 (35%)	59 (79%)	15 (20%)	1 (1%)	9	17
44	BD	155/159 (98%)	153 (99%)	2 (1%)	0	100	100
45	BE	234/237 (99%)	223 (95%)	11 (5%)	0	100	100
46	BF	192/202 (95%)	181 (94%)	11 (6%)	0	100	100
47	BG	138/151 (91%)	131 (95%)	7 (5%)	0	100	100
48	BH	218/223 (98%)	204 (94%)	14 (6%)	0	100	100
49	BI	127/130 (98%)	121 (95%)	6 (5%)	0	100	100
50	BJ	128/131 (98%)	123 (96%)	5 (4%)	0	100	100
51	BK	132/142 (93%)	119 (90%)	11 (8%)	2 (2%)	8	15
52	BL	36/106 (34%)	31 (86%)	4 (11%)	1 (3%)	4	5
53	BM	123/141 (87%)	116 (94%)	7 (6%)	0	100	100
54	BN	142/147 (97%)	131 (92%)	10 (7%)	1 (1%)	18	32
55	BO	141/153 (92%)	134 (95%)	6 (4%)	1 (1%)	18	32
56	BP	27/54 (50%)	18 (67%)	8 (30%)	1 (4%)	2	3
57	BQ	147/151 (97%)	145 (99%)	2 (1%)	0	100	100
58	BR	142/147 (97%)	136 (96%)	6 (4%)	0	100	100
59	BS	62/71 (87%)	59 (95%)	3 (5%)	0	100	100
60	BT	133/158 (84%)	126 (95%)	5 (4%)	2 (2%)	8	15
61	BU	153/158 (97%)	147 (96%)	6 (4%)	0	100	100
62	BV	113/128 (88%)	110 (97%)	3 (3%)	0	100	100
63	BW	66/110 (60%)	61 (92%)	4 (6%)	1 (2%)	8	15
64	BX	93/100 (93%)	69 (74%)	19 (20%)	5 (5%)	1	1
65	BY	63/67 (94%)	57 (90%)	6 (10%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
66	BZ	69/77 (90%)	60 (87%)	8 (12%)	1 (1%)	9	16
67	Ba	41/54 (76%)	39 (95%)	2 (5%)	0	100	100
68	Bb	58/68 (85%)	58 (100%)	0	0	100	100
69	Bc	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
All	All	8622/9723 (89%)	8249 (96%)	352 (4%)	21 (0%)	44	62

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
51	BK	10	ASN
52	BL	59	SER
54	BN	6	SER
55	BO	112	LEU
64	BX	29	VAL
64	BX	47	PRO
2	3	568	SER
14	AK	38	GLY
14	AK	41	SER
56	BP	29	ILE
43	BC	183	PRO
66	BZ	71	ALA
25	AV	3	PHE
28	AY	24	THR
51	BK	11	PRO
64	BX	5	ARG
64	BX	42	TYR
60	BT	86	LYS
60	BT	114	THR
63	BW	43	ILE
64	BX	53	LEU

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	3	249/552 (45%)	234 (94%)	15 (6%)	17	34
5	AA	181/186 (97%)	179 (99%)	2 (1%)	65	83
6	AB	280/282 (99%)	271 (97%)	9 (3%)	34	60
7	AC	226/231 (98%)	220 (97%)	6 (3%)	39	65
8	AD	149/149 (100%)	143 (96%)	6 (4%)	28	51
9	AE	165/165 (100%)	162 (98%)	3 (2%)	51	75
10	AF	115/118 (98%)	113 (98%)	2 (2%)	53	77
11	AG	163/165 (99%)	159 (98%)	4 (2%)	42	67
12	AH	133/135 (98%)	129 (97%)	4 (3%)	36	62
13	AI	115/118 (98%)	113 (98%)	2 (2%)	53	77
14	AJ	87/89 (98%)	83 (95%)	4 (5%)	24	45
14	AK	77/89 (86%)	75 (97%)	2 (3%)	40	66
15	AL	121/125 (97%)	116 (96%)	5 (4%)	27	50
16	AM	161/165 (98%)	159 (99%)	2 (1%)	63	82
17	AN	134/140 (96%)	128 (96%)	6 (4%)	24	46
18	AO	166/169 (98%)	163 (98%)	3 (2%)	51	75
19	AP	99/100 (99%)	97 (98%)	2 (2%)	48	73
20	AQ	127/128 (99%)	125 (98%)	2 (2%)	55	78
21	AR	69/71 (97%)	67 (97%)	2 (3%)	37	63
22	AS	84/85 (99%)	82 (98%)	2 (2%)	43	69
23	AT	157/158 (99%)	154 (98%)	3 (2%)	50	74
24	AU	71/71 (100%)	70 (99%)	1 (1%)	59	80
25	AV	107/112 (96%)	101 (94%)	6 (6%)	19	37
26	AW	48/53 (91%)	43 (90%)	5 (10%)	7	13
27	AX	58/65 (89%)	56 (97%)	2 (3%)	32	57
28	AY	147/152 (97%)	144 (98%)	3 (2%)	48	73
29	AZ	77/79 (98%)	71 (92%)	6 (8%)	11	23
30	Aa	78/81 (96%)	74 (95%)	4 (5%)	21	41
31	Ab	125/137 (91%)	125 (100%)	0	100	100
32	Ac	67/68 (98%)	63 (94%)	4 (6%)	17	34
33	Ad	44/44 (100%)	44 (100%)	0	100	100
34	Ae	60/61 (98%)	56 (93%)	4 (7%)	15	29

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	Af	42/43 (98%)	42 (100%)	0	100	100
36	Ag	46/49 (94%)	46 (100%)	0	100	100
37	Ah	82/82 (100%)	82 (100%)	0	100	100
38	Ai	77/80 (96%)	77 (100%)	0	100	100
39	Aj	161/162 (99%)	155 (96%)	6 (4%)	30	54
40	Ak	79/82 (96%)	76 (96%)	3 (4%)	29	53
41	BA	157/181 (87%)	150 (96%)	7 (4%)	24	46
42	BB	174/182 (96%)	168 (97%)	6 (3%)	32	57
43	BC	63/183 (34%)	55 (87%)	8 (13%)	4	8
44	BD	136/138 (99%)	131 (96%)	5 (4%)	30	54
45	BE	203/204 (100%)	198 (98%)	5 (2%)	42	67
46	BF	161/169 (95%)	151 (94%)	10 (6%)	16	32
47	BG	114/121 (94%)	107 (94%)	7 (6%)	17	33
48	BH	191/193 (99%)	187 (98%)	4 (2%)	47	72
49	BI	109/110 (99%)	104 (95%)	5 (5%)	24	45
50	BJ	105/106 (99%)	101 (96%)	4 (4%)	29	53
51	BK	110/117 (94%)	105 (96%)	5 (4%)	24	46
52	BL	34/94 (36%)	29 (85%)	5 (15%)	3	5
53	BM	93/106 (88%)	91 (98%)	2 (2%)	45	71
54	BN	117/120 (98%)	114 (97%)	3 (3%)	40	66
55	BO	113/119 (95%)	104 (92%)	9 (8%)	11	22
56	BP	25/48 (52%)	24 (96%)	1 (4%)	28	51
57	BQ	135/137 (98%)	129 (96%)	6 (4%)	25	47
58	BR	131/134 (98%)	125 (95%)	6 (5%)	24	45
59	BS	55/59 (93%)	54 (98%)	1 (2%)	51	75
60	BT	120/137 (88%)	115 (96%)	5 (4%)	26	49
61	BU	127/130 (98%)	121 (95%)	6 (5%)	23	44
62	BV	101/111 (91%)	93 (92%)	8 (8%)	11	22
63	BW	59/94 (63%)	55 (93%)	4 (7%)	14	28
64	BX	85/89 (96%)	80 (94%)	5 (6%)	18	35
65	BY	55/57 (96%)	48 (87%)	7 (13%)	4	8

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
66	BZ	59/63 (94%)	58 (98%)	1 (2%)	53 77
67	Ba	39/44 (89%)	38 (97%)	1 (3%)	40 66
68	Bb	49/56 (88%)	49 (100%)	0	100 100
69	Bc	51/52 (98%)	49 (96%)	2 (4%)	28 52
All	All	7398/8195 (90%)	7130 (96%)	268 (4%)	32 55

All (268) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	3	325	VAL
2	3	341	VAL
2	3	351	SER
2	3	385	SER
2	3	423	THR
2	3	468	VAL
2	3	509	THR
2	3	512	ILE
2	3	531	VAL
2	3	559	VAL
2	3	564	THR
2	3	588	ASP
2	3	594	ASN
2	3	609	VAL
2	3	610	VAL
5	AA	83	ASP
5	AA	127	ILE
6	AB	34	VAL
6	AB	70	VAL
6	AB	91	THR
6	AB	117	VAL
6	AB	187	LYS
6	AB	215	VAL
6	AB	221	VAL
6	AB	247	LEU
6	AB	278	GLU
7	AC	13	LEU
7	AC	43	ASP
7	AC	110	CYS
7	AC	168	SER
7	AC	169	LEU
7	AC	275	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	AD	28	VAL
8	AD	58	SER
8	AD	112	LYS
8	AD	126	VAL
8	AD	132	ASP
8	AD	146	LEU
9	AE	31	LYS
9	AE	61	VAL
9	AE	164	GLU
10	AF	4	THR
10	AF	100	LYS
11	AG	17	GLU
11	AG	55	VAL
11	AG	107	VAL
11	AG	143	LEU
12	AH	18	VAL
12	AH	37	LEU
12	AH	38	ASN
12	AH	82	THR
13	AI	70	ARG
13	AI	96	ASP
14	AJ	4	VAL
14	AJ	27	ASP
14	AJ	73	VAL
14	AJ	98	THR
14	AK	22	LYS
14	AK	46	ARG
15	AL	2	VAL
15	AL	9	THR
15	AL	46	SER
15	AL	58	TRP
15	AL	124	VAL
16	AM	26	SER
16	AM	148	SER
17	AN	11	ARG
17	AN	100	GLU
17	AN	111	ARG
17	AN	114	GLU
17	AN	164	THR
17	AN	169	GLU
18	AO	50	ILE
18	AO	168	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
18	AO	175	LEU
19	AP	116	SER
19	AP	122	ILE
20	AQ	2	VAL
20	AQ	95	VAL
21	AR	56	VAL
21	AR	75	VAL
22	AS	15	LEU
22	AS	89	THR
23	AT	9	THR
23	AT	19	LYS
23	AT	161	VAL
24	AU	7	ILE
25	AV	37	GLN
25	AV	53	VAL
25	AV	85	THR
25	AV	87	SER
25	AV	90	GLN
25	AV	101	VAL
26	AW	3	ILE
26	AW	5	LYS
26	AW	25	ASP
26	AW	49	LYS
26	AW	56	LYS
27	AX	25	GLN
27	AX	62	GLU
28	AY	34	ASP
28	AY	112	SER
28	AY	154	VAL
29	AZ	8	LEU
29	AZ	28	LEU
29	AZ	29	LEU
29	AZ	69	ILE
29	AZ	92	SER
29	AZ	94	ILE
30	Aa	8	VAL
30	Aa	10	THR
30	Aa	26	THR
30	Aa	59	GLU
32	Ac	51	VAL
32	Ac	57	SER
32	Ac	72	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	Ac	84	ARG
34	Ae	8	VAL
34	Ae	28	ASP
34	Ae	52	GLN
34	Ae	55	SER
39	Aj	42	VAL
39	Aj	53	SER
39	Aj	109	LYS
39	Aj	165	VAL
39	Aj	169	THR
39	Aj	182	GLU
40	Ak	37	THR
40	Ak	55	LYS
40	Ak	60	VAL
41	BA	104	LEU
41	BA	116	THR
41	BA	122	ASP
41	BA	137	ARG
41	BA	167	LEU
41	BA	189	MET
41	BA	206	GLU
42	BB	95	CYS
42	BB	108	THR
42	BB	112	LEU
42	BB	151	THR
42	BB	160	ILE
42	BB	169	SER
43	BC	142	VAL
43	BC	149	GLU
43	BC	164	ILE
43	BC	177	VAL
43	BC	181	LEU
43	BC	193	THR
43	BC	199	TYR
43	BC	200	SER
44	BD	18	LYS
44	BD	66	GLU
44	BD	93	ASP
44	BD	97	SER
44	BD	154	LYS
45	BE	29	THR
45	BE	126	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
45	BE	149	VAL
45	BE	159	VAL
45	BE	234	VAL
46	BF	13	THR
46	BF	26	THR
46	BF	47	LEU
46	BF	70	ASN
46	BF	82	ASP
46	BF	95	VAL
46	BF	111	THR
46	BF	159	VAL
46	BF	172	VAL
46	BF	176	THR
47	BG	13	SER
47	BG	34	ILE
47	BG	36	GLU
47	BG	55	ILE
47	BG	63	VAL
47	BG	113	ILE
47	BG	139	LEU
48	BH	9	LEU
48	BH	88	VAL
48	BH	145	THR
48	BH	156	VAL
49	BI	14	ILE
49	BI	47	VAL
49	BI	54	ASP
49	BI	76	ARG
49	BI	129	VAL
50	BJ	41	LEU
50	BJ	65	ARG
50	BJ	76	ARG
50	BJ	114	VAL
51	BK	4	VAL
51	BK	10	ASN
51	BK	24	VAL
51	BK	59	LEU
51	BK	135	SER
52	BL	45	LEU
52	BL	47	THR
52	BL	65	THR
52	BL	74	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
52	BL	77	LEU
53	BM	81	ASN
53	BM	93	TYR
54	BN	66	ASN
54	BN	85	THR
54	BN	105	ILE
55	BO	8	ILE
55	BO	34	ILE
55	BO	94	ILE
55	BO	96	SER
55	BO	108	LEU
55	BO	126	VAL
55	BO	131	THR
55	BO	137	PHE
55	BO	143	VAL
56	BP	44	VAL
57	BQ	63	VAL
57	BQ	71	LEU
57	BQ	80	ILE
57	BQ	86	GLU
57	BQ	118	VAL
57	BQ	147	SER
58	BR	8	SER
58	BR	17	THR
58	BR	128	ILE
58	BR	133	ASP
58	BR	134	VAL
58	BR	135	VAL
59	BS	40	ASP
60	BT	87	VAL
60	BT	103	VAL
60	BT	113	ILE
60	BT	136	THR
60	BT	139	VAL
61	BU	10	ASP
61	BU	59	ILE
61	BU	69	VAL
61	BU	115	THR
61	BU	124	THR
61	BU	153	VAL
62	BV	23	LYS
62	BV	25	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
62	BV	52	VAL
62	BV	63	LYS
62	BV	79	THR
62	BV	86	VAL
62	BV	100	GLU
62	BV	102	LYS
63	BW	53	THR
63	BW	59	GLN
63	BW	65	THR
63	BW	96	VAL
64	BX	17	ARG
64	BX	30	VAL
64	BX	39	THR
64	BX	40	VAL
64	BX	92	VAL
65	BY	18	VAL
65	BY	21	ARG
65	BY	22	CYS
65	BY	31	THR
65	BY	38	VAL
65	BY	48	LEU
65	BY	62	VAL
66	BZ	49	THR
67	Ba	3	SER
69	Bc	28	ARG
69	Bc	31	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
5	AA	33	ASN
6	AB	6	ASN
6	AB	243	GLN
8	AD	145	GLN
9	AE	160	GLN
12	AH	8	GLN
12	AH	153	ASN
17	AN	30	GLN
17	AN	113	GLN
20	AQ	64	HIS
23	AT	12	GLN
24	AU	50	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
25	AV	90	GLN
27	AX	36	GLN
31	Ab	49	GLN
36	Ag	16	HIS
36	Ag	25	ASN
37	Ah	24	ASN
37	Ah	62	ASN
39	Aj	105	ASN
39	Aj	155	GLN
39	Aj	161	ASN
41	BA	136	HIS
44	BD	89	ASN
46	BF	56	ASN
46	BF	63	GLN
49	BI	91	GLN
50	BJ	57	HIS
51	BK	8	GLN
51	BK	10	ASN
51	BK	100	GLN
53	BM	28	ASN
55	BO	120	HIS
57	BQ	7	HIS
57	BQ	27	GLN
59	BS	48	ASN
62	BV	49	GLN
66	BZ	20	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	128/129 (99%)	9 (7%)	1 (0%)
3	1	2844/3024 (94%)	353 (12%)	25 (0%)
4	4	1426/1498 (95%)	261 (18%)	32 (2%)
All	All	4398/4651 (94%)	623 (14%)	58 (1%)

All (623) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	8	A
1	2	25	G
1	2	28	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2	59	U
1	2	60	A
1	2	76	U
1	2	77	C
1	2	98	G
1	2	117	G
3	1	2	A
3	1	29	G
3	1	38	5MC
3	1	43	G
3	1	63	A
3	1	66	A
3	1	67	G
3	1	75	U
3	1	76	A
3	1	77	G
3	1	83	G
3	1	109	A
3	1	110	A
3	1	111	U
3	1	118	U
3	1	134	U
3	1	154	G
3	1	162	A
3	1	177	A
3	1	196	G
3	1	197	A
3	1	203	A
3	1	204	G
3	1	208	A
3	1	211	G
3	1	229	G
3	1	233	C
3	1	247	G
3	1	258	A
3	1	269	A
3	1	270	C
3	1	292	U
3	1	294	G
3	1	303	C
3	1	304	A
3	1	305	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	1	328	G
3	1	329	U
3	1	330	G
3	1	335	G
3	1	358	A
3	1	359	U
3	1	366	G
3	1	373	A
3	1	374	A
3	1	389	A
3	1	390	G
3	1	399	U
3	1	406	G
3	1	422	U
3	1	423	U
3	1	435	G
3	1	436	C
3	1	437	G
3	1	442	C
3	1	457	G
3	1	487	U
3	1	488	A
3	1	489	G
3	1	504	G
3	1	512	G
3	1	523	G
3	1	534	A
3	1	535	G
3	1	558	G
3	1	575	G
3	1	576	G
3	1	606	C
3	1	613	G
3	1	614	U
3	1	629	C
3	1	643	U
3	1	644	A
3	1	655	C
3	1	656	A
3	1	668	G
3	1	669	U
3	1	684	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	1	685	G
3	1	698	A
3	1	723	C
3	1	724	A
3	1	725	G
3	1	740	A
3	1	772	A
3	1	803	U
3	1	826	G
3	1	847	C
3	1	860	U
3	1	865	U
3	1	881	G
3	1	893	G
3	1	894	G
3	1	900	A
3	1	902	OMG
3	1	903	A
3	1	907	A
3	1	910	A
3	1	923	G
3	1	930	C
3	1	945	C
3	1	946	U
3	1	965	G
3	1	968	G
3	1	978	G
3	1	989	A
3	1	1021	C
3	1	1029	A
3	1	1031	C
3	1	1053	G
3	1	1067	G
3	1	1074	U
3	1	1075	G
3	1	1082	G
3	1	1095	G
3	1	1101	A
3	1	1104	A
3	1	1129	A
3	1	1132	U
3	1	1133	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	1	1147	A
3	1	1160	G
3	1	1171	A
3	1	1172	A
3	1	1173	G
3	1	1176	A
3	1	1177	G
3	1	1238	G
3	1	1254	G
3	1	1255	A
3	1	1256	U
3	1	1259	A
3	1	1260	C
3	1	1262	G
3	1	1268	A
3	1	1301	U
3	1	1302	U
3	1	1303	G
3	1	1312	G
3	1	1322	G
3	1	1323	G
3	1	1328	G
3	1	1338	A
3	1	1354	G
3	1	1365	C
3	1	1382	U
3	1	1383	C
3	1	1389	G
3	1	1393	G
3	1	1402	A
3	1	1417	C
3	1	1424	G
3	1	1428	G
3	1	1429	A
3	1	1430	A
3	1	1431	A
3	1	1470	U
3	1	1474	C
3	1	1480	U
3	1	1483	G
3	1	1500	A
3	1	1508	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	1	1510	A
3	1	1514	A
3	1	1515	A
3	1	1526	A
3	1	1527	U
3	1	1549	U
3	1	1550	C
3	1	1551	U
3	1	1559	C
3	1	1562	A
3	1	1564	G
3	1	1577	C
3	1	1578	G
3	1	1602	U
3	1	1604	C
3	1	1623	A
3	1	1632	G
3	1	1633	A
3	1	1635	U
3	1	1636	G
3	1	1644	G
3	1	1668	A
3	1	1669	U
3	1	1680	U
3	1	1681	U
3	1	1698	U
3	1	1712	A
3	1	1728	C
3	1	1752	A
3	1	1757	C
3	1	1760	A
3	1	1764	G
3	1	1765	C
3	1	1777	A
3	1	1786	G
3	1	1789	G
3	1	1790	C
3	1	1791	U
3	1	1792	C
3	1	1818	G
3	1	1840	G
3	1	1860	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	1	1867	U
3	1	1868	A
3	1	1869	U
3	1	1870	A
3	1	1892	G
3	1	1900	G
3	1	1909	A
3	1	1916	A
3	1	1918	C
3	1	1920	A
3	1	1922	A
3	1	1927	A
3	1	1936	C
3	1	1938	A
3	1	1947	OMG
3	1	1975	A
3	1	1999	A
3	1	2022	A
3	1	2023	G
3	1	2024	G
3	1	2027	G
3	1	2028	G
3	1	2029	G
3	1	2030	G
3	1	2031	G
3	1	2032	U
3	1	2034	A
3	1	2041	C
3	1	2043	C
3	1	2047	U
3	1	2048	A
3	1	2051	G
3	1	2054	G
3	1	2058	A
3	1	2061	G
3	1	2062	C
3	1	2076	U
3	1	2084	U
3	1	2085	G
3	1	2088	OMU
3	1	2091	A
3	1	2092	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	1	2093	G
3	1	2103	OMG
3	1	2112	U
3	1	2114	U
3	1	2116	OMC
3	1	2118	G
3	1	2142	U
3	1	2151	A
3	1	2153	A
3	1	2175	C
3	1	2176	OMG
3	1	2180	A
3	1	2181	G
3	1	2189	G
3	1	2199	A
3	1	2213	G
3	1	2318	A
3	1	2336	A
3	1	2337	C
3	1	2350	G
3	1	2357	G
3	1	2361	G
3	1	2362	OMG
3	1	2391	G
3	1	2395	C
3	1	2399	A
3	1	2400	A
3	1	2417	U
3	1	2421	A
3	1	2422	A
3	1	2432	A
3	1	2434	A
3	1	2446	A
3	1	2447	A
3	1	2457	G
3	1	2498	G
3	1	2500	C
3	1	2507	A
3	1	2537	OMG
3	1	2540	U
3	1	2541	G
3	1	2546	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	1	2547	A
3	1	2548	A
3	1	2555	OMC
3	1	2559	G
3	1	2561	A
3	1	2562	A
3	1	2582	G
3	1	2589	C
3	1	2590	C
3	1	2594	C
3	1	2606	U
3	1	2608	OMG
3	1	2612	C
3	1	2616	G
3	1	2617	A
3	1	2632	A
3	1	2643	G
3	1	2644	C
3	1	2680	A
3	1	2681	G
3	1	2687	C
3	1	2696	G
3	1	2699	U
3	1	2717	G
3	1	2723	U
3	1	2724	C
3	1	2727	U
3	1	2735	G
3	1	2743	U
3	1	2744	G
3	1	2754	G
3	1	2758	A
3	1	2759	A
3	1	2760	G
3	1	2770	G
3	1	2788	G
3	1	2804	U
3	1	2825	C
3	1	2826	U
3	1	2827	G
3	1	2846	G
3	1	2854	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	1	2860	A
3	1	2863	G
3	1	2869	A
3	1	2877	A
3	1	2878	G
3	1	2890	A
3	1	2903	U
3	1	2913	G
3	1	2915	A
3	1	2929	A
3	1	2939	U
3	1	2952	U
3	1	2953	G
3	1	2954	A
3	1	2982	U
3	1	2983	U
3	1	2985	C
3	1	2995	A
3	1	2996	G
3	1	3000	G
3	1	3007	C
3	1	3013	G
3	1	3019	G
4	4	3	A
4	4	8	U
4	4	9	U
4	4	12	U
4	4	13	C
4	4	14	C
4	4	16	G
4	4	17	C
4	4	19	OMG
4	4	33	U
4	4	56	A
4	4	72	G
4	4	73	C
4	4	74	G
4	4	75	C
4	4	89	A
4	4	101	C
4	4	102	A
4	4	110	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	4	111	A
4	4	112	C
4	4	117	C
4	4	137	C
4	4	138	G
4	4	144	C
4	4	154	U
4	4	155	C
4	4	172	C
4	4	179	A
4	4	181	G
4	4	193	A
4	4	195	A
4	4	196	G
4	4	209	A
4	4	211	C
4	4	212	C
4	4	213	G
4	4	214	C
4	4	246	A
4	4	248	C
4	4	250	G
4	4	254	G
4	4	269	G
4	4	270	C
4	4	283	A
4	4	284	G
4	4	292	G
4	4	296	C
4	4	304	G
4	4	308	C
4	4	309	G
4	4	332	C
4	4	333	A
4	4	349	C
4	4	356	C
4	4	359	C
4	4	371	C
4	4	376	C
4	4	377	A
4	4	401	A
4	4	410	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	4	418	A
4	4	431	U
4	4	455	A
4	4	456	A
4	4	457	U
4	4	463	G
4	4	465	OMG
4	4	471	G
4	4	472	U
4	4	479	U
4	4	488	G
4	4	491	G
4	4	492	U
4	4	493	A
4	4	494	A
4	4	496	A2M
4	4	508	M7A
4	4	511	OMG
4	4	524	A
4	4	525	C
4	4	533	A
4	4	534	A
4	4	537	C
4	4	542	G
4	4	557	A
4	4	594	G
4	4	600	G
4	4	614	A
4	4	623	G
4	4	626	A
4	4	627	G
4	4	636	U
4	4	647	U
4	4	648	A
4	4	649	G
4	4	656	A
4	4	662	U
4	4	664	A
4	4	665	A
4	4	679	A
4	4	683	G
4	4	685	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	4	692	G
4	4	695	G
4	4	704	A
4	4	709	G
4	4	710	C
4	4	716	G
4	4	723	G
4	4	738	A
4	4	742	A
4	4	748	A
4	4	753	A
4	4	754	U
4	4	755	A
4	4	778	C
4	4	781	U
4	4	789	A
4	4	790	G
4	4	807	G
4	4	808	G
4	4	832	C
4	4	841	C
4	4	855	G
4	4	856	U
4	4	867	G
4	4	879	A2M
4	4	887	G
4	4	891	G
4	4	899	C
4	4	901	A
4	4	924	A
4	4	926	U
4	4	927	U
4	4	928	G
4	4	929	G
4	4	930	A
4	4	944	A
4	4	1007	G
4	4	1008	A
4	4	1009	G
4	4	1012	G
4	4	1013	C
4	4	1023	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	4	1024	U
4	4	1025	C
4	4	1037	U
4	4	1040	G
4	4	1045	OMC
4	4	1051	A
4	4	1053	G
4	4	1054	U
4	4	1058	G
4	4	1060	A2M
4	4	1068	A
4	4	1069	G
4	4	1073	C
4	4	1084	U
4	4	1085	U
4	4	1086	G
4	4	1089	A
4	4	1090	C
4	4	1091	C
4	4	1092	C
4	4	1093	C
4	4	1099	A
4	4	1100	C
4	4	1101	G
4	4	1102	G
4	4	1113	A
4	4	1119	G
4	4	1125	C
4	4	1126	U
4	4	1127	G
4	4	1135	A
4	4	1136	A
4	4	1137	G
4	4	1149	A
4	4	1150	G
4	4	1162	A
4	4	1163	OMG
4	4	1164	G
4	4	1166	C
4	4	1167	A
4	4	1168	G
4	4	1175	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	4	1177	G
4	4	1178	A
4	4	1179	A
4	4	1180	A
4	4	1181	C
4	4	1182	C
4	4	1183	C
4	4	1192	C
4	4	1193	A
4	4	1199	G
4	4	1201	U
4	4	1202	OMG
4	4	1204	A
4	4	1211	OMG
4	4	1214	A
4	4	1223	U
4	4	1226	G
4	4	1236	G
4	4	1246	A
4	4	1252	U
4	4	1265	A
4	4	1266	G
4	4	1268	A
4	4	1271	G
4	4	1286	C
4	4	1301	G
4	4	1302	U
4	4	1319	G
4	4	1325	C
4	4	1326	A
4	4	1330	A
4	4	1336	G
4	4	1345	G
4	4	1360	A
4	4	1364	A
4	4	1366	C
4	4	1385	G
4	4	1416	G
4	4	1417	U
4	4	1418	G
4	4	1419	G
4	4	1422	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	4	1427	A
4	4	1430	A
4	4	1431	G
4	4	1432	G
4	4	1433	G
4	4	1435	G
4	4	1436	C
4	4	1437	U
4	4	1440	C
4	4	1442	A
4	4	1445	G
4	4	1447	G
4	4	1449	U
4	4	1450	G
4	4	1451	A
4	4	1452	A
4	4	1453	G
4	4	1456	G
4	4	1458	A
4	4	1462	A
4	4	1463	G
4	4	1464	G
4	4	1465	U
4	4	1466	A
4	4	1476	G
4	4	1479	C
4	4	1488	G
4	4	1489	G
4	4	1490	A
4	4	1491	U
4	4	1493	A
4	4	1494	C

All (58) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	7	A
3	1	117	U
3	1	434	C
3	1	456	G
3	1	533	A
3	1	541	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	1	575	G
3	1	613	G
3	1	668	G
3	1	724	A
3	1	859	C
3	1	880	U
3	1	902	OMG
3	1	1253	A
3	1	1337	C
3	1	1514	A
3	1	1526	A
3	1	2022	A
3	1	2102	A
3	1	2361	G
3	1	2420	G
3	1	2431	U
3	1	2868	U
3	1	2914	C
3	1	2984	C
3	1	2995	A
4	4	16	G
4	4	73	C
4	4	101	C
4	4	212	C
4	4	213	G
4	4	358	G
4	4	471	G
4	4	510	U
4	4	593	C
4	4	663	U
4	4	664	A
4	4	678	C
4	4	855	G
4	4	928	G
4	4	1007	G
4	4	1023	G
4	4	1053	G
4	4	1090	C
4	4	1091	C
4	4	1098	U
4	4	1134	U
4	4	1162	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	4	1174	C
4	4	1176	C
4	4	1178	A
4	4	1179	A
4	4	1251	G
4	4	1417	U
4	4	1421	G
4	4	1444	G
4	4	1448	G
4	4	1464	G

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

106 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	$\# Z > 2$
4	MA6	4	1478	4	23,26,27	0.35	0	33,38,41	0.81	1 (3%)
3	5MC	1	2056	71,3	19,22,23	1.53	3 (15%)	26,32,35	1.17	3 (11%)
3	OMU	1	2574	3	19,22,23	1.28	4 (21%)	25,31,34	1.80	4 (16%)
3	OMC	1	2704	3	19,22,23	0.81	0	25,31,34	0.81	0
4	OMG	4	1289	4,71	23,26,27	1.22	3 (13%)	32,38,41	2.00	5 (15%)
4	OMC	4	572	4	19,22,23	0.80	0	25,31,34	0.89	1 (4%)
3	OMG	1	2176	71,3	23,26,27	1.22	4 (17%)	32,38,41	1.98	6 (18%)
3	UR3	1	2698	3	19,22,23	0.94	1 (5%)	26,32,35	1.69	3 (11%)
3	PSU	1	2607	3	18,21,22	0.96	1 (5%)	21,30,33	0.75	0
3	OMC	1	2885	3	19,22,23	0.81	0	25,31,34	0.78	0
4	OMG	4	19	4	23,26,27	1.22	4 (17%)	32,38,41	2.01	5 (15%)
4	OMG	4	1211	4	23,26,27	1.24	3 (13%)	32,38,41	2.05	7 (21%)
3	OMU	1	2707	3	19,22,23	1.31	3 (15%)	25,31,34	1.88	5 (20%)
3	OMG	1	902	71,3	23,26,27	1.20	4 (17%)	32,38,41	1.98	6 (18%)
3	OMG	1	2066	3	23,26,27	1.25	4 (17%)	32,38,41	2.01	7 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
53	IAS	BM	128	53	6,7,8	1.32	1 (16%)	3,8,10	1.21	0
4	MA6	4	1477	4	23,26,27	0.35	0	33,38,41	0.76	1 (3%)
4	M7A	4	508	4	19,25,26	0.29	0	25,37,40	0.59	0
4	OMC	4	514	4	19,22,23	0.83	0	25,31,34	0.92	1 (4%)
3	OMG	1	2366	3	23,26,27	1.19	3 (13%)	32,38,41	1.96	6 (18%)
3	PSU	1	2571	3	18,21,22	0.92	1 (5%)	21,30,33	0.68	0
3	OMG	1	2667	3	23,26,27	1.22	3 (13%)	32,38,41	2.04	6 (18%)
3	OMU	1	2408	3	19,22,23	1.25	3 (15%)	25,31,34	1.88	5 (20%)
3	A2M	1	2059	71,3	22,25,26	0.27	0	30,36,39	0.61	0
4	A2M	4	880	4	22,25,26	0.20	0	30,36,39	0.45	0
3	5MC	1	38	3	19,22,23	1.47	3 (15%)	26,32,35	1.33	5 (19%)
3	OMC	1	1816	3	19,22,23	0.79	0	25,31,34	0.74	0
3	OMG	1	2103	3	23,26,27	1.23	4 (17%)	32,38,41	1.99	5 (15%)
3	OMU	1	908	71,3	19,22,23	1.33	4 (21%)	25,31,34	2.00	7 (28%)
3	A2M	1	2011	3	22,25,26	0.21	0	30,36,39	0.45	0
4	OMC	4	1034	4	19,22,23	0.82	1 (5%)	25,31,34	0.83	0
3	OMG	1	1949	3	23,26,27	1.23	3 (13%)	32,38,41	1.96	6 (18%)
3	OMC	1	872	3	19,22,23	0.79	0	25,31,34	0.83	0
3	G7M	1	3023	3	23,26,27	1.84	2 (8%)	34,39,42	1.06	2 (5%)
3	PSU	1	2610	3	18,21,22	0.94	1 (5%)	21,30,33	0.73	0
3	A2M	1	1990	3	22,25,26	0.19	0	30,36,39	0.47	0
4	OMG	4	7	4	23,26,27	1.23	3 (13%)	32,38,41	2.01	6 (18%)
3	B8T	1	79	3	19,22,23	0.40	0	25,31,34	0.35	0
3	OMC	1	2624	3	19,22,23	0.83	1 (5%)	25,31,34	0.74	0
3	OMG	1	2608	3	23,26,27	1.19	4 (17%)	32,38,41	1.96	6 (18%)
4	OMG	4	465	4	23,26,27	1.22	4 (17%)	32,38,41	1.94	6 (18%)
4	OMG	4	462	4	23,26,27	1.21	3 (13%)	32,38,41	1.97	6 (18%)
4	PSU	4	263	4	18,21,22	0.92	1 (5%)	21,30,33	0.58	0
4	OMG	4	1210	4	23,26,27	1.23	3 (13%)	32,38,41	2.00	7 (21%)
3	OMC	1	2538	3	19,22,23	0.79	0	25,31,34	0.79	0
4	OMG	4	511	4	23,26,27	1.20	4 (17%)	32,38,41	1.96	6 (18%)
4	OMC	4	1368	4	19,22,23	0.83	1 (5%)	25,31,34	0.77	0
3	OMC	1	2116	3	19,22,23	0.83	0	25,31,34	0.64	0
3	B8T	1	2937	3	19,22,23	0.40	0	25,31,34	0.31	0
3	OMG	1	2537	3	23,26,27	1.19	3 (13%)	32,38,41	1.99	6 (18%)
4	OMU	4	15	4	19,22,23	1.37	4 (21%)	25,31,34	1.91	5 (20%)
4	OMG	4	674	4	23,26,27	1.22	3 (13%)	32,38,41	2.01	5 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	OMG	1	2601	71,3	23,26,27	1.20	3 (13%)	32,38,41	2.02	7 (21%)
3	4AC	1	2016	3	21,24,25	0.39	0	28,34,37	0.57	0
3	OMG	1	1957	3	23,26,27	1.19	4 (17%)	32,38,41	2.00	6 (18%)
4	4AC	4	1318	4	21,24,25	0.39	0	28,34,37	0.73	0
4	A2M	4	496	4	22,25,26	0.21	0	30,36,39	0.46	0
4	A2M	4	879	4	22,25,26	0.22	0	30,36,39	0.38	0
3	PSU	1	2625	3	18,21,22	0.93	1 (5%)	21,30,33	0.70	0
3	OMU	1	2088	3	19,22,23	1.29	3 (15%)	25,31,34	1.81	5 (20%)
3	PSU	1	2044	3	18,21,22	0.94	1 (5%)	21,30,33	0.57	0
3	OMC	1	2143	3	19,22,23	0.29	0	25,31,34	0.35	0
3	OMU	1	2155	3	19,22,23	1.27	3 (15%)	25,31,34	1.88	5 (20%)
3	OMU	1	875	3	19,22,23	1.31	4 (21%)	25,31,34	1.91	5 (20%)
4	B8T	4	1469	4	19,22,23	0.44	0	25,31,34	0.39	0
3	OMC	1	2884	3	19,22,23	0.81	0	25,31,34	0.83	1 (4%)
3	OMC	1	493	3	19,22,23	0.79	0	25,31,34	0.83	0
3	OMC	1	1976	3	19,22,23	0.84	2 (10%)	25,31,34	0.80	0
4	A2M	4	569	4,71	22,25,26	0.20	0	30,36,39	0.48	0
3	OMG	1	2104	3	23,26,27	1.21	4 (17%)	32,38,41	2.00	6 (18%)
3	OMU	1	2666	3	19,22,23	1.28	3 (15%)	25,31,34	1.89	5 (20%)
3	OMC	1	2720	3	19,22,23	0.78	0	25,31,34	0.89	0
4	OMG	4	908	4	23,26,27	1.21	4 (17%)	32,38,41	2.02	6 (18%)
3	OMG	1	1971	3	23,26,27	1.22	3 (13%)	32,38,41	2.01	7 (21%)
4	OMG	4	1212	4	23,26,27	1.20	4 (17%)	32,38,41	2.03	7 (21%)
3	OMG	1	2071	3	23,26,27	1.20	4 (17%)	32,38,41	1.89	6 (18%)
4	OMU	4	877	4	19,22,23	1.29	4 (21%)	25,31,34	1.90	5 (20%)
4	OMG	4	467	4	23,26,27	1.25	4 (17%)	32,38,41	1.93	5 (15%)
4	OMG	4	1202	4,71	23,26,27	1.23	3 (13%)	32,38,41	2.08	7 (21%)
3	OMC	1	2115	3	19,22,23	0.81	0	25,31,34	0.76	0
3	OMU	1	2623	3	19,22,23	1.27	4 (21%)	25,31,34	1.87	4 (16%)
4	OMC	4	1184	4	19,22,23	0.78	0	25,31,34	0.73	0
4	OMG	4	1163	4	23,26,27	1.26	3 (13%)	32,38,41	2.10	6 (18%)
3	OMG	1	2017	3	23,26,27	1.24	3 (13%)	32,38,41	2.00	6 (18%)
3	OMC	1	673	3	19,22,23	0.79	0	25,31,34	0.79	0
3	OMG	1	1947	3	23,26,27	1.20	4 (17%)	32,38,41	2.04	7 (21%)
3	OMU	1	2851	3	19,22,23	1.28	4 (21%)	25,31,34	1.82	5 (20%)
3	OMU	1	2628	3	19,22,23	1.25	3 (15%)	25,31,34	1.84	6 (24%)
4	OMG	4	475	4	23,26,27	1.21	3 (13%)	32,38,41	2.00	7 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	OMU	1	2077	3	19,22,23	1.34	4 (21%)	25,31,34	1.83	5 (20%)
4	4AC	4	5	4	21,24,25	0.41	0	28,34,37	0.70	0
3	PSU	1	1911	3	18,21,22	0.94	1 (5%)	21,30,33	0.76	0
3	PSU	1	1987	3	18,21,22	0.91	1 (5%)	21,30,33	0.70	0
4	OMC	4	1045	4	19,22,23	0.82	0	25,31,34	0.85	1 (4%)
3	OMG	1	2388	3	23,26,27	1.21	4 (17%)	32,38,41	2.03	7 (21%)
4	OMG	4	906	4	23,26,27	1.23	3 (13%)	32,38,41	2.03	7 (21%)
4	A2M	4	1060	4	22,25,26	0.23	0	30,36,39	0.72	2 (6%)
3	A2M	1	2691	71,3	22,25,26	0.20	0	30,36,39	0.36	0
3	OMC	1	492	3	19,22,23	0.76	0	25,31,34	0.82	1 (4%)
4	OMC	4	489	4	19,22,23	0.85	1 (5%)	25,31,34	1.03	2 (8%)
4	6MZ	4	1459	4,71	22,25,26	1.45	5 (22%)	29,36,39	2.18	8 (27%)
3	OMC	1	2555	3	19,22,23	0.83	0	25,31,34	1.01	1 (4%)
4	B8T	4	1035	4	19,22,23	0.44	0	25,31,34	0.53	0
4	A2M	4	40	4	22,25,26	0.18	0	30,36,39	0.39	0
3	OMG	1	2362	3	23,26,27	1.22	3 (13%)	32,38,41	2.05	6 (18%)
3	OMC	1	2018	3	19,22,23	0.80	0	25,31,34	0.72	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MA6	4	1478	4	-	2/11/29/30	0/3/3/3
3	5MC	1	2056	71,3	-	1/7/25/26	0/2/2/2
3	OMU	1	2574	3	-	0/9/27/28	0/2/2/2
3	OMC	1	2704	3	-	0/9/27/28	0/2/2/2
4	OMG	4	1289	4,71	-	0/9/27/28	0/3/3/3
4	OMC	4	572	4	-	0/9/27/28	0/2/2/2
3	OMG	1	2176	71,3	-	0/9/27/28	0/3/3/3
3	UR3	1	2698	3	-	0/7/25/26	0/2/2/2
3	PSU	1	2607	3	-	0/7/25/26	0/2/2/2
3	OMC	1	2885	3	-	0/9/27/28	0/2/2/2
4	OMG	4	19	4	-	2/9/27/28	0/3/3/3
4	OMG	4	1211	4	-	3/9/27/28	0/3/3/3
3	OMU	1	2707	3	-	0/9/27/28	0/2/2/2
3	OMG	1	902	71,3	-	0/9/27/28	0/3/3/3
3	OMG	1	2066	3	-	0/9/27/28	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
53	IAS	BM	128	53	-	1/7/7/8	-
4	MA6	4	1477	4	-	0/11/29/30	0/3/3/3
4	M7A	4	508	4	-	4/7/37/38	0/3/3/3
4	OMC	4	514	4	-	0/9/27/28	0/2/2/2
3	OMG	1	2366	3	-	1/9/27/28	0/3/3/3
3	PSU	1	2571	3	-	0/7/25/26	0/2/2/2
3	OMG	1	2667	3	-	0/9/27/28	0/3/3/3
3	OMU	1	2408	3	-	0/9/27/28	0/2/2/2
3	A2M	1	2059	71,3	-	1/9/27/28	0/3/3/3
4	A2M	4	880	4	-	0/9/27/28	0/3/3/3
3	5MC	1	38	3	-	1/7/25/26	0/2/2/2
3	OMC	1	1816	3	-	0/9/27/28	0/2/2/2
3	OMG	1	2103	3	-	0/9/27/28	0/3/3/3
3	OMU	1	908	71,3	-	4/9/27/28	0/2/2/2
3	A2M	1	2011	3	-	1/9/27/28	0/3/3/3
4	OMC	4	1034	4	-	0/9/27/28	0/2/2/2
3	OMG	1	1949	3	-	0/9/27/28	0/3/3/3
3	OMC	1	872	3	-	0/9/27/28	0/2/2/2
3	G7M	1	3023	3	-	2/7/25/26	0/3/3/3
3	PSU	1	2610	3	-	0/7/25/26	0/2/2/2
3	A2M	1	1990	3	-	0/9/27/28	0/3/3/3
4	OMG	4	7	4	-	0/9/27/28	0/3/3/3
3	B8T	1	79	3	-	0/7/27/28	0/2/2/2
3	OMC	1	2624	3	-	0/9/27/28	0/2/2/2
3	OMG	1	2608	3	-	2/9/27/28	0/3/3/3
4	OMG	4	465	4	-	2/9/27/28	0/3/3/3
4	OMG	4	462	4	-	0/9/27/28	0/3/3/3
4	PSU	4	263	4	-	0/7/25/26	0/2/2/2
4	OMG	4	1210	4	-	1/9/27/28	0/3/3/3
3	OMC	1	2538	3	-	0/9/27/28	0/2/2/2
4	OMG	4	511	4	-	3/9/27/28	0/3/3/3
4	OMC	4	1368	4	-	2/9/27/28	0/2/2/2
3	OMC	1	2116	3	-	2/9/27/28	0/2/2/2
3	B8T	1	2937	3	-	2/7/27/28	0/2/2/2
3	OMG	1	2537	3	-	2/9/27/28	0/3/3/3
4	OMU	4	15	4	-	0/9/27/28	0/2/2/2
4	OMG	4	674	4	-	0/9/27/28	0/3/3/3
3	OMG	1	2601	71,3	-	0/9/27/28	0/3/3/3
3	4AC	1	2016	3	-	0/11/29/30	0/2/2/2
3	OMG	1	1957	3	-	0/9/27/28	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	4AC	4	1318	4	-	0/11/29/30	0/2/2/2
4	A2M	4	496	4	-	3/9/27/28	0/3/3/3
4	A2M	4	879	4	-	4/9/27/28	0/3/3/3
3	PSU	1	2625	3	-	0/7/25/26	0/2/2/2
3	OMU	1	2088	3	-	1/9/27/28	0/2/2/2
3	PSU	1	2044	3	-	2/7/25/26	0/2/2/2
3	OMC	1	2143	3	-	0/9/27/28	0/2/2/2
3	OMU	1	2155	3	-	2/9/27/28	0/2/2/2
3	OMU	1	875	3	-	0/9/27/28	0/2/2/2
4	B8T	4	1469	4	-	0/7/27/28	0/2/2/2
3	OMC	1	2884	3	-	0/9/27/28	0/2/2/2
3	OMC	1	493	3	-	1/9/27/28	0/2/2/2
3	OMC	1	1976	3	-	0/9/27/28	0/2/2/2
4	A2M	4	569	4,71	-	0/9/27/28	0/3/3/3
3	OMG	1	2104	3	-	1/9/27/28	0/3/3/3
3	OMU	1	2666	3	-	0/9/27/28	0/2/2/2
3	OMC	1	2720	3	-	0/9/27/28	0/2/2/2
4	OMG	4	908	4	-	3/9/27/28	0/3/3/3
3	OMG	1	1971	3	-	0/9/27/28	0/3/3/3
4	OMG	4	1212	4	-	0/9/27/28	0/3/3/3
3	OMG	1	2071	3	-	0/9/27/28	0/3/3/3
4	OMU	4	877	4	-	0/9/27/28	0/2/2/2
4	OMG	4	467	4	-	1/9/27/28	0/3/3/3
4	OMG	4	1202	4,71	-	2/9/27/28	0/3/3/3
3	OMC	1	2115	3	-	0/9/27/28	0/2/2/2
3	OMU	1	2623	3	-	0/9/27/28	0/2/2/2
4	OMC	4	1184	4	-	0/9/27/28	0/2/2/2
4	OMG	4	1163	4	-	4/9/27/28	0/3/3/3
3	OMG	1	2017	3	-	1/9/27/28	0/3/3/3
3	OMC	1	673	3	-	0/9/27/28	0/2/2/2
3	OMG	1	1947	3	-	2/9/27/28	0/3/3/3
3	OMU	1	2851	3	-	0/9/27/28	0/2/2/2
3	OMU	1	2628	3	-	2/9/27/28	0/2/2/2
4	OMG	4	475	4	-	0/9/27/28	0/3/3/3
3	OMU	1	2077	3	-	1/9/27/28	0/2/2/2
4	4AC	4	5	4	-	0/11/29/30	0/2/2/2
3	PSU	1	1911	3	-	0/7/25/26	0/2/2/2
3	PSU	1	1987	3	-	0/7/25/26	0/2/2/2
4	OMC	4	1045	4	-	3/9/27/28	0/2/2/2
3	OMG	1	2388	3	-	1/9/27/28	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	OMG	4	906	4	-	0/9/27/28	0/3/3/3
4	A2M	4	1060	4	-	4/9/27/28	0/3/3/3
3	A2M	1	2691	71,3	-	1/9/27/28	0/3/3/3
3	OMC	1	492	3	-	1/9/27/28	0/2/2/2
4	OMC	4	489	4	-	0/9/27/28	0/2/2/2
4	6MZ	4	1459	4,71	-	0/9/27/28	0/3/3/3
3	OMC	1	2555	3	-	1/9/27/28	0/2/2/2
4	B8T	4	1035	4	-	2/7/27/28	0/2/2/2
4	A2M	4	40	4	-	0/9/27/28	0/3/3/3
3	OMG	1	2362	3	-	3/9/27/28	0/3/3/3
3	OMC	1	2018	3	-	0/9/27/28	0/2/2/2

All (197) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	1	3023	G7M	C8-N7	7.56	1.45	1.33
3	1	2056	5MC	C5-C4	5.41	1.48	1.44
3	1	38	5MC	C5-C4	5.06	1.47	1.44
3	1	3023	G7M	C8-N9	4.03	1.46	1.35
4	4	1459	6MZ	C5-C4	4.03	1.46	1.39
3	1	2625	PSU	C6-C5	3.63	1.39	1.35
3	1	2607	PSU	C6-C5	3.63	1.39	1.35
3	1	1911	PSU	C6-C5	3.61	1.39	1.35
3	1	2610	PSU	C6-C5	3.59	1.39	1.35
3	1	2044	PSU	C6-C5	3.57	1.39	1.35
4	4	263	PSU	C6-C5	3.56	1.39	1.35
3	1	2571	PSU	C6-C5	3.56	1.39	1.35
3	1	1987	PSU	C6-C5	3.47	1.39	1.35
4	4	15	OMU	C4-N3	-3.37	1.32	1.38
4	4	1163	OMG	C5-C4	3.16	1.47	1.38
3	1	2707	OMU	C4-N3	-3.14	1.33	1.38
3	1	875	OMU	C4-N3	-3.12	1.33	1.38
4	4	1459	6MZ	C5-N7	-3.09	1.33	1.39
3	1	2574	OMU	C4-N3	-3.08	1.33	1.38
4	4	877	OMU	C4-N3	-3.07	1.33	1.38
3	1	2077	OMU	C4-N3	-3.06	1.33	1.38
3	1	908	OMU	C4-N3	-3.03	1.33	1.38
3	1	2666	OMU	C4-N3	-3.03	1.33	1.38
3	1	2667	OMG	C5-C4	3.00	1.47	1.38
4	4	1202	OMG	C6-N1	-2.99	1.33	1.38
3	1	2088	OMU	C4-N3	-2.98	1.33	1.38
3	1	2623	OMU	C4-N3	-2.97	1.33	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	1	1949	OMG	C6-N1	-2.97	1.33	1.38
3	1	1971	OMG	C6-N1	-2.96	1.33	1.38
4	4	674	OMG	C5-C4	2.96	1.46	1.38
4	4	467	OMG	C6-N1	-2.96	1.33	1.38
3	1	2103	OMG	C6-N1	-2.95	1.33	1.38
3	1	2155	OMU	C4-N3	-2.95	1.33	1.38
3	1	2017	OMG	C5-C4	2.94	1.46	1.38
3	1	2066	OMG	C6-N1	-2.94	1.33	1.38
3	1	2176	OMG	C6-N1	-2.94	1.33	1.38
4	4	475	OMG	C5-C4	2.94	1.46	1.38
3	1	2851	OMU	C4-N3	-2.92	1.33	1.38
4	4	906	OMG	C6-N1	-2.92	1.33	1.38
4	4	1210	OMG	C6-N1	-2.90	1.33	1.38
4	4	1211	OMG	C6-N1	-2.90	1.33	1.38
3	1	2608	OMG	C5-C4	2.89	1.46	1.38
4	4	7	OMG	C6-N1	-2.87	1.33	1.38
4	4	1289	OMG	C6-N1	-2.87	1.33	1.38
4	4	465	OMG	C5-C4	2.87	1.46	1.38
3	1	2366	OMG	C5-C4	2.87	1.46	1.38
4	4	462	OMG	C5-C4	2.87	1.46	1.38
4	4	511	OMG	C5-C4	2.86	1.46	1.38
3	1	38	5MC	C6-N1	-2.86	1.33	1.38
3	1	2537	OMG	C5-C4	2.86	1.46	1.38
3	1	2408	OMU	C4-N3	-2.85	1.33	1.38
4	4	908	OMG	C6-N1	-2.84	1.33	1.38
4	4	465	OMG	C6-N1	-2.83	1.33	1.38
3	1	2362	OMG	C5-C4	2.82	1.46	1.38
3	1	2017	OMG	C6-N1	-2.82	1.33	1.38
4	4	1163	OMG	C6-N1	-2.82	1.33	1.38
3	1	2601	OMG	C6-N1	-2.81	1.33	1.38
3	1	2667	OMG	C6-N1	-2.81	1.33	1.38
3	1	2103	OMG	C5-C4	2.81	1.46	1.38
3	1	1949	OMG	C5-C4	2.81	1.46	1.38
4	4	15	OMU	C2-N3	-2.80	1.33	1.38
4	4	1212	OMG	C6-N1	-2.80	1.33	1.38
3	1	2104	OMG	C6-N1	-2.80	1.33	1.38
4	4	19	OMG	C6-N1	-2.80	1.33	1.38
3	1	2628	OMU	C4-N3	-2.80	1.33	1.38
4	4	877	OMU	C2-N3	-2.79	1.33	1.38
4	4	7	OMG	C5-C4	2.79	1.46	1.38
3	1	1957	OMG	C5-C4	2.79	1.46	1.38
3	1	2176	OMG	C5-C4	2.79	1.46	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	4	1289	OMG	C5-C4	2.79	1.46	1.38
3	1	2601	OMG	C5-C4	2.79	1.46	1.38
3	1	1957	OMG	C6-N1	-2.78	1.33	1.38
3	1	1971	OMG	C5-C4	2.78	1.46	1.38
3	1	2707	OMU	C2-N3	-2.78	1.33	1.38
3	1	2366	OMG	C6-N1	-2.77	1.33	1.38
4	4	19	OMG	C5-C4	2.76	1.46	1.38
4	4	467	OMG	C5-C4	2.75	1.46	1.38
4	4	475	OMG	C6-N1	-2.75	1.33	1.38
4	4	674	OMG	C6-N1	-2.75	1.33	1.38
4	4	462	OMG	C6-N1	-2.74	1.33	1.38
3	1	2056	5MC	C6-N1	-2.74	1.33	1.38
3	1	1947	OMG	C5-C4	2.74	1.46	1.38
3	1	2071	OMG	C6-N1	-2.74	1.33	1.38
3	1	1947	OMG	C6-N1	-2.74	1.33	1.38
3	1	902	OMG	C6-N1	-2.74	1.33	1.38
4	4	1211	OMG	C5-C4	2.73	1.46	1.38
3	1	2155	OMU	C2-N3	-2.73	1.33	1.38
3	1	2077	OMU	C2-N3	-2.73	1.33	1.38
3	1	2388	OMG	C6-N1	-2.73	1.33	1.38
3	1	2362	OMG	C6-N1	-2.72	1.33	1.38
3	1	2071	OMG	C5-C4	2.72	1.46	1.38
3	1	2088	OMU	C2-N3	-2.71	1.33	1.38
4	4	908	OMG	C5-C4	2.70	1.46	1.38
4	4	1202	OMG	C5-C4	2.70	1.46	1.38
3	1	2066	OMG	C5-C4	2.70	1.46	1.38
3	1	902	OMG	C5-C4	2.67	1.46	1.38
4	4	906	OMG	C5-C4	2.67	1.46	1.38
4	4	1210	OMG	C5-C4	2.67	1.46	1.38
3	1	2388	OMG	C5-C4	2.67	1.46	1.38
3	1	2537	OMG	C6-N1	-2.63	1.33	1.38
4	4	511	OMG	C6-N1	-2.61	1.34	1.38
3	1	2666	OMU	C2-N3	-2.60	1.33	1.38
3	1	2104	OMG	C5-C4	2.60	1.45	1.38
3	1	2574	OMU	C2-N3	-2.60	1.33	1.38
3	1	875	OMU	C2-N3	-2.58	1.33	1.38
3	1	2608	OMG	C6-N1	-2.57	1.34	1.38
4	4	1212	OMG	C5-C4	2.55	1.45	1.38
3	1	2623	OMU	C2-N3	-2.53	1.33	1.38
3	1	2851	OMU	C2-N3	-2.52	1.33	1.38
3	1	2066	OMG	C5-N7	-2.52	1.34	1.39
4	4	7	OMG	C5-N7	-2.51	1.34	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	1	908	OMU	C2-N3	-2.50	1.33	1.38
3	1	2017	OMG	C5-N7	-2.50	1.34	1.39
3	1	908	OMU	C5-C4	-2.45	1.38	1.43
4	4	1459	6MZ	C8-N9	-2.45	1.33	1.37
4	4	1210	OMG	C5-N7	-2.44	1.34	1.39
3	1	1971	OMG	C5-N7	-2.44	1.34	1.39
3	1	2574	OMU	C5-C4	-2.44	1.38	1.43
4	4	908	OMG	C5-N7	-2.43	1.34	1.39
3	1	1949	OMG	C5-N7	-2.43	1.34	1.39
3	1	2408	OMU	C2-N3	-2.42	1.33	1.38
3	1	2628	OMU	C2-N3	-2.42	1.33	1.38
4	4	1163	OMG	C5-N7	-2.41	1.34	1.39
3	1	2088	OMU	C5-C4	-2.41	1.38	1.43
4	4	467	OMG	C5-N7	-2.41	1.34	1.39
4	4	511	OMG	C5-N7	-2.40	1.34	1.39
3	1	2628	OMU	C5-C4	-2.40	1.38	1.43
3	1	902	OMG	C5-N7	-2.40	1.34	1.39
3	1	875	OMU	C5-C4	-2.39	1.38	1.43
3	1	2362	OMG	C5-N7	-2.39	1.34	1.39
4	4	1202	OMG	C5-N7	-2.38	1.34	1.39
4	4	15	OMU	C5-C4	-2.38	1.38	1.43
3	1	2707	OMU	C5-C4	-2.36	1.38	1.43
3	1	2103	OMG	C5-N7	-2.36	1.34	1.39
4	4	1211	OMG	C5-N7	-2.34	1.34	1.39
3	1	902	OMG	C4-N9	-2.34	1.32	1.38
3	1	2077	OMU	C5-C4	-2.34	1.38	1.43
3	1	2388	OMG	C4-N9	-2.33	1.32	1.38
4	4	906	OMG	C5-N7	-2.33	1.34	1.39
4	4	465	OMG	C5-N7	-2.32	1.34	1.39
3	1	2104	OMG	C5-N7	-2.32	1.34	1.39
3	1	2366	OMG	C5-N7	-2.32	1.34	1.39
3	1	2388	OMG	C5-N7	-2.30	1.34	1.39
3	1	2071	OMG	C4-N9	-2.29	1.32	1.38
3	1	2408	OMU	C5-C4	-2.29	1.38	1.43
3	1	2176	OMG	C5-N7	-2.29	1.34	1.39
4	4	674	OMG	C5-N7	-2.28	1.34	1.39
3	1	2667	OMG	C5-N7	-2.28	1.34	1.39
3	1	2537	OMG	C5-N7	-2.28	1.34	1.39
3	1	2623	OMU	C5-C4	-2.27	1.38	1.43
4	4	462	OMG	C5-N7	-2.27	1.34	1.39
3	1	2851	OMU	C5-C4	-2.27	1.38	1.43
4	4	475	OMG	C5-N7	-2.25	1.34	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	1	1947	OMG	C5-N7	-2.25	1.34	1.39
3	1	2601	OMG	C5-N7	-2.23	1.34	1.39
4	4	1212	OMG	C4-N9	-2.23	1.32	1.38
3	1	2608	OMG	C5-N7	-2.23	1.34	1.39
3	1	2056	5MC	C6-C5	2.22	1.38	1.34
4	4	19	OMG	C5-N7	-2.22	1.34	1.39
4	4	1289	OMG	C5-N7	-2.22	1.34	1.39
3	1	2071	OMG	C5-N7	-2.21	1.34	1.39
3	1	2666	OMU	C5-C4	-2.21	1.38	1.43
3	1	2155	OMU	C5-C4	-2.19	1.38	1.43
3	1	2104	OMG	C4-N9	-2.19	1.32	1.38
3	1	1957	OMG	C5-N7	-2.19	1.34	1.39
4	4	467	OMG	C4-N9	-2.18	1.32	1.38
4	4	877	OMU	C5-C4	-2.17	1.39	1.43
4	4	489	OMC	C6-N1	-2.14	1.33	1.38
4	4	1368	OMC	C6-N1	-2.14	1.33	1.38
3	1	1947	OMG	C4-N9	-2.13	1.32	1.38
4	4	1459	6MZ	C5-C6	2.13	1.47	1.41
4	4	1212	OMG	C5-N7	-2.13	1.34	1.39
3	1	38	5MC	C6-C5	2.11	1.38	1.34
53	BM	128	IAS	CB-CG	2.11	1.55	1.50
3	1	2624	OMC	C6-N1	-2.10	1.33	1.38
3	1	1976	OMC	C6-N1	-2.09	1.33	1.38
3	1	1976	OMC	C5-C4	-2.09	1.38	1.42
4	4	1034	OMC	C6-N1	-2.09	1.33	1.38
4	4	15	OMU	C6-N1	-2.09	1.33	1.38
4	4	465	OMG	C4-N9	-2.09	1.32	1.38
3	1	2077	OMU	C6-N1	-2.08	1.33	1.38
4	4	1459	6MZ	C4-N9	-2.08	1.33	1.37
3	1	2608	OMG	C4-N9	-2.08	1.32	1.38
3	1	1957	OMG	C4-N9	-2.07	1.32	1.38
3	1	908	OMU	C2-N1	2.07	1.41	1.38
4	4	877	OMU	C6-N1	-2.07	1.33	1.38
4	4	511	OMG	C4-N9	-2.06	1.32	1.38
3	1	2066	OMG	C4-N9	-2.06	1.32	1.38
3	1	2176	OMG	C4-N9	-2.04	1.32	1.38
4	4	19	OMG	C4-N9	-2.03	1.32	1.38
3	1	2103	OMG	C4-N9	-2.03	1.32	1.38
3	1	875	OMU	C6-N1	-2.03	1.33	1.38
3	1	2698	UR3	C5-C4	-2.03	1.38	1.43
3	1	2623	OMU	C6-N1	-2.02	1.33	1.38
4	4	908	OMG	C4-N9	-2.02	1.32	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	1	2851	OMU	C6-N1	-2.01	1.33	1.38
3	1	2574	OMU	C6-N1	-2.01	1.33	1.38

All (314) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	4	1163	OMG	C5-C4-N3	-6.70	117.72	128.39
3	1	2698	UR3	C4-N3-C2	-6.47	119.38	124.58
3	1	2017	OMG	C5-C4-N3	-6.45	118.13	128.39
3	1	2667	OMG	C5-C4-N3	-6.44	118.14	128.39
4	4	1459	6MZ	C5-C4-N3	-6.37	117.94	126.72
4	4	674	OMG	C5-C4-N3	-6.37	118.25	128.39
4	4	1202	OMG	C5-C4-N3	-6.33	118.32	128.39
3	1	2362	OMG	C5-C4-N3	-6.27	118.41	128.39
3	1	1971	OMG	C5-C4-N3	-6.23	118.48	128.39
4	4	906	OMG	C5-C4-N3	-6.20	118.52	128.39
4	4	1289	OMG	C5-C4-N3	-6.19	118.54	128.39
4	4	908	OMG	C5-C4-N3	-6.19	118.55	128.39
3	1	2601	OMG	C5-C4-N3	-6.15	118.60	128.39
4	4	475	OMG	C5-C4-N3	-6.13	118.63	128.39
4	4	7	OMG	C5-C4-N3	-6.12	118.66	128.39
3	1	2537	OMG	C5-C4-N3	-6.08	118.72	128.39
3	1	2066	OMG	C5-C4-N3	-6.07	118.73	128.39
3	1	1949	OMG	C5-C4-N3	-6.05	118.77	128.39
4	4	1211	OMG	C5-C4-N3	-6.04	118.78	128.39
3	1	2366	OMG	C5-C4-N3	-6.01	118.83	128.39
4	4	1210	OMG	C5-C4-N3	-6.00	118.84	128.39
3	1	2103	OMG	C5-C4-N3	-5.95	118.92	128.39
4	4	462	OMG	C5-C4-N3	-5.94	118.94	128.39
4	4	511	OMG	C5-C4-N3	-5.93	118.95	128.39
4	4	19	OMG	C5-C4-N3	-5.92	118.97	128.39
3	1	1957	OMG	C5-C4-N3	-5.89	119.02	128.39
4	4	465	OMG	C5-C4-N3	-5.88	119.03	128.39
3	1	2176	OMG	C5-C4-N3	-5.88	119.03	128.39
4	4	467	OMG	C5-C4-N3	-5.80	119.16	128.39
3	1	2608	OMG	C5-C4-N3	-5.76	119.22	128.39
3	1	2104	OMG	C5-C4-N3	-5.73	119.26	128.39
3	1	1947	OMG	C5-C4-N3	-5.71	119.30	128.39
3	1	2388	OMG	C5-C4-N3	-5.70	119.31	128.39
4	4	1212	OMG	C5-C4-N3	-5.60	119.47	128.39
4	4	1459	6MZ	N3-C4-N9	5.59	136.67	127.17
3	1	902	OMG	C5-C4-N3	-5.58	119.51	128.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	1	2071	OMG	C5-C4-N3	-5.40	119.79	128.39
4	4	1163	OMG	N9-C4-N3	5.33	136.62	125.95
4	4	877	OMU	C4-N3-C2	-5.28	120.05	126.61
4	4	1202	OMG	C2-N3-C4	5.27	121.37	112.30
4	4	674	OMG	C2-N3-C4	5.22	121.28	112.30
4	4	15	OMU	C4-N3-C2	-5.21	120.15	126.61
4	4	908	OMG	C2-N3-C4	5.19	121.23	112.30
3	1	2601	OMG	C2-N3-C4	5.18	121.22	112.30
3	1	2667	OMG	C2-N3-C4	5.16	121.19	112.30
3	1	2155	OMU	C4-N3-C2	-5.14	120.23	126.61
3	1	875	OMU	C4-N3-C2	-5.14	120.23	126.61
4	4	906	OMG	C2-N3-C4	5.13	121.14	112.30
4	4	1163	OMG	C2-N3-C4	5.13	121.13	112.30
4	4	511	OMG	C2-N3-C4	5.13	121.13	112.30
3	1	2362	OMG	C2-N3-C4	5.13	121.13	112.30
4	4	475	OMG	C2-N3-C4	5.12	121.12	112.30
3	1	2537	OMG	C2-N3-C4	5.11	121.11	112.30
3	1	2666	OMU	C4-N3-C2	-5.11	120.27	126.61
3	1	2623	OMU	C4-N3-C2	-5.10	120.28	126.61
4	4	19	OMG	C2-N3-C4	5.07	121.04	112.30
4	4	1289	OMG	C2-N3-C4	5.07	121.04	112.30
3	1	1957	OMG	C2-N3-C4	5.05	120.99	112.30
3	1	2707	OMU	C4-N3-C2	-5.04	120.35	126.61
3	1	2176	OMG	C2-N3-C4	5.04	120.98	112.30
4	4	1210	OMG	C2-N3-C4	5.03	120.97	112.30
3	1	1947	OMG	C2-N3-C4	5.03	120.97	112.30
3	1	2017	OMG	N9-C4-N3	5.03	136.00	125.95
3	1	2388	OMG	C2-N3-C4	5.02	120.95	112.30
3	1	1949	OMG	C2-N3-C4	5.02	120.94	112.30
4	4	1211	OMG	C2-N3-C4	5.01	120.93	112.30
3	1	1971	OMG	C2-N3-C4	5.01	120.92	112.30
3	1	2608	OMG	C2-N3-C4	5.00	120.91	112.30
3	1	2104	OMG	C2-N3-C4	4.99	120.90	112.30
3	1	2408	OMU	C4-N3-C2	-4.99	120.41	126.61
3	1	2017	OMG	C2-N3-C4	4.99	120.90	112.30
4	4	7	OMG	C2-N3-C4	4.96	120.85	112.30
3	1	2851	OMU	C4-N3-C2	-4.96	120.45	126.61
3	1	2366	OMG	C2-N3-C4	4.94	120.81	112.30
3	1	2103	OMG	C2-N3-C4	4.94	120.81	112.30
3	1	2066	OMG	C2-N3-C4	4.94	120.81	112.30
3	1	902	OMG	C2-N3-C4	4.94	120.80	112.30
4	4	1212	OMG	C2-N3-C4	4.91	120.75	112.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	1	2667	OMG	N9-C4-N3	4.89	135.72	125.95
4	4	462	OMG	C2-N3-C4	4.88	120.70	112.30
4	4	465	OMG	C2-N3-C4	4.83	120.61	112.30
3	1	1971	OMG	N9-C4-N3	4.79	135.52	125.95
3	1	908	OMU	C1'-N1-C2	4.75	126.13	117.59
3	1	2071	OMG	C2-N3-C4	4.73	120.45	112.30
3	1	2362	OMG	N9-C4-N3	4.72	135.38	125.95
3	1	2574	OMU	C4-N3-C2	-4.69	120.79	126.61
4	4	467	OMG	C2-N3-C4	4.68	120.36	112.30
3	1	2628	OMU	C4-N3-C2	-4.67	120.82	126.61
4	4	1211	OMG	N9-C4-N3	4.64	135.24	125.95
4	4	7	OMG	N9-C4-N3	4.64	135.23	125.95
3	1	2088	OMU	C4-N3-C2	-4.64	120.85	126.61
3	1	2601	OMG	N9-C4-N3	4.63	135.20	125.95
4	4	1210	OMG	N9-C4-N3	4.62	135.18	125.95
3	1	2077	OMU	C4-N3-C2	-4.61	120.89	126.61
3	1	875	OMU	C5-C4-N3	4.58	121.22	114.80
4	4	674	OMG	N9-C4-N3	4.56	135.06	125.95
4	4	1289	OMG	N9-C4-N3	4.56	135.06	125.95
4	4	908	OMG	N9-C4-N3	4.55	135.05	125.95
3	1	1949	OMG	N9-C4-N3	4.54	135.03	125.95
4	4	475	OMG	N9-C4-N3	4.53	135.02	125.95
4	4	906	OMG	N9-C4-N3	4.51	134.97	125.95
3	1	2066	OMG	N9-C4-N3	4.49	134.94	125.95
4	4	462	OMG	N9-C4-N3	4.48	134.92	125.95
3	1	2155	OMU	C5-C4-N3	4.45	121.03	114.80
3	1	2366	OMG	N9-C4-N3	4.45	134.85	125.95
4	4	1202	OMG	N9-C4-N3	4.43	134.81	125.95
4	4	465	OMG	N9-C4-N3	4.42	134.80	125.95
3	1	2176	OMG	N9-C4-N3	4.42	134.79	125.95
3	1	2537	OMG	N9-C4-N3	4.41	134.78	125.95
4	4	15	OMU	C5-C4-N3	4.41	120.97	114.80
4	4	877	OMU	C5-C4-N3	4.40	120.97	114.80
4	4	15	OMU	N3-C2-N1	4.39	120.61	114.89
3	1	2707	OMU	C5-C4-N3	4.34	120.88	114.80
4	4	467	OMG	N9-C4-N3	4.32	134.60	125.95
3	1	2666	OMU	C5-C4-N3	4.31	120.84	114.80
3	1	2103	OMG	N9-C4-N3	4.31	134.57	125.95
4	4	511	OMG	N9-C4-N3	4.30	134.54	125.95
4	4	19	OMG	N9-C4-N3	4.27	134.50	125.95
3	1	1957	OMG	N9-C4-N3	4.26	134.47	125.95
3	1	2408	OMU	C5-C4-N3	4.23	120.73	114.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	1	3023	G7M	N9-C8-N7	-4.23	102.21	112.48
3	1	2608	OMG	N9-C4-N3	4.23	134.41	125.95
3	1	2851	OMU	C5-C4-N3	4.23	120.72	114.80
3	1	2666	OMU	N3-C2-N1	4.21	120.37	114.89
3	1	2088	OMU	C5-C4-N3	4.20	120.68	114.80
3	1	908	OMU	C4-N3-C2	-4.20	121.40	126.61
3	1	1947	OMG	N9-C4-N3	4.17	134.29	125.95
3	1	2104	OMG	N9-C4-N3	4.14	134.23	125.95
3	1	2574	OMU	C5-C4-N3	4.12	120.58	114.80
4	4	877	OMU	N3-C2-N1	4.12	120.26	114.89
3	1	2623	OMU	N3-C2-N1	4.11	120.25	114.89
4	4	1212	OMG	N9-C4-N3	4.11	134.18	125.95
3	1	2077	OMU	C5-C4-N3	4.11	120.56	114.80
3	1	2155	OMU	N3-C2-N1	4.10	120.23	114.89
3	1	902	OMG	N9-C4-N3	4.09	134.14	125.95
3	1	2707	OMU	N3-C2-N1	4.09	120.21	114.89
3	1	2628	OMU	N3-C2-N1	4.05	120.16	114.89
3	1	2088	OMU	N3-C2-N1	4.02	120.13	114.89
3	1	875	OMU	N3-C2-N1	4.00	120.10	114.89
3	1	2574	OMU	N3-C2-N1	3.99	120.08	114.89
3	1	908	OMU	C5-C4-N3	3.99	120.39	114.80
3	1	2623	OMU	C5-C4-N3	3.98	120.38	114.80
3	1	2388	OMG	N9-C4-N3	3.95	133.84	125.95
3	1	2071	OMG	N9-C4-N3	3.92	133.79	125.95
3	1	2628	OMU	C5-C4-N3	3.92	120.29	114.80
3	1	2408	OMU	N3-C2-N1	3.89	119.96	114.89
3	1	2077	OMU	N3-C2-N1	3.85	119.90	114.89
3	1	2851	OMU	N3-C2-N1	3.72	119.74	114.89
3	1	2388	OMG	C6-C5-N7	3.71	137.05	130.29
3	1	38	5MC	C5-C6-N1	-3.70	119.29	123.31
4	4	1459	6MZ	C2-N3-C4	3.68	120.82	111.83
3	1	902	OMG	C6-C5-N7	3.65	136.94	130.29
3	1	1947	OMG	C6-C5-N7	3.63	136.89	130.29
4	4	1212	OMG	C6-C5-N7	3.61	136.85	130.29
3	1	2104	OMG	C6-C5-N7	3.60	136.84	130.29
3	1	908	OMU	N3-C2-N1	3.59	119.57	114.89
3	1	1957	OMG	C6-C5-N7	3.58	136.81	130.29
4	4	1202	OMG	C6-C5-N7	3.58	136.81	130.29
4	4	19	OMG	C6-C5-N7	3.57	136.78	130.29
3	1	2698	UR3	C5-C4-N3	3.56	119.73	115.04
3	1	2103	OMG	C6-C5-N7	3.54	136.73	130.29
3	1	2608	OMG	C6-C5-N7	3.48	136.62	130.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	1	2071	OMG	C6-C5-N7	3.47	136.61	130.29
3	1	2408	OMU	O4-C4-C5	-3.43	119.24	125.16
3	1	2176	OMG	C6-C5-N7	3.41	136.49	130.29
3	1	2537	OMG	C6-C5-N7	3.40	136.48	130.29
3	1	875	OMU	O4-C4-C5	-3.36	119.37	125.16
4	4	906	OMG	C6-C5-N7	3.35	136.38	130.29
4	4	1211	OMG	C6-C5-N7	3.34	136.38	130.29
3	1	2601	OMG	C6-C5-N7	3.34	136.37	130.29
4	4	1289	OMG	C6-C5-N7	3.33	136.35	130.29
4	4	674	OMG	C6-C5-N7	3.33	136.34	130.29
3	1	2628	OMU	O4-C4-C5	-3.32	119.43	125.16
4	4	467	OMG	C6-C5-N7	3.31	136.32	130.29
3	1	2066	OMG	C6-C5-N7	3.29	136.28	130.29
4	4	908	OMG	C6-C5-N7	3.29	136.27	130.29
3	1	908	OMU	O4-C4-C5	-3.29	119.50	125.16
4	4	475	OMG	C6-C5-N7	3.26	136.22	130.29
3	1	2362	OMG	C6-C5-N7	3.26	136.22	130.29
4	4	462	OMG	C6-C5-N7	3.25	136.21	130.29
4	4	511	OMG	C6-C5-N7	3.25	136.21	130.29
3	1	1949	OMG	C6-C5-N7	3.25	136.21	130.29
3	1	2366	OMG	C6-C5-N7	3.25	136.21	130.29
3	1	2623	OMU	O4-C4-C5	-3.22	119.60	125.16
4	4	465	OMG	C6-C5-N7	3.22	136.15	130.29
3	1	2666	OMU	O4-C4-C5	-3.21	119.63	125.16
4	4	1210	OMG	C6-C5-N7	3.19	136.09	130.29
3	1	2155	OMU	O4-C4-C5	-3.17	119.70	125.16
3	1	2088	OMU	O4-C4-C5	-3.16	119.72	125.16
3	1	1971	OMG	C6-C5-N7	3.14	136.00	130.29
3	1	2574	OMU	O4-C4-C5	-3.14	119.75	125.16
4	4	877	OMU	O4-C4-C5	-3.13	119.77	125.16
3	1	2056	5MC	C5-C6-N1	-3.12	119.92	123.31
3	1	2707	OMU	O4-C4-C5	-3.11	119.79	125.16
3	1	2851	OMU	O4-C4-C5	-3.10	119.81	125.16
3	1	2667	OMG	C6-C5-N7	3.09	135.91	130.29
4	4	7	OMG	C6-C5-N7	3.08	135.90	130.29
4	4	1477	MA6	C2-N1-C6	3.05	119.28	111.83
4	4	1478	MA6	C2-N1-C6	3.05	119.28	111.83
3	1	2077	OMU	O4-C4-C5	-3.04	119.93	125.16
4	4	1459	6MZ	N1-C2-N3	-2.94	124.13	128.58
4	4	15	OMU	O4-C4-C5	-2.87	120.21	125.16
3	1	2555	OMC	O2-C2-N3	-2.82	117.89	122.33
3	1	908	OMU	C1'-N1-C6	-2.81	114.77	120.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	4	1202	OMG	C4-C5-N7	-2.79	106.25	110.67
3	1	38	5MC	C5-C4-N3	-2.76	118.93	121.75
3	1	2017	OMG	C6-C5-N7	2.73	135.26	130.29
3	1	2056	5MC	C5-C4-N3	-2.72	118.97	121.75
3	1	2103	OMG	C4-C5-N7	-2.70	106.39	110.67
4	4	674	OMG	C4-C5-N7	-2.69	106.41	110.67
4	4	19	OMG	C4-C5-N7	-2.67	106.44	110.67
3	1	2537	OMG	C4-C5-N7	-2.65	106.47	110.67
3	1	2104	OMG	C4-C5-N7	-2.65	106.47	110.67
3	1	2388	OMG	C4-C5-N7	-2.65	106.47	110.67
4	4	1289	OMG	C4-C5-N7	-2.64	106.49	110.67
3	1	1957	OMG	C4-C5-N7	-2.62	106.51	110.67
3	1	2362	OMG	C4-C5-N7	-2.62	106.51	110.67
4	4	1459	6MZ	C4-N9-C8	2.62	108.49	105.74
4	4	1459	6MZ	C4-C5-N7	-2.62	107.59	110.58
4	4	906	OMG	C4-C5-N7	-2.59	106.57	110.67
4	4	467	OMG	C4-C5-N7	-2.58	106.58	110.67
3	1	2366	OMG	C4-C5-N7	-2.58	106.59	110.67
3	1	1947	OMG	C4-C5-N7	-2.57	106.61	110.67
4	4	908	OMG	C4-C5-N7	-2.56	106.62	110.67
3	1	2066	OMG	C4-C5-N7	-2.55	106.62	110.67
4	4	1212	OMG	C4-C5-N7	-2.55	106.63	110.67
3	1	2608	OMG	C4-C5-N7	-2.55	106.64	110.67
3	1	2077	OMU	C1'-N1-C2	2.53	122.14	117.59
3	1	902	OMG	C4-C5-N7	-2.53	106.66	110.67
4	4	1060	A2M	C3'-C2'-C1'	-2.52	97.98	102.81
3	1	2667	OMG	C4-C5-N7	-2.52	106.68	110.67
4	4	1459	6MZ	C1'-N9-C8	-2.51	121.53	127.09
4	4	1163	OMG	C6-C5-N7	2.50	134.83	130.29
3	1	2666	OMU	O2-C2-N1	-2.49	119.56	122.80
4	4	1211	OMG	C4-C5-N7	-2.48	106.73	110.67
4	4	462	OMG	C4-C5-N7	-2.48	106.74	110.67
4	4	1045	OMC	O2-C2-N3	-2.48	118.42	122.33
3	1	1949	OMG	C4-C5-N7	-2.45	106.78	110.67
4	4	15	OMU	O2-C2-N1	-2.45	119.61	122.80
3	1	2601	OMG	C4-C5-N7	-2.44	106.80	110.67
4	4	475	OMG	C4-C5-N7	-2.42	106.83	110.67
3	1	2071	OMG	C4-C5-N7	-2.42	106.84	110.67
4	4	465	OMG	C4-C5-N7	-2.41	106.86	110.67
4	4	511	OMG	C4-C5-N7	-2.40	106.86	110.67
3	1	1971	OMG	C4-C5-N7	-2.39	106.88	110.67
3	1	2176	OMG	C4-C5-N7	-2.38	106.89	110.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	1	2056	5MC	CM5-C5-C6	-2.36	119.66	122.85
4	4	7	OMG	C4-C5-N7	-2.36	106.93	110.67
4	4	1212	OMG	C2'-C1'-N9	-2.35	109.78	114.24
4	4	511	OMG	O6-C6-C5	-2.34	120.34	126.53
4	4	1210	OMG	C4-C5-N7	-2.33	106.98	110.67
3	1	2388	OMG	O6-C6-C5	-2.33	120.39	126.53
3	1	2698	UR3	C1'-N1-C2	2.31	120.83	117.04
3	1	1947	OMG	C2'-C1'-N9	-2.31	109.85	114.24
4	4	489	OMC	O2-C2-N3	-2.31	118.69	122.33
3	1	38	5MC	CM5-C5-C6	-2.30	119.74	122.85
3	1	2601	OMG	O6-C6-C5	-2.30	120.47	126.53
4	4	1163	OMG	O6-C6-C5	-2.28	120.50	126.53
3	1	2017	OMG	C4-C5-N7	-2.27	107.07	110.67
4	4	7	OMG	O6-C6-C5	-2.24	120.61	126.53
4	4	877	OMU	O2-C2-N1	-2.23	119.89	122.80
3	1	2066	OMG	O6-C6-C5	-2.22	120.66	126.53
3	1	902	OMG	O6-C6-C5	-2.22	120.67	126.53
3	1	38	5MC	O2-C2-N3	-2.22	118.84	122.33
3	1	2017	OMG	O6-C6-C5	-2.21	120.70	126.53
3	1	2408	OMU	O2-C2-N1	-2.21	119.93	122.80
3	1	1971	OMG	O6-C6-C5	-2.20	120.72	126.53
3	1	1947	OMG	O6-C6-C5	-2.20	120.73	126.53
4	4	1060	A2M	O2'-C2'-C1'	2.19	113.15	108.99
3	1	2628	OMU	O2-C2-N1	-2.19	119.95	122.80
4	4	465	OMG	O6-C6-C5	-2.18	120.77	126.53
3	1	38	5MC	C1'-N1-C6	-2.18	117.56	121.15
4	4	1210	OMG	O6-C6-C5	-2.18	120.79	126.53
3	1	2707	OMU	O2-C2-N1	-2.17	119.97	122.80
3	1	2362	OMG	O6-C6-C5	-2.17	120.81	126.53
3	1	2366	OMG	O6-C6-C5	-2.17	120.81	126.53
3	1	875	OMU	O2-C2-N1	-2.17	119.97	122.80
3	1	2071	OMG	O6-C6-C5	-2.16	120.84	126.53
3	1	2851	OMU	O2-C2-N1	-2.15	120.00	122.80
3	1	1957	OMG	O6-C6-C5	-2.14	120.88	126.53
4	4	906	OMG	O6-C6-C5	-2.14	120.88	126.53
3	1	492	OMC	O2-C2-N3	-2.13	118.97	122.33
3	1	2066	OMG	CM2-O2'-C2'	-2.13	109.01	114.47
4	4	1211	OMG	O6-C6-C5	-2.13	120.92	126.53
3	1	2155	OMU	O2-C2-N1	-2.12	120.04	122.80
3	1	2628	OMU	C1'-N1-C2	2.12	121.39	117.59
3	1	2104	OMG	O6-C6-C5	-2.11	120.95	126.53
4	4	572	OMC	O2-C2-N3	-2.11	119.00	122.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	4	908	OMG	O6-C6-C5	-2.11	120.97	126.53
3	1	2608	OMG	O6-C6-C5	-2.11	120.97	126.53
3	1	2884	OMC	O2-C2-N3	-2.10	119.02	122.33
4	4	514	OMC	O2-C2-N3	-2.10	119.02	122.33
3	1	2667	OMG	O6-C6-C5	-2.09	121.01	126.53
4	4	462	OMG	O6-C6-C5	-2.09	121.02	126.53
4	4	1202	OMG	C5-C6-N1	2.09	118.57	113.25
4	4	1202	OMG	O6-C6-C5	-2.09	121.02	126.53
4	4	489	OMC	C1'-N1-C2	2.08	123.04	118.44
3	1	2601	OMG	C5-C6-N1	2.08	118.55	113.25
3	1	908	OMU	O2-C2-N3	-2.07	117.67	121.49
4	4	1212	OMG	O6-C6-C5	-2.07	121.08	126.53
3	1	1971	OMG	C5-C6-N1	2.06	118.51	113.25
3	1	2176	OMG	O6-C6-C5	-2.06	121.08	126.53
4	4	1163	OMG	C4-C5-N7	-2.06	107.41	110.67
4	4	475	OMG	O6-C6-C5	-2.06	121.10	126.53
3	1	2388	OMG	C5-C6-N1	2.04	118.44	113.25
3	1	2537	OMG	O6-C6-C5	-2.04	121.16	126.53
4	4	906	OMG	C5-C6-N1	2.04	118.44	113.25
4	4	1459	6MZ	C5-N7-C8	2.03	106.65	103.45
3	1	3023	G7M	C8-N7-C5	2.03	110.32	107.78
4	4	475	OMG	C5-C6-N1	2.02	118.41	113.25
3	1	1949	OMG	O6-C6-C5	-2.02	121.21	126.53
3	1	2088	OMU	C1'-N1-C2	2.02	121.22	117.59
4	4	1210	OMG	C5-C6-N1	2.01	118.38	113.25
4	4	1211	OMG	C5-C6-N1	2.01	118.36	113.25

There are no chirality outliers.

All (85) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	4	496	A2M	C1'-C2'-O2'-CM'
4	4	879	A2M	C3'-C4'-C5'-O5'
4	4	879	A2M	C1'-C2'-O2'-CM'
4	4	1045	OMC	O4'-C4'-C5'-O5'
4	4	1060	A2M	C1'-C2'-O2'-CM'
4	4	1202	OMG	O4'-C4'-C5'-O5'
4	4	1211	OMG	O4'-C4'-C5'-O5'
3	1	1947	OMG	O4'-C4'-C5'-O5'
3	1	2011	A2M	C1'-C2'-O2'-CM'
3	1	2537	OMG	O4'-C4'-C5'-O5'
3	1	2608	OMG	O4'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	1	2691	A2M	C1'-C2'-O2'-CM'
4	4	19	OMG	O4'-C4'-C5'-O5'
4	4	19	OMG	C3'-C4'-C5'-O5'
4	4	465	OMG	O4'-C4'-C5'-O5'
4	4	1060	A2M	O4'-C4'-C5'-O5'
4	4	1202	OMG	C3'-C4'-C5'-O5'
4	4	1211	OMG	C3'-C4'-C5'-O5'
3	1	1947	OMG	C3'-C4'-C5'-O5'
3	1	2116	OMC	O4'-C4'-C5'-O5'
3	1	2608	OMG	C3'-C4'-C5'-O5'
4	4	508	M7A	O4'-C4'-C5'-O5'
4	4	511	OMG	O4'-C4'-C5'-O5'
4	4	511	OMG	C3'-C4'-C5'-O5'
4	4	879	A2M	O4'-C4'-C5'-O5'
4	4	1060	A2M	C3'-C4'-C5'-O5'
4	4	1163	OMG	C3'-C4'-C5'-O5'
4	4	1368	OMC	O4'-C4'-C5'-O5'
4	4	1478	MA6	O4'-C4'-C5'-O5'
4	4	496	A2M	O4'-C4'-C5'-O5'
4	4	508	M7A	C3'-C4'-C5'-O5'
4	4	1045	OMC	C3'-C4'-C5'-O5'
3	1	2537	OMG	C3'-C4'-C5'-O5'
4	4	465	OMG	C3'-C4'-C5'-O5'
3	1	2937	B8T	C3'-C4'-C5'-O5'
3	1	38	5MC	C4'-C5'-O5'-P
4	4	1035	B8T	O4'-C4'-C5'-O5'
3	1	2116	OMC	C3'-C4'-C5'-O5'
3	1	2362	OMG	O4'-C4'-C5'-O5'
3	1	3023	G7M	O4'-C4'-C5'-O5'
4	4	1035	B8T	C3'-C4'-C5'-O5'
4	4	1163	OMG	O4'-C4'-C5'-O5'
3	1	2628	OMU	O4'-C4'-C5'-O5'
4	4	1478	MA6	C3'-C4'-C5'-O5'
3	1	2044	PSU	O4'-C4'-C5'-O5'
4	4	1368	OMC	C3'-C4'-C5'-O5'
3	1	492	OMC	O4'-C4'-C5'-O5'
4	4	908	OMG	C3'-C4'-C5'-O5'
3	1	2388	OMG	C4'-C5'-O5'-P
3	1	2044	PSU	C3'-C4'-C5'-O5'
53	BM	128	IAS	CA-CB-CG-OD1
3	1	2056	5MC	O4'-C4'-C5'-O5'
4	4	511	OMG	C4'-C5'-O5'-P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	1	908	OMU	O4'-C1'-N1-C2
4	4	467	OMG	C3'-C2'-O2'-CM2
3	1	2059	A2M	C3'-C2'-O2'-CM'
3	1	2555	OMC	C4'-C5'-O5'-P
4	4	496	A2M	C3'-C4'-C5'-O5'
3	1	908	OMU	O4'-C1'-N1-C6
3	1	908	OMU	C2'-C1'-N1-C2
4	4	508	M7A	C4'-C5'-O5'-P
3	1	2362	OMG	C4'-C5'-O5'-P
3	1	3023	G7M	C3'-C4'-C5'-O5'
3	1	493	OMC	C3'-C2'-O2'-CM2
3	1	2017	OMG	C3'-C2'-O2'-CM2
3	1	2077	OMU	C3'-C2'-O2'-CM2
3	1	908	OMU	C2'-C1'-N1-C6
4	4	908	OMG	O4'-C4'-C5'-O5'
3	1	2366	OMG	O4'-C4'-C5'-O5'
4	4	879	A2M	C4'-C5'-O5'-P
4	4	1060	A2M	C4'-C5'-O5'-P
4	4	1163	OMG	C4'-C5'-O5'-P
3	1	2937	B8T	O4'-C4'-C5'-O5'
4	4	1163	OMG	C2'-C1'-N9-C4
4	4	908	OMG	C4'-C5'-O5'-P
4	4	1211	OMG	C3'-C2'-O2'-CM2
3	1	2155	OMU	C2'-C1'-N1-C6
4	4	1045	OMC	C2'-C1'-N1-C2
3	1	2362	OMG	C3'-C4'-C5'-O5'
3	1	2155	OMU	O4'-C1'-N1-C6
4	4	508	M7A	C2'-C1'-N9-C8
3	1	2104	OMG	C3'-C2'-O2'-CM2
4	4	1210	OMG	C3'-C4'-C5'-O5'
3	1	2628	OMU	C3'-C4'-C5'-O5'
3	1	2088	OMU	C4'-C5'-O5'-P

There are no ring outliers.

80 monomers are involved in 128 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	4	1478	MA6	2	0
3	1	2056	5MC	1	0
3	1	2704	OMC	3	0
4	4	1289	OMG	3	0
4	4	572	OMC	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	1	2698	UR3	1	0
3	1	2607	PSU	1	0
3	1	2885	OMC	3	0
4	4	1211	OMG	4	0
3	1	2707	OMU	1	0
3	1	902	OMG	3	0
53	BM	128	IAS	1	0
4	4	1477	MA6	2	0
4	4	514	OMC	1	0
3	1	2366	OMG	2	0
3	1	2667	OMG	2	0
3	1	2408	OMU	2	0
3	1	2059	A2M	1	0
4	4	880	A2M	4	0
3	1	1816	OMC	1	0
3	1	2103	OMG	1	0
3	1	2011	A2M	2	0
4	4	1034	OMC	1	0
3	1	872	OMC	1	0
3	1	3023	G7M	1	0
3	1	2610	PSU	1	0
3	1	1990	A2M	4	0
4	4	7	OMG	3	0
3	1	2624	OMC	2	0
3	1	2608	OMG	1	0
4	4	465	OMG	2	0
4	4	462	OMG	1	0
4	4	263	PSU	2	0
4	4	1210	OMG	4	0
3	1	2538	OMC	2	0
4	4	1368	OMC	1	0
3	1	2537	OMG	1	0
4	4	15	OMU	1	0
4	4	674	OMG	1	0
3	1	1957	OMG	1	0
4	4	1318	4AC	1	0
4	4	879	A2M	3	0
3	1	2088	OMU	2	0
3	1	2044	PSU	2	0
3	1	2155	OMU	1	0
3	1	875	OMU	3	0
3	1	2884	OMC	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	1	493	OMC	1	0
3	1	1976	OMC	1	0
3	1	2104	OMG	3	0
3	1	2720	OMC	1	0
4	4	908	OMG	1	0
3	1	1971	OMG	1	0
4	4	1212	OMG	2	0
3	1	2071	OMG	1	0
4	4	877	OMU	2	0
4	4	467	OMG	1	0
4	4	1202	OMG	2	0
3	1	2115	OMC	1	0
3	1	2623	OMU	2	0
4	4	1184	OMC	3	0
4	4	1163	OMG	2	0
3	1	2017	OMG	1	0
3	1	1947	OMG	1	0
3	1	2851	OMU	4	0
3	1	2628	OMU	3	0
4	4	475	OMG	5	0
3	1	2077	OMU	1	0
4	4	5	4AC	1	0
4	4	1045	OMC	1	0
3	1	2388	OMG	1	0
4	4	906	OMG	1	0
4	4	1060	A2M	1	0
3	1	492	OMC	2	0
4	4	489	OMC	1	0
4	4	1459	6MZ	2	0
3	1	2555	OMC	2	0
4	4	1035	B8T	1	0
3	1	2362	OMG	1	0
3	1	2018	OMC	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 326 ligands modelled in this entry, 262 are monoatomic - leaving 64 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	$\# Z > 2$
70	SPM	1	3131	-	13,13,13	0.17	0	12,12,12	0.23	0
70	SPM	1	3114	-	13,13,13	0.17	0	12,12,12	0.47	0
70	SPM	4	3014	-	13,13,13	0.16	0	12,12,12	0.44	0
70	SPM	4	3015	-	13,13,13	0.15	0	12,12,12	0.37	0
70	SPM	Ah	101	-	13,13,13	0.17	0	12,12,12	0.20	0
70	SPM	1	3116	-	13,13,13	0.16	0	12,12,12	0.31	0
70	SPM	1	3107	-	13,13,13	0.17	0	12,12,12	0.20	0
70	SPM	1	3130	-	13,13,13	0.15	0	12,12,12	0.13	0
70	SPM	1	3142	-	13,13,13	0.16	0	12,12,12	0.38	0
70	SPM	1	3127	-	13,13,13	0.16	0	12,12,12	0.35	0
70	SPM	1	3120	-	13,13,13	0.17	0	12,12,12	0.23	0
70	SPM	1	3132	-	13,13,13	0.14	0	12,12,12	0.20	0
70	SPM	1	3140	-	13,13,13	0.15	0	12,12,12	0.32	0
70	SPM	4	3004	-	13,13,13	0.17	0	12,12,12	0.16	0
70	SPM	4	3018	-	13,13,13	0.16	0	12,12,12	0.34	0
70	SPM	4	3016	-	13,13,13	0.15	0	12,12,12	0.20	0
70	SPM	4	3013	-	13,13,13	0.16	0	12,12,12	0.26	0
70	SPM	1	3102	-	13,13,13	0.18	0	12,12,12	0.42	0
70	SPM	1	3103	-	13,13,13	0.17	0	12,12,12	0.49	0
70	SPM	1	3115	-	13,13,13	0.17	0	12,12,12	0.42	0
70	SPM	4	3005	-	13,13,13	0.14	0	12,12,12	0.23	0
70	SPM	1	3109	-	13,13,13	0.18	0	12,12,12	0.31	0
70	SPM	1	3129	-	13,13,13	0.16	0	12,12,12	0.39	0
70	SPM	1	3134	-	13,13,13	0.19	0	12,12,12	0.38	0
70	SPM	1	3123	-	13,13,13	0.16	0	12,12,12	0.39	0
70	SPM	1	3125	-	13,13,13	0.16	0	12,12,12	0.28	0
70	SPM	1	3137	-	13,13,13	0.16	0	12,12,12	0.34	0
70	SPM	AL	201	-	13,13,13	0.16	0	12,12,12	0.32	0
70	SPM	AM	201	-	13,13,13	0.17	0	12,12,12	0.43	0
70	SPM	1	3117	-	13,13,13	0.17	0	12,12,12	0.32	0
70	SPM	1	3112	-	13,13,13	0.17	0	12,12,12	0.29	0
70	SPM	1	3139	-	13,13,13	0.16	0	12,12,12	0.23	0
70	SPM	1	3122	-	13,13,13	0.18	0	12,12,12	0.28	0
70	SPM	1	3105	-	13,13,13	0.15	0	12,12,12	0.18	0
70	SPM	4	3003	-	13,13,13	0.18	0	12,12,12	0.20	0
70	SPM	1	3104	-	13,13,13	0.18	0	12,12,12	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
70	SPM	1	3128	-	13,13,13	0.16	0	12,12,12	0.22	0
70	SPM	1	3106	3	13,13,13	0.15	0	12,12,12	0.34	0
70	SPM	4	3012	-	13,13,13	0.17	0	12,12,12	0.10	0
70	SPM	1	3108	-	13,13,13	0.18	0	12,12,12	0.53	0
70	SPM	1	3121	-	13,13,13	0.24	0	12,12,12	0.27	0
70	SPM	1	3133	-	13,13,13	0.17	0	12,12,12	0.29	0
70	SPM	4	3011	-	13,13,13	0.15	0	12,12,12	0.42	0
70	SPM	1	3135	-	13,13,13	0.16	0	12,12,12	0.60	0
70	SPM	4	3006	-	13,13,13	0.15	0	12,12,12	0.27	0
70	SPM	4	3010	-	13,13,13	0.16	0	12,12,12	0.65	0
70	SPM	1	3113	-	13,13,13	0.16	0	12,12,12	0.29	0
70	SPM	1	3126	-	13,13,13	0.16	0	12,12,12	0.50	0
70	SPM	4	3001	-	13,13,13	0.16	0	12,12,12	0.35	0
70	SPM	4	3009	-	13,13,13	0.19	0	12,12,12	0.36	0
70	SPM	1	3141	-	13,13,13	0.17	0	12,12,12	0.59	0
70	SPM	1	3138	-	13,13,13	0.18	0	12,12,12	0.65	0
70	SPM	1	3110	-	13,13,13	0.16	0	12,12,12	0.18	0
70	SPM	1	3119	-	13,13,13	0.19	0	12,12,12	0.31	0
70	SPM	4	3002	-	13,13,13	0.18	0	12,12,12	0.41	0
70	SPM	4	3007	-	13,13,13	0.21	0	12,12,12	0.55	0
70	SPM	1	3111	-	13,13,13	0.16	0	12,12,12	0.26	0
70	SPM	4	3017	-	13,13,13	0.24	0	12,12,12	1.59	1 (8%)
70	SPM	1	3124	-	13,13,13	0.15	0	12,12,12	0.26	0
70	SPM	4	3008	-	13,13,13	0.15	0	12,12,12	0.18	0
70	SPM	1	3143	-	13,13,13	0.18	0	12,12,12	0.42	0
70	SPM	1	3101	-	13,13,13	0.17	0	12,12,12	0.45	0
70	SPM	1	3118	-	13,13,13	0.16	0	12,12,12	0.20	0
70	SPM	1	3136	-	13,13,13	0.15	0	12,12,12	0.44	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
70	SPM	1	3131	-	-	0/11/11/11	-
70	SPM	1	3114	-	-	2/11/11/11	-
70	SPM	4	3014	-	-	3/11/11/11	-
70	SPM	4	3015	-	-	1/11/11/11	-
70	SPM	Ah	101	-	-	2/11/11/11	-
70	SPM	1	3116	-	-	2/11/11/11	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
70	SPM	1	3107	-	-	1/11/11/11	-
70	SPM	1	3130	-	-	0/11/11/11	-
70	SPM	1	3142	-	-	1/11/11/11	-
70	SPM	1	3127	-	-	0/11/11/11	-
70	SPM	1	3120	-	-	2/11/11/11	-
70	SPM	1	3132	-	-	5/11/11/11	-
70	SPM	1	3140	-	-	1/11/11/11	-
70	SPM	4	3004	-	-	0/11/11/11	-
70	SPM	4	3018	-	-	0/11/11/11	-
70	SPM	4	3016	-	-	1/11/11/11	-
70	SPM	4	3013	-	-	1/11/11/11	-
70	SPM	1	3102	-	-	0/11/11/11	-
70	SPM	1	3103	-	-	0/11/11/11	-
70	SPM	1	3115	-	-	1/11/11/11	-
70	SPM	4	3005	-	-	1/11/11/11	-
70	SPM	1	3109	-	-	1/11/11/11	-
70	SPM	1	3129	-	-	1/11/11/11	-
70	SPM	1	3134	-	-	2/11/11/11	-
70	SPM	1	3123	-	-	2/11/11/11	-
70	SPM	1	3125	-	-	1/11/11/11	-
70	SPM	1	3137	-	-	2/11/11/11	-
70	SPM	AL	201	-	-	1/11/11/11	-
70	SPM	AM	201	-	-	1/11/11/11	-
70	SPM	1	3117	-	-	2/11/11/11	-
70	SPM	1	3112	-	-	1/11/11/11	-
70	SPM	1	3139	-	-	0/11/11/11	-
70	SPM	1	3122	-	-	0/11/11/11	-
70	SPM	1	3105	-	-	1/11/11/11	-
70	SPM	4	3003	-	-	4/11/11/11	-
70	SPM	1	3104	-	-	2/11/11/11	-
70	SPM	1	3128	-	-	1/11/11/11	-
70	SPM	1	3106	3	-	2/11/11/11	-
70	SPM	4	3012	-	-	2/11/11/11	-
70	SPM	1	3108	-	-	3/11/11/11	-
70	SPM	1	3121	-	-	1/11/11/11	-
70	SPM	1	3133	-	-	3/11/11/11	-
70	SPM	4	3011	-	-	2/11/11/11	-
70	SPM	1	3135	-	-	0/11/11/11	-
70	SPM	4	3006	-	-	2/11/11/11	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
70	SPM	4	3010	-	-	3/11/11/11	-
70	SPM	1	3113	-	-	2/11/11/11	-
70	SPM	1	3126	-	-	3/11/11/11	-
70	SPM	4	3001	-	-	0/11/11/11	-
70	SPM	4	3009	-	-	2/11/11/11	-
70	SPM	1	3141	-	-	4/11/11/11	-
70	SPM	1	3138	-	-	5/11/11/11	-
70	SPM	1	3110	-	-	0/11/11/11	-
70	SPM	1	3119	-	-	3/11/11/11	-
70	SPM	4	3002	-	-	2/11/11/11	-
70	SPM	4	3007	-	-	5/11/11/11	-
70	SPM	1	3111	-	-	0/11/11/11	-
70	SPM	4	3017	-	-	5/11/11/11	-
70	SPM	1	3124	-	-	0/11/11/11	-
70	SPM	4	3008	-	-	0/11/11/11	-
70	SPM	1	3143	-	-	2/11/11/11	-
70	SPM	1	3101	-	-	4/11/11/11	-
70	SPM	1	3118	-	-	1/11/11/11	-
70	SPM	1	3136	-	-	1/11/11/11	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
70	4	3017	SPM	C7-C8-C9	5.12	137.21	113.56

There are no chirality outliers.

All (103) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
70	4	3017	SPM	C6-C7-C8-C9
70	1	3138	SPM	N5-C6-C7-C8
70	4	3007	SPM	C7-C8-C9-N10
70	AL	201	SPM	N10-C11-C12-C13
70	1	3134	SPM	N5-C6-C7-C8
70	4	3009	SPM	C7-C8-C9-N10
70	1	3137	SPM	C7-C8-C9-N10
70	4	3005	SPM	N5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
70	1	3101	SPM	C7-C8-C9-N10
70	4	3003	SPM	N5-C6-C7-C8
70	4	3017	SPM	C7-C8-C9-N10
70	1	3106	SPM	N10-C11-C12-C13
70	1	3128	SPM	C2-C3-C4-N5
70	1	3136	SPM	N10-C11-C12-C13
70	4	3003	SPM	C2-C3-C4-N5
70	1	3108	SPM	N5-C6-C7-C8
70	1	3142	SPM	N5-C6-C7-C8
70	4	3017	SPM	N10-C11-C12-C13
70	1	3116	SPM	N5-C6-C7-C8
70	4	3012	SPM	N10-C11-C12-C13
70	1	3121	SPM	C7-C8-C9-N10
70	1	3133	SPM	N5-C6-C7-C8
70	1	3129	SPM	C12-C11-N10-C9
70	1	3132	SPM	N5-C6-C7-C8
70	1	3101	SPM	C12-C11-N10-C9
70	1	3138	SPM	C7-C8-C9-N10
70	1	3133	SPM	N10-C11-C12-C13
70	AM	201	SPM	C7-C6-N5-C4
70	1	3119	SPM	C7-C8-C9-N10
70	1	3114	SPM	C6-C7-C8-C9
70	1	3132	SPM	C7-C8-C9-N10
70	1	3101	SPM	C7-C6-N5-C4
70	1	3109	SPM	N10-C11-C12-C13
70	4	3015	SPM	N10-C11-C12-C13
70	1	3133	SPM	C6-C7-C8-C9
70	1	3143	SPM	C6-C7-C8-C9
70	4	3014	SPM	C2-C3-C4-N5
70	1	3113	SPM	N10-C11-C12-C13
70	1	3104	SPM	C8-C9-N10-C11
70	1	3117	SPM	C12-C11-N10-C9
70	1	3132	SPM	C11-C12-C13-N14
70	4	3002	SPM	C6-C7-C8-C9
70	1	3138	SPM	C6-C7-C8-C9
70	1	3107	SPM	C6-C7-C8-C9
70	1	3105	SPM	C8-C9-N10-C11
70	1	3108	SPM	C3-C4-N5-C6
70	4	3009	SPM	C8-C9-N10-C11
70	Ah	101	SPM	C7-C6-N5-C4
70	Ah	101	SPM	C6-C7-C8-C9
70	4	3010	SPM	N10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
70	1	3141	SPM	C2-C3-C4-N5
70	4	3006	SPM	C6-C7-C8-C9
70	1	3125	SPM	C6-C7-C8-C9
70	1	3104	SPM	C6-C7-C8-C9
70	4	3014	SPM	C12-C11-N10-C9
70	1	3126	SPM	C2-C3-C4-N5
70	4	3016	SPM	C11-C12-C13-N14
70	1	3120	SPM	C7-C6-N5-C4
70	1	3143	SPM	C2-C3-C4-N5
70	4	3011	SPM	N10-C11-C12-C13
70	1	3132	SPM	C6-C7-C8-C9
70	1	3138	SPM	C8-C9-N10-C11
70	1	3141	SPM	C8-C9-N10-C11
70	4	3002	SPM	C3-C4-N5-C6
70	4	3007	SPM	C2-C3-C4-N5
70	1	3115	SPM	C12-C11-N10-C9
70	1	3140	SPM	C3-C4-N5-C6
70	4	3007	SPM	C6-C7-C8-C9
70	1	3138	SPM	N10-C11-C12-C13
70	1	3141	SPM	N5-C6-C7-C8
70	1	3101	SPM	C3-C4-N5-C6
70	1	3134	SPM	C12-C11-N10-C9
70	1	3141	SPM	C3-C4-N5-C6
70	4	3007	SPM	C11-C12-C13-N14
70	4	3014	SPM	C8-C9-N10-C11
70	1	3123	SPM	C2-C3-C4-N5
70	4	3003	SPM	N10-C11-C12-C13
70	1	3112	SPM	C8-C9-N10-C11
70	1	3119	SPM	C12-C11-N10-C9
70	1	3137	SPM	C12-C11-N10-C9
70	4	3006	SPM	C8-C9-N10-C11
70	4	3010	SPM	C7-C6-N5-C4
70	4	3012	SPM	C3-C4-N5-C6
70	4	3013	SPM	C3-C4-N5-C6
70	1	3108	SPM	C6-C7-C8-C9
70	1	3117	SPM	C7-C8-C9-N10
70	4	3010	SPM	C12-C11-N10-C9
70	4	3017	SPM	C3-C4-N5-C6
70	1	3113	SPM	C7-C8-C9-N10
70	4	3007	SPM	C8-C9-N10-C11
70	1	3119	SPM	C8-C9-N10-C11
70	4	3017	SPM	C7-C6-N5-C4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
70	1	3116	SPM	C6-C7-C8-C9
70	1	3123	SPM	N5-C6-C7-C8
70	1	3132	SPM	C8-C9-N10-C11
70	4	3011	SPM	C12-C11-N10-C9
70	1	3118	SPM	C7-C8-C9-N10
70	1	3114	SPM	C2-C3-C4-N5
70	1	3120	SPM	C12-C11-N10-C9
70	1	3126	SPM	C7-C6-N5-C4
70	4	3003	SPM	C12-C11-N10-C9
70	1	3126	SPM	C7-C8-C9-N10
70	1	3106	SPM	C7-C8-C9-N10

There are no ring outliers.

22 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
70	1	3114	SPM	2	0
70	4	3014	SPM	2	0
70	1	3116	SPM	1	0
70	1	3107	SPM	1	0
70	1	3120	SPM	1	0
70	1	3140	SPM	1	0
70	1	3102	SPM	1	0
70	1	3103	SPM	1	0
70	4	3005	SPM	2	0
70	1	3134	SPM	1	0
70	1	3125	SPM	1	0
70	AL	201	SPM	2	0
70	1	3117	SPM	1	0
70	1	3139	SPM	1	0
70	1	3128	SPM	2	0
70	1	3106	SPM	2	0
70	4	3012	SPM	2	0
70	1	3108	SPM	1	0
70	1	3121	SPM	1	0
70	1	3126	SPM	1	0
70	4	3017	SPM	2	0
70	4	3008	SPM	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

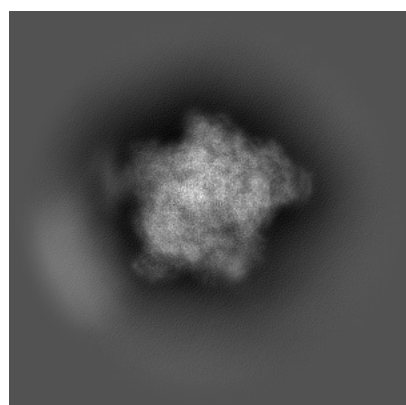
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47668. These allow visual inspection of the internal detail of the map and identification of artifacts.

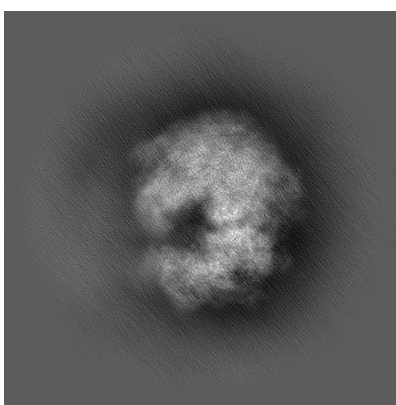
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

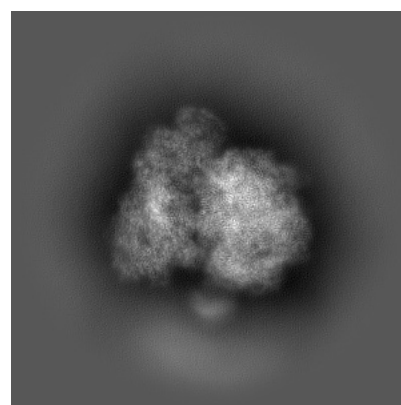
6.1.1 Primary map



X



Y

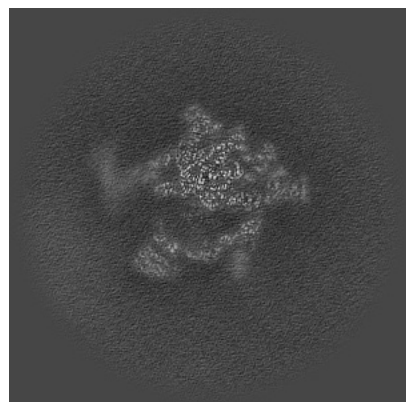


Z

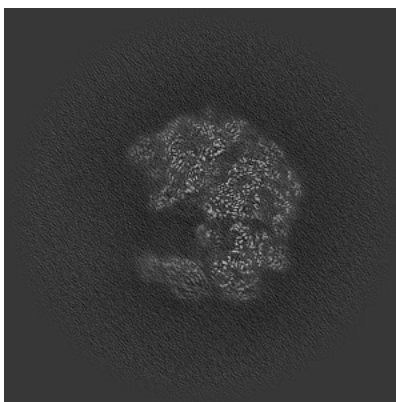
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

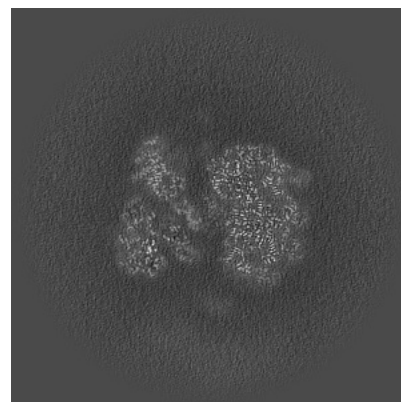
6.2.1 Primary map



X Index: 304



Y Index: 304

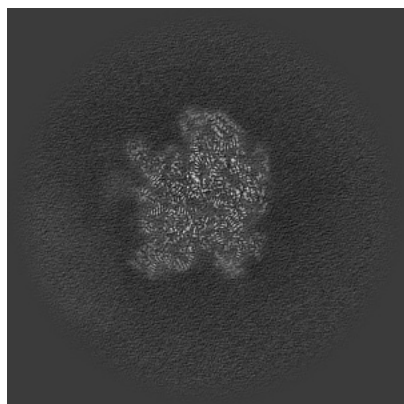


Z Index: 304

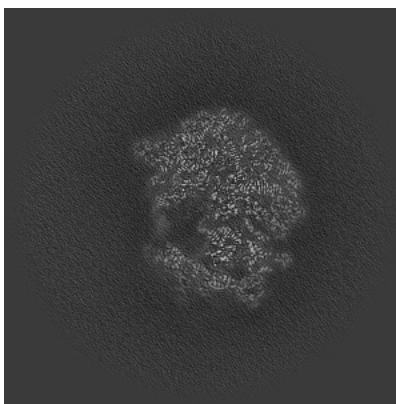
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

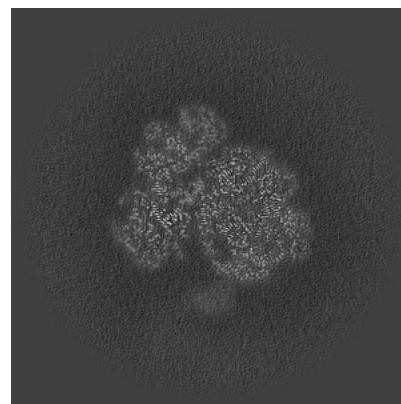
6.3.1 Primary map



X Index: 334



Y Index: 288

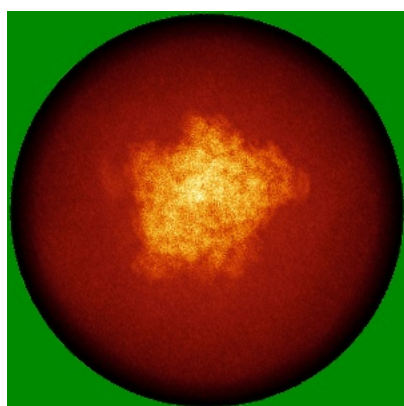


Z Index: 326

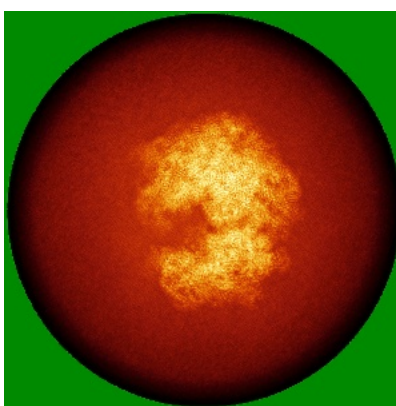
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

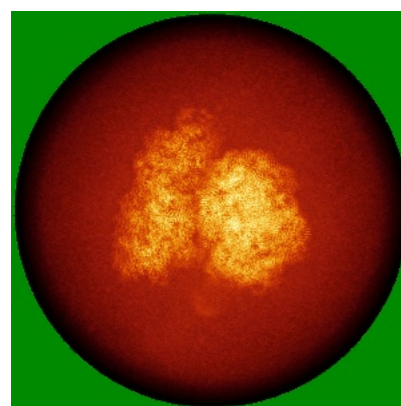
6.4.1 Primary map



X



Y

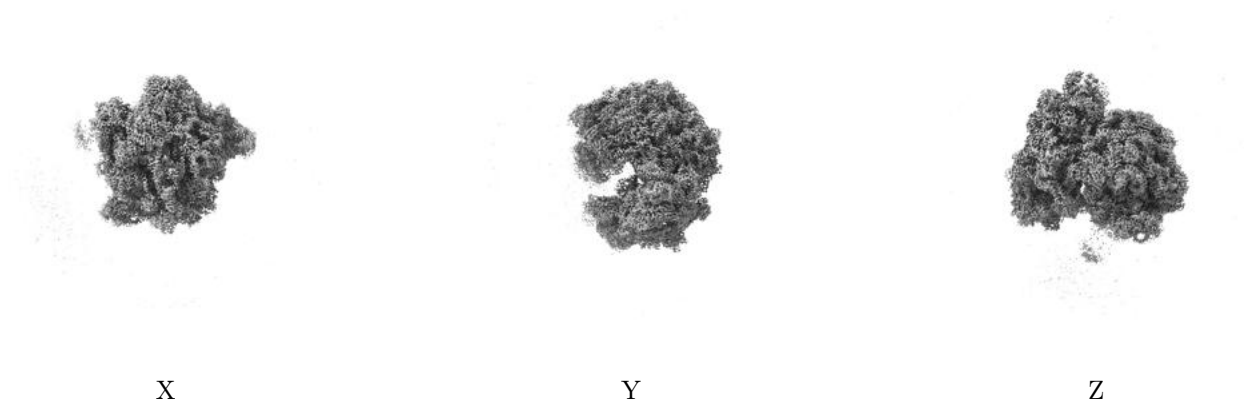


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.188. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

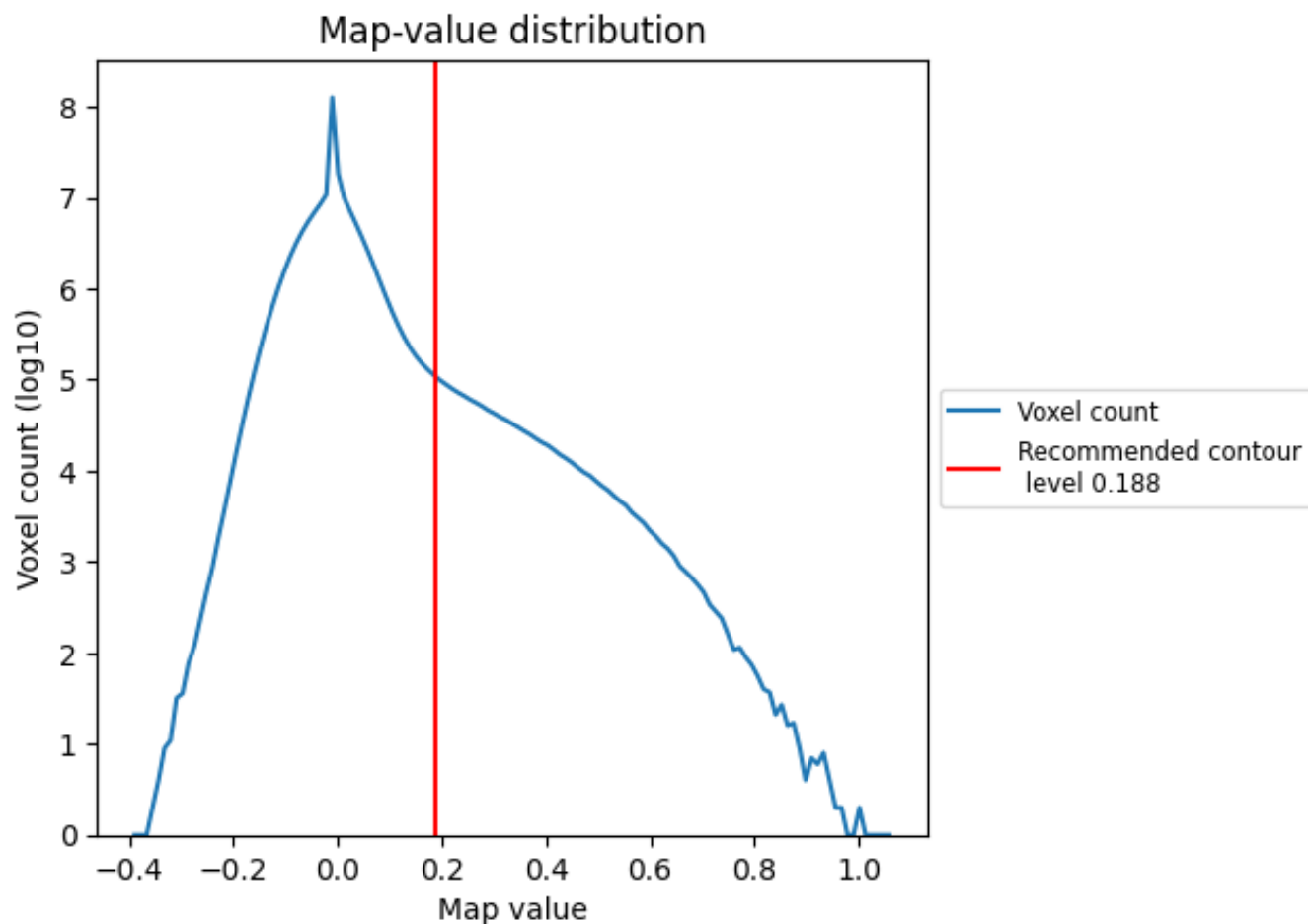
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

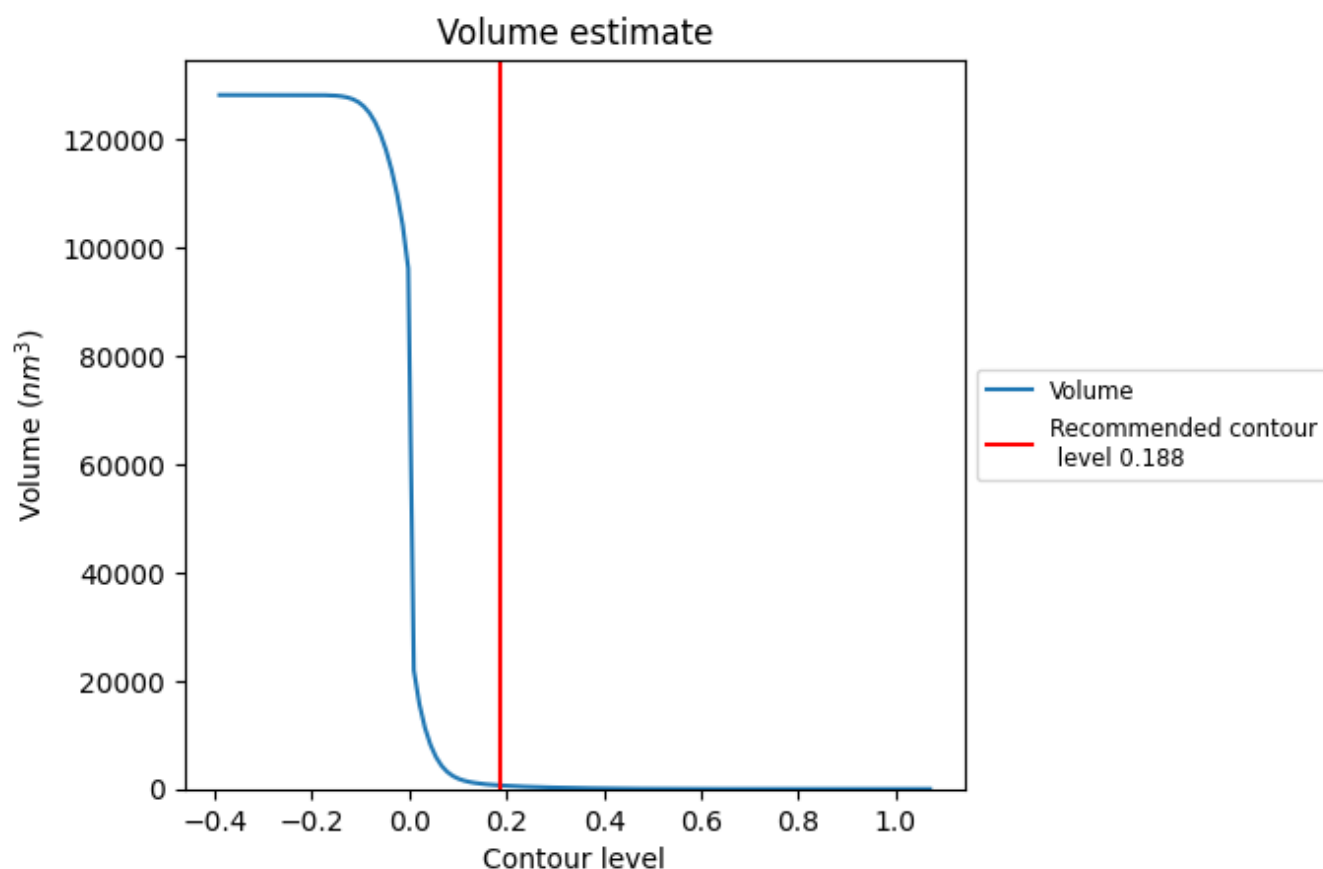
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

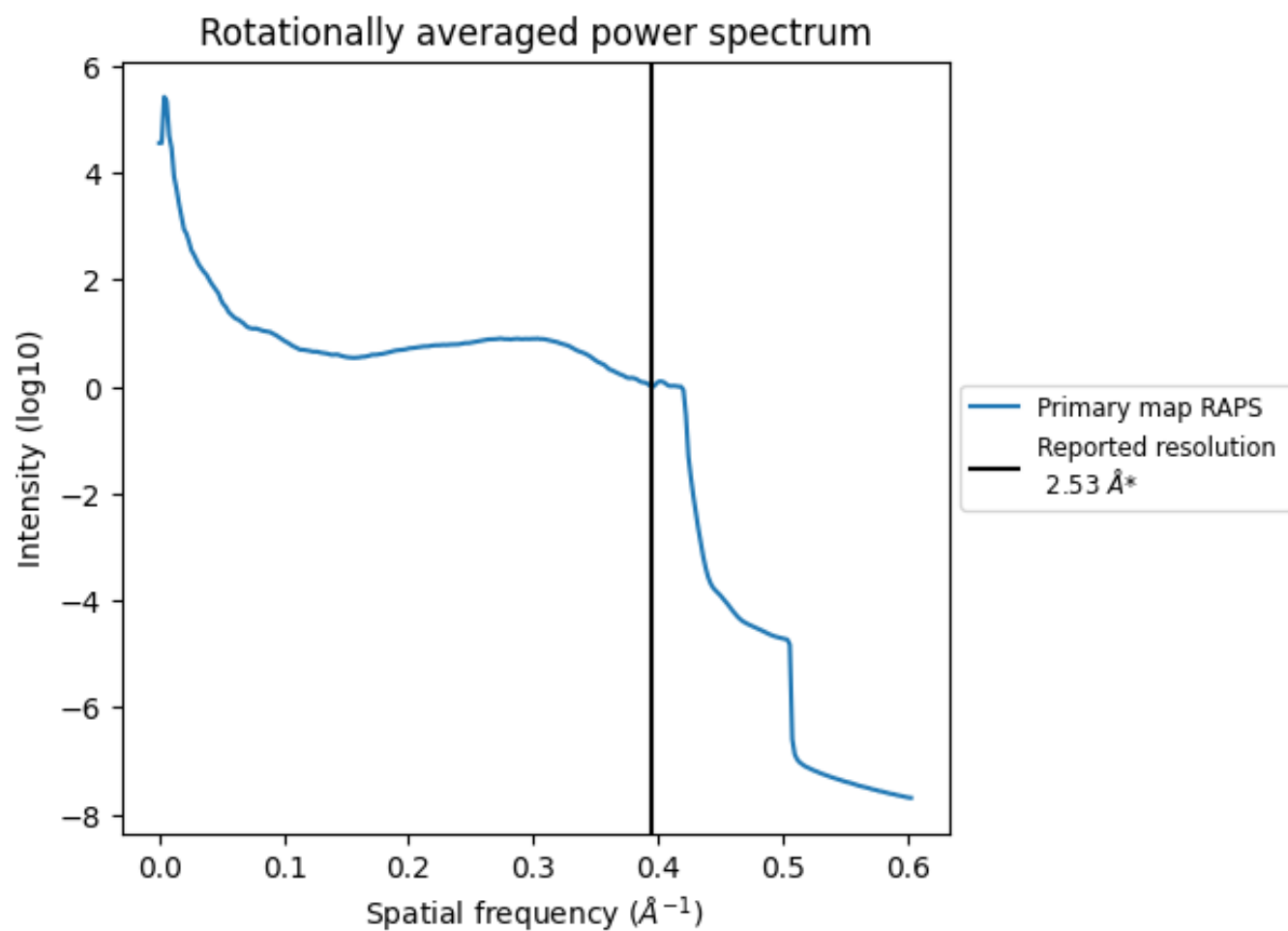
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 654 nm^3 ; this corresponds to an approximate mass of 590 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.395 Å⁻¹

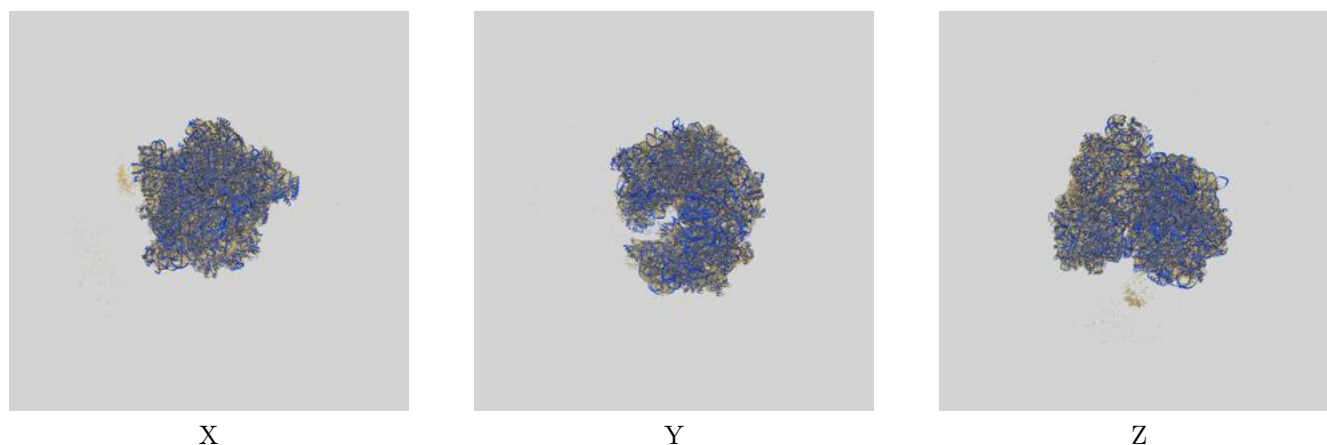
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

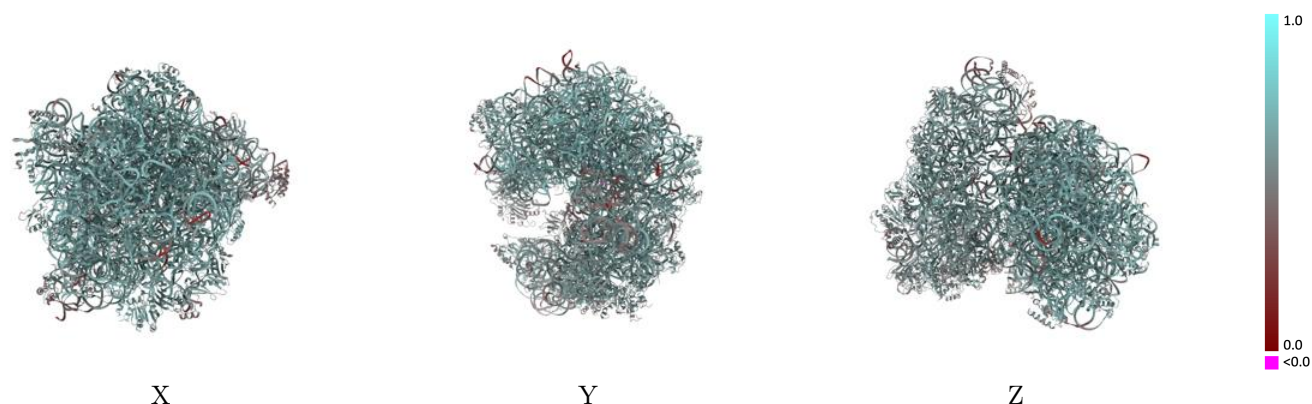
This section contains information regarding the fit between EMDB map EMD-47668 and PDB model 9E7F. Per-residue inclusion information can be found in section [3](#) on page [24](#).

9.1 Map-model overlay [i](#)



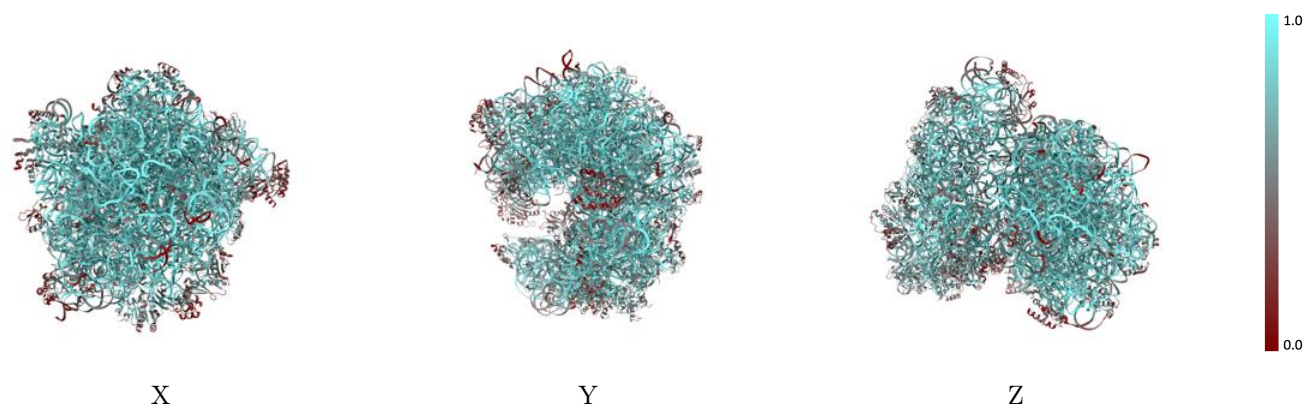
The images above show the 3D surface view of the map at the recommended contour level 0.188 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



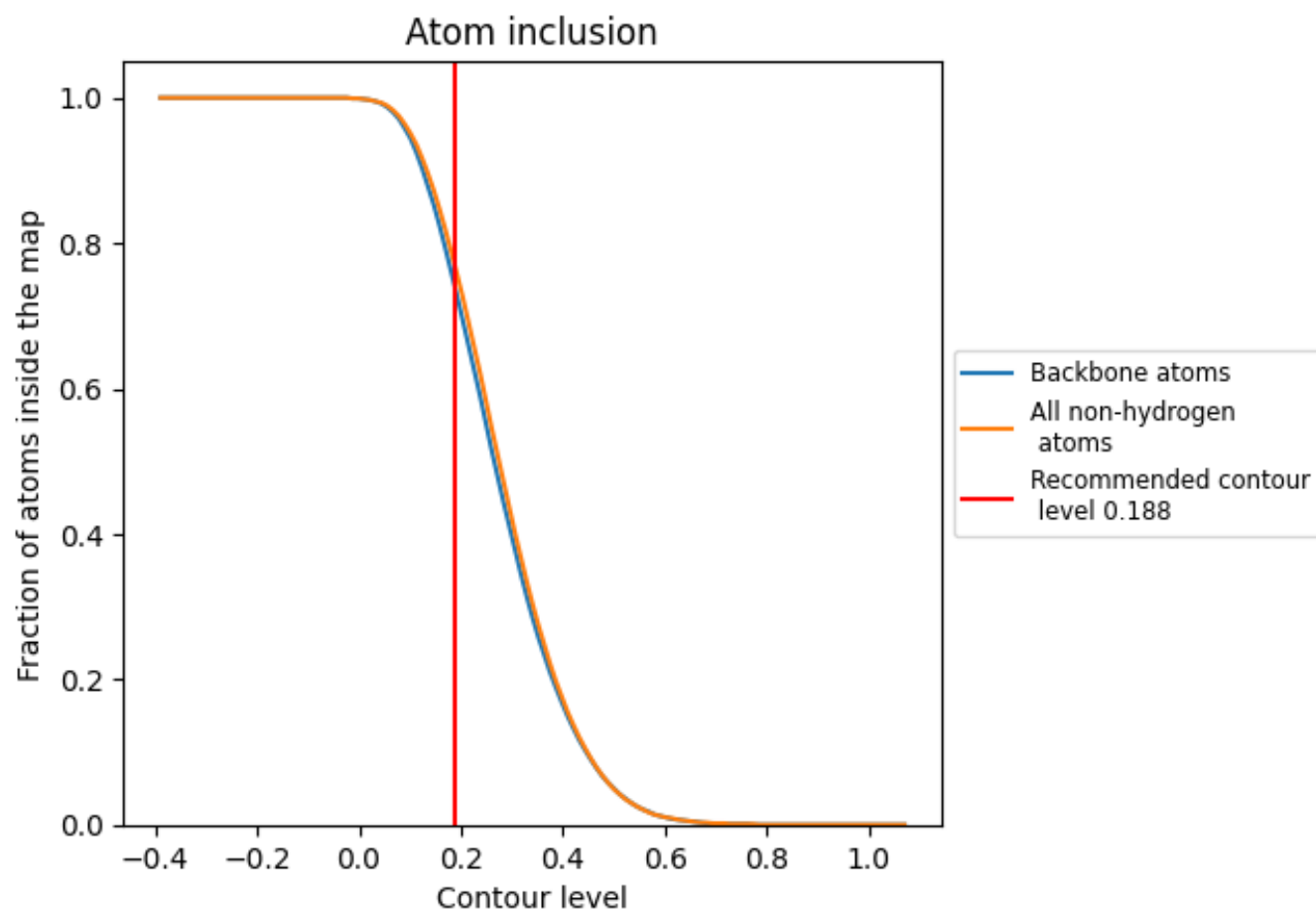
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.188).

9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 77% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.188) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7700	 0.6030
1	 0.8910	 0.6350
2	 0.6920	 0.5650
3	 0.4220	 0.4750
4	 0.8440	 0.5760
AA	 0.8280	 0.6530
AB	 0.7950	 0.6530
AC	 0.7410	 0.6350
AD	 0.2020	 0.4570
AE	 0.5100	 0.5950
AF	 0.4580	 0.5650
AG	 0.7480	 0.6370
AH	 0.7520	 0.6410
AI	 0.7720	 0.6440
AJ	 0.4840	 0.5610
AK	 0.4310	 0.5540
AL	 0.6600	 0.6120
AM	 0.8060	 0.6480
AN	 0.6810	 0.6320
AO	 0.4550	 0.5580
AP	 0.7480	 0.6370
AQ	 0.7460	 0.6310
AR	 0.5790	 0.6000
AS	 0.8260	 0.6540
AT	 0.8300	 0.6600
AU	 0.7370	 0.6420
AV	 0.7000	 0.6210
AW	 0.7970	 0.6430
AX	 0.6020	 0.5970
AY	 0.7730	 0.6370
AZ	 0.6060	 0.5870
Aa	 0.7480	 0.6340
Ab	 0.7570	 0.6390
Ac	 0.8410	 0.6380
Ad	 0.9560	 0.6920



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Ae	 0.6530	 0.6210
Af	 0.8930	 0.6670
Ag	 0.5960	 0.6070
Ah	 0.7760	 0.6480
Ai	 0.7470	 0.6250
Aj	 0.5370	 0.5970
Ak	 0.6110	 0.6030
BA	 0.5380	 0.5450
BB	 0.5530	 0.5340
BC	 0.3510	 0.4920
BD	 0.6750	 0.5850
BE	 0.6780	 0.5920
BF	 0.6970	 0.5820
BG	 0.3110	 0.4760
BH	 0.6850	 0.5780
BI	 0.7840	 0.5970
BJ	 0.6580	 0.5920
BK	 0.6830	 0.5600
BL	 0.4290	 0.5440
BM	 0.6520	 0.5560
BN	 0.6300	 0.5750
BO	 0.5240	 0.5370
BP	 0.4430	 0.4860
BQ	 0.6230	 0.5750
BR	 0.6240	 0.5800
BS	 0.3820	 0.4680
BT	 0.5620	 0.5480
BU	 0.7270	 0.5880
BV	 0.4530	 0.5290
BW	 0.5990	 0.5550
BX	 0.2620	 0.4780
BY	 0.6170	 0.5730
BZ	 0.5740	 0.5300
Ba	 0.5430	 0.5440
Bb	 0.2580	 0.4540
Bc	 0.6290	 0.5630