



Full wwPDB EM Validation Report ⓘ

Aug 9, 2026 – 04:17 PM JST

PDB ID : 9VXM / pdb_00009vxm
EMDB ID : EMD-65433
Title : Human mitoribosome in a non-rotated state, with multiple neomycin molecules bound, featuring A/A-site and P/P-site tRNAs
Authors : Zhu, L.; Jia, C.; Wu, M.; Li, W.
Deposited on : 2025-07-19
Resolution : 2.90 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 : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

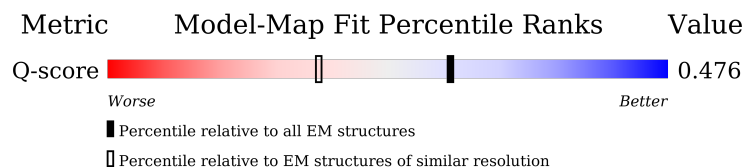
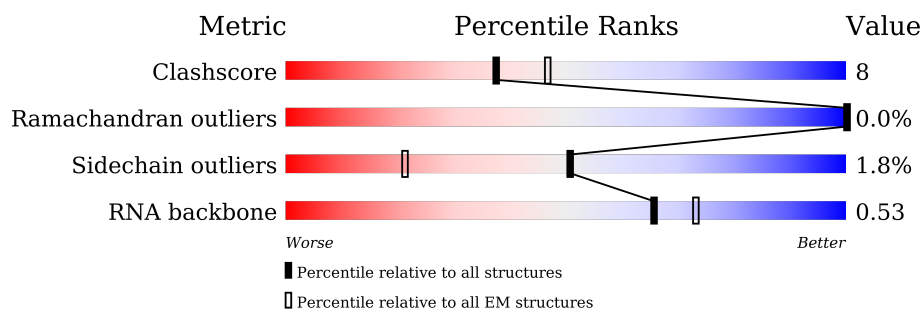
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 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	13054 (2.40 - 3.40)

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	0	188	
2	1	65	
3	2	92	

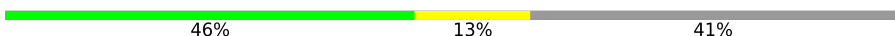
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	3	188	
5	4	103	
6	5	423	
7	6	380	
8	7	338	
9	8	206	
10	9	137	
11	A	1561	
12	D	305	
13	E	348	
14	F	311	
15	H	267	
16	I	261	
17	J	192	
18	k	178	
19	L	145	
20	M	296	
21	N	251	
22	O	175	
23	P	180	
24	Q	292	
25	R	149	
26	S	205	
27	T	206	
28	U	153	

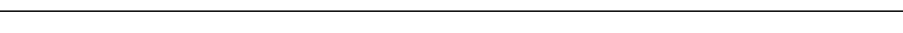
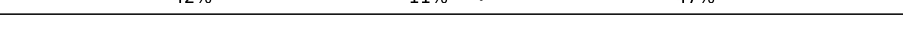
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	W	148	
30	X	256	
31	Y	250	
32	Z	161	
33	V	216	
34	b	215	
35	e	279	
36	g	166	
37	h	158	
38	i	128	
39	j	123	
40	n	112	
41	l	138	
42	m	128	
43	o	102	
44	q	222	
45	r	196	
46	AA	954	
47	AB	296	
48	AC	167	
49	AD	430	
50	AE	125	
51	AF	242	
52	AG	396	
53	AH	201	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
54	AI	194	
55	AJ	138	
56	AK	128	
57	AL	257	
58	AM	137	
59	AN	130	
60	AO	258	
61	AP	142	
62	C	87	
63	AR	360	
64	AS	190	
65	AT	173	
66	AU	205	
67	AV	414	
68	AW	187	
69	AX	398	
70	AY	395	
71	AZ	106	
72	A0	217	
73	A1	323	
74	G	118	
75	A3	199	
76	A4	689	
77	Az	32	
78	Aw	68	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
79	Ax	70	
80	B	72	
81	a	142	
82	c	332	
83	d	306	
84	f	212	
85	p	206	
86	s	439	

2 Entry composition

There are 98 unique types of molecules in this entry. The entry contains 176080 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 protein called Large ribosomal subunit protein bL32m.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	110	Total	C	N	O	S	0	0
			898	554	176	162	6		

- Molecule 2 is a protein called Large ribosomal subunit protein bL33m.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	56	Total	C	N	O	S	0	0
			464	296	89	77	2		

- Molecule 3 is a protein called Large ribosomal subunit protein bL34m.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	46	Total	C	N	O	S	0	0
			377	233	83	60	1		

- Molecule 4 is a protein called Large ribosomal subunit protein bL35m.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	95	Total	C	N	O	S	0	0
			832	539	162	128	3		

- Molecule 5 is a protein called Large ribosomal subunit protein bL36m.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	38	Total	C	N	O	S	0	0
			342	217	72	49	4		

- Molecule 6 is a protein called Large ribosomal subunit protein mL37.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	5	394	Total	C	N	O	S	0	0
			3210	2073	560	566	11		

- Molecule 7 is a protein called Large ribosomal subunit protein mL38.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	354	Total	C	N	O	S	0	0
			2948	1881	525	533	9		

- Molecule 8 is a protein called Large ribosomal subunit protein mL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7	294	Total	C	N	O	S	0	0
			2390	1529	405	438	18		

- Molecule 9 is a protein called Large ribosomal subunit protein mL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	8	157	Total	C	N	O	S	0	0
			1327	844	235	246	2		

- Molecule 10 is a protein called Large ribosomal subunit protein mL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	9	124	Total	C	N	O	S	0	0
			997	644	170	181	2		

- Molecule 11 is a RNA chain called 16S mitochondrial rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	A	1558	Total	C	N	O	P	0	0
			33070	14843	5963	10706	1558		

- Molecule 12 is a protein called Large ribosomal subunit protein uL2m.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	D	238	Total	C	N	O	S	0	0
			1859	1157	376	317	9		

- Molecule 13 is a protein called Large ribosomal subunit protein uL3m.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	E	305	Total	C	N	O	S	0	0
			2406	1545	418	432	11		

- Molecule 14 is a protein called Large ribosomal subunit protein uL4m.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	F	252	Total	C	N	O	S	0	0
			2031	1305	370	350	6		

- Molecule 15 is a protein called Large ribosomal subunit protein bL9m.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	H	202	Total	C	N	O	S	0	0
			1661	1067	304	286	4		

- Molecule 16 is a protein called Large ribosomal subunit protein uL10m.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	I	168	Total	C	N	O	S	0	0
			1351	870	245	226	10		

- Molecule 17 is a protein called Large ribosomal subunit protein uL11m.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	J	175	Total	C	N	O	S	0	0
			1330	847	237	244	2		

- Molecule 18 is a protein called Large ribosomal subunit protein uL13m.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	k	178	Total	C	N	O	S	0	0
			1455	936	259	253	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
k	1	ACE	-	acetylation	UNP Q9BYD1

- Molecule 19 is a protein called Large ribosomal subunit protein uL14m.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	L	115	Total	C	N	O	S	0	0
			890	559	171	155	5		

- Molecule 20 is a protein called Large ribosomal subunit protein uL15m.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	M	289	Total	C	N	O	S	0	0
			2314	1476	427	405	6		

- Molecule 21 is a protein called Large ribosomal subunit protein uL16m.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	N	222	Total	C	N	O	S	0	0
			1786	1143	326	307	10		

- Molecule 22 is a protein called Large ribosomal subunit protein bL17m.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	O	154	Total	C	N	O	S	0	0
			1259	792	241	219	7		

- Molecule 23 is a protein called Large ribosomal subunit protein uL18m.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	P	144	Total	C	N	O	S	0	0
			1173	733	224	211	5		

- Molecule 24 is a protein called Large ribosomal subunit protein bL19m.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Q	239	Total	C	N	O	S	0	0
			1990	1277	353	351	9		

- Molecule 25 is a protein called Large ribosomal subunit protein bL20m.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	R	140	Total	C	N	O	S	0	0
			1154	732	231	187	4		

- Molecule 26 is a protein called Large ribosomal subunit protein bL21m.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	S	161	Total	C	N	O	S	0	0
			1293	835	227	227	4		

- Molecule 27 is a protein called Large ribosomal subunit protein uL22m.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	T	166	Total	C	N	O	S	0	0
			1369	875	254	233	7		

- Molecule 28 is a protein called Large ribosomal subunit protein uL23m.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	U	153	Total	C	N	O	S	0	0
			1251	788	234	226	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	2	ACE	-	acetylation	UNP Q16540

- Molecule 29 is a protein called Large ribosomal subunit protein bL27m.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	W	116	Total	C	N	O	S	0	0
			904	577	171	153	3		

- Molecule 30 is a protein called Large ribosomal subunit protein bL28m.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	X	244	Total	C	N	O	S	0	0
			2044	1322	352	365	5		

- Molecule 31 is a protein called Large ribosomal subunit protein uL29m.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Y	181	Total	C	N	O	S	0	0
			1556	995	298	259	4		

- Molecule 32 is a protein called Large ribosomal subunit protein uL30m.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Z	122	Total	C	N	O	S	0	0
			996	636	186	171	3		

- Molecule 33 is a protein called Large ribosomal subunit protein uL24m.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	V	205	Total	C	N	O	S	0	0
			1676	1068	298	302	8		

- Molecule 34 is a protein called Large ribosomal subunit protein mL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	b	151	Total	C	N	O	S	0	0
			1196	744	231	218	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
b	2	ACE	-	acetylation	UNP Q8N983

- Molecule 35 is a protein called Large ribosomal subunit protein mL46.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	e	238	Total	C	N	O	S	0	0
			1931	1222	339	364	6		

- Molecule 36 is a protein called Large ribosomal subunit protein mL49.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	g	134	Total	C	N	O	S	0	0
			1113	719	193	199	2		

- Molecule 37 is a protein called Large ribosomal subunit protein mL50.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	h	110	Total	C	N	O	S	0	0
			895	568	156	168	3		

- Molecule 38 is a protein called Large ribosomal subunit protein mL51.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	i	97	Total	C	N	O	S	0	0
			828	532	165	127	4		

- Molecule 39 is a protein called Large ribosomal subunit protein mL52.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	j	94	Total	C	N	O	S	0	0
			745	463	144	136	2		

- Molecule 40 is a protein called Large ribosomal subunit protein mL53.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	n	102	Total	C	N	O	S	0	0
			774	479	148	142	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
n	2	ACE	-	acetylation	UNP Q96EL3

- Molecule 41 is a protein called Large ribosomal subunit protein mL54.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	l	82	Total	C	N	O	S	0	0
			688	437	120	128	3		

- Molecule 42 is a protein called Large ribosomal subunit protein mL55.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	m	92	Total	C	N	O	S	0	0
			791	488	159	142	2		

- Molecule 43 is a protein called Large ribosomal subunit protein mL63.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	o	94	Total	C	N	O	S	0	0
			798	501	165	129	3		

- Molecule 44 is a protein called Large ribosomal subunit protein mL64.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	q	128	Total	C	N	O	S	0	0
			1076	671	208	192	5		

- Molecule 45 is a protein called Large ribosomal subunit protein mL66.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	r	162	Total	C	N	O	S	0	0
			1322	839	252	223	8		

- Molecule 46 is a RNA chain called 12S mitochondrial rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	AA	954	Total	C	N	O	P	0	0
			20260	9088	3647	6571	954		

- Molecule 47 is a protein called Small ribosomal subunit protein uS2m.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	AB	224	Total	C	N	O	S	0	0
			1818	1158	328	322	10		

- Molecule 48 is a protein called Small ribosomal subunit protein uS3m.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	AC	132	Total	C	N	O	S	0	0
			1083	699	195	185	4		

- Molecule 49 is a protein called Small ribosomal subunit protein uS5m.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	AD	343	Total	C	N	O	S	0	0
			2731	1713	518	487	13		

- Molecule 50 is a protein called Small ribosomal subunit protein bS6m.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	AE	122	Total	C	N	O	S	0	0
			972	614	177	177	4		

- Molecule 51 is a protein called Small ribosomal subunit protein uS7m.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	AF	208	Total	C	N	O	S	0	0
			1725	1104	312	298	11		

- Molecule 52 is a protein called Small ribosomal subunit protein uS9m.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	AG	327	Total	C	N	O	S	0	0
			2688	1710	477	487	14		

- Molecule 53 is a protein called Small ribosomal subunit protein uS10m.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	AH	140	Total	C	N	O	S	0	0
			1152	745	194	210	3		

- Molecule 54 is a protein called Small ribosomal subunit protein uS11m.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	AI	137	Total	C	N	O	S	0	0
			1020	642	192	182	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AI	184	5F0	ASN	conflict	UNP P82912

- Molecule 55 is a protein called Small ribosomal subunit protein uS12m.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	AJ	108	Total	C	N	O	S	0	0
			839	521	169	143	6		

- Molecule 56 is a protein called Small ribosomal subunit protein uS14m.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	AK	101	Total	C	N	O	S	0	0
			862	537	179	141	5		

- Molecule 57 is a protein called Small ribosomal subunit protein uS15m.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	AL	174	Total	C	N	O	S	0	0
			1453	925	270	251	7		

- Molecule 58 is a protein called Small ribosomal subunit protein bS16m.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	AM	119	Total	C	N	O	S	0	0
			942	594	185	157	6		

- Molecule 59 is a protein called Small ribosomal subunit protein uS17m.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	AN	110	Total	C	N	O	S	0	0
			868	562	156	147	3		

- Molecule 60 is a protein called Small ribosomal subunit protein mS40.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	AO	193	Total	C	N	O	S	0	0
			1592	1014	294	277	7		

- Molecule 61 is a protein called Small ribosomal subunit protein bS18m.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	AP	97	Total	C	N	O	S	0	0
			781	501	134	138	8		

- Molecule 62 is a protein called Small ribosomal subunit protein bS21m.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	C	87	Total	C	N	O	S	0	0
			744	460	150	126	8		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	2	ACE	-	acetylation	UNP P82921
C	50	ARG	CYS	variant	UNP P82921

- Molecule 63 is a protein called Small ribosomal subunit protein mS22.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	AR	295	Total	C	N	O	S	0	0
			2409	1533	413	455	8		

- Molecule 64 is a protein called Small ribosomal subunit protein mS23.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	AS	135	Total	C	N	O	S	0	0
			1111	716	198	196	1		

- Molecule 65 is a protein called Small ribosomal subunit protein mS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	AT	168	Total	C	N	O	S	0	0
			1371	877	239	244	11		

- Molecule 66 is a protein called Small ribosomal subunit protein mS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	AU	176	Total	C	N	O	S	0	0
			1488	916	301	267	4		

- Molecule 67 is a protein called Small ribosomal subunit protein mS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	AV	362	Total	C	N	O	S	0	0
			2969	1904	495	558	12		

- Molecule 68 is a protein called Small ribosomal subunit protein bS1m.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	AW	100	Total	C	N	O	S	0	0
			789	498	141	146	4		

- Molecule 69 is a protein called Small ribosomal subunit protein mS29.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	AX	352	Total	C	N	O	S	0	0
			2849	1822	499	517	11		

- Molecule 70 is a protein called Small ribosomal subunit protein mS31.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	AY	149	Total	C	N	O	S	0	0
			1246	801	207	234	4		

- Molecule 71 is a protein called Small ribosomal subunit protein mS33.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	AZ	100	Total	C	N	O	S	0	0
			839	534	153	148	4		

- Molecule 72 is a protein called Small ribosomal subunit protein mS34.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	A0	215	Total	C	N	O	S	0	0
			1787	1130	339	313	5		

- Molecule 73 is a protein called Small ribosomal subunit protein mS35.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	A1	279	Total	C	N	O	S	0	0
			2265	1435	387	432	11		

- Molecule 74 is a protein called Small ribosomal subunit protein mS37.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	G	118	Total	C	N	O	S	0	0
			935	579	182	166	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	2	ACE	-	acetylation	UNP Q96BP2

- Molecule 75 is a protein called Small ribosomal subunit protein mS38.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	A3	70	Total	C	N	O	S	0	0
			625	401	134	89	1		

- Molecule 76 is a protein called Small ribosomal subunit protein mS39.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	A4	588	Total	C	N	O	S	0	0
			4768	3053	808	879	28		

- Molecule 77 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	Az	16	Total	C	N	O	P	0	0
			339	152	56	115	16		

- Molecule 78 is a RNA chain called A/A-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	Aw	68	Total	C	N	O	P	0	0
			1434	646	248	472	68		

- Molecule 79 is a RNA chain called P/P-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	Ax	70	Total	C	N	O	P	0	0
			1482	665	260	487	70		

- Molecule 80 is a RNA chain called mitochondrial tRNA^{Val}.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	B	72	Total	C	N	O	P	0	0
			1524	685	269	498	72		

- Molecule 81 is a protein called Large ribosomal subunit protein mL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	a	100	Total	C	N	O	S	0	0
			840	529	152	154	5		

- Molecule 82 is a protein called Large ribosomal subunit protein mL44.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	c	286	Total	C	N	O	S	0	0
			2299	1470	397	423	9		

- Molecule 83 is a protein called Large ribosomal subunit protein mL45.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	d	241	Total	C	N	O	S	0	0
			1985	1273	340	359	13		

- Molecule 84 is a protein called Large ribosomal subunit protein mL48.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	f	157	Total	C	N	O	S	0	0
			1252	799	207	242	4		

- Molecule 85 is a protein called Large ribosomal subunit protein mL62.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	p	147	Total	C	N	O	S	0	0
			1205	748	228	225	4		

- Molecule 86 is a protein called Large ribosomal subunit protein mL65.

Mol	Chain	Residues	Atoms					AltConf	Trace
86	s	386	Total	C	N	O	S	0	0
			3155	2023	559	559	14		

- Molecule 87 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
87	0	1	Total	Zn	0
			1	1	
87	4	1	Total	Zn	0
			1	1	
87	AO	1	Total	Zn	0
			1	1	

- Molecule 88 is POTASSIUM ION (CCD ID: K) (formula: K).

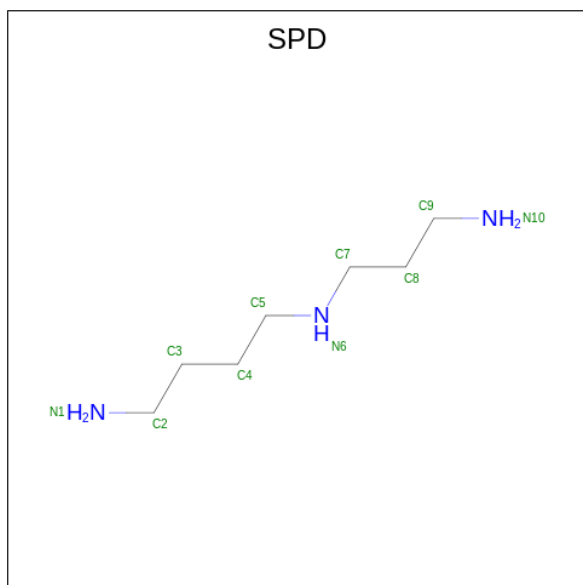
Mol	Chain	Residues	Atoms		AltConf
88	3	1	Total	K	0
			1	1	
88	6	1	Total	K	0
			1	1	
88	A	28	Total	K	0
			28	28	
88	D	1	Total	K	0
			1	1	
88	M	1	Total	K	0
			1	1	
88	N	1	Total	K	0
			1	1	
88	W	1	Total	K	0
			1	1	

Continued on next page...

Continued from previous page...

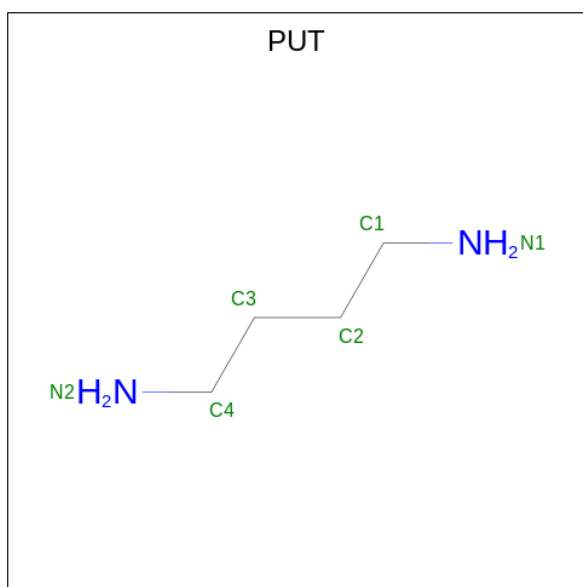
Mol	Chain	Residues	Atoms	AltConf
88	i	1	Total K 1 1	0
88	o	1	Total K 1 1	0
88	AA	17	Total K 17 17	0

- Molecule 89 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$).



Mol	Chain	Residues	Atoms	AltConf
89	A	1	Total C N 10 7 3	0
89	A	1	Total C N 10 7 3	0
89	A	1	Total C N 10 7 3	0
89	AA	1	Total C N 10 7 3	0

- Molecule 90 is 1,4-DIAMINOBUTANE (CCD ID: PUT) (formula: $C_4H_{12}N_2$).

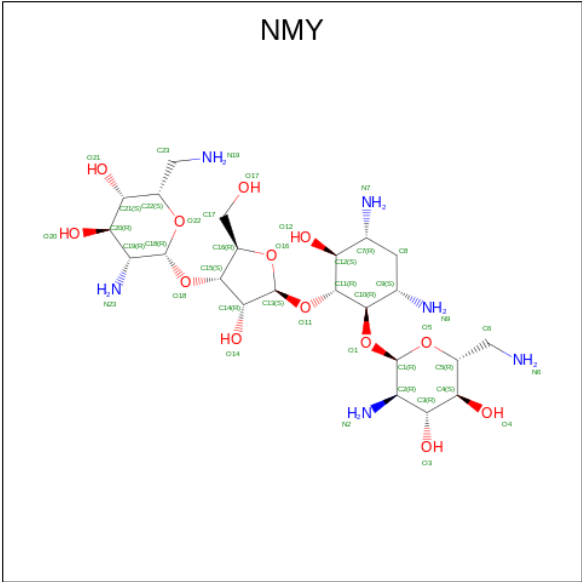


Mol	Chain	Residues	Atoms			AltConf
90	A	1	Total	C	N	0
			6	4	2	

- Molecule 91 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

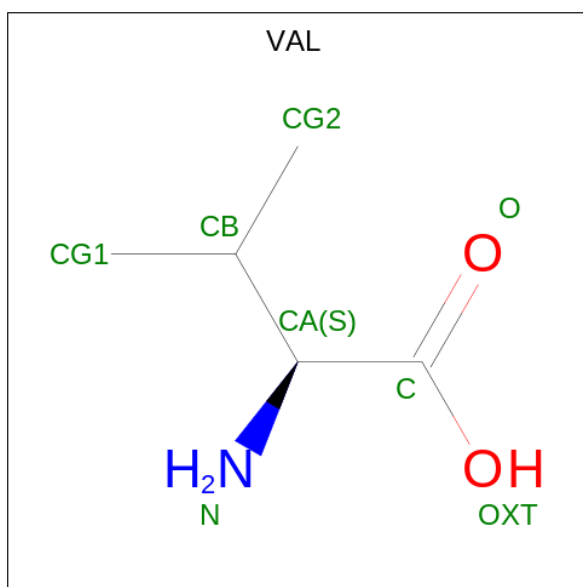
Mol	Chain	Residues	Atoms		AltConf
91	A	138	Total	Mg	0
			138	138	
91	D	2	Total	Mg	0
			2	2	
91	g	1	Total	Mg	0
			1	1	
91	o	1	Total	Mg	0
			1	1	
91	AA	62	Total	Mg	0
			62	62	
91	AB	1	Total	Mg	0
			1	1	
91	AX	1	Total	Mg	0
			1	1	
91	A3	1	Total	Mg	0
			1	1	
91	Az	1	Total	Mg	0
			1	1	

- Molecule 92 is NEOMYCIN (CCD ID: NMY) (formula: C₂₃H₄₆N₆O₁₃) (labeled as "Ligand of Interest" by depositor).



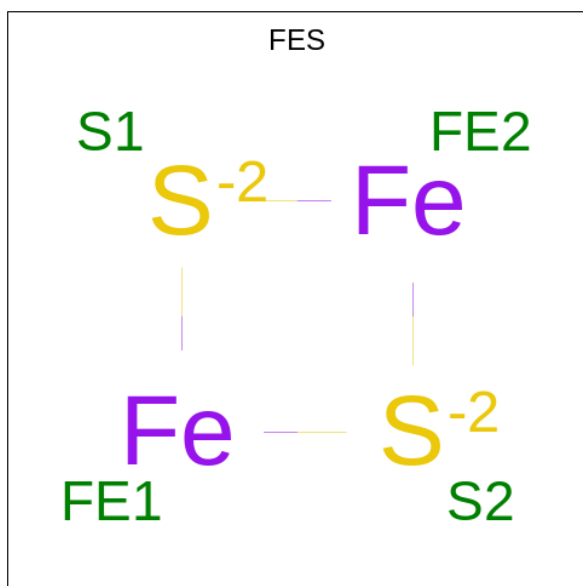
Mol	Chain	Residues	Atoms				AltConf
92	A	1	Total	C	N	O	0
			42	23	6	13	
92	A	1	Total	C	N	O	0
			42	23	6	13	
92	A	1	Total	C	N	O	0
			42	23	6	13	
92	A	1	Total	C	N	O	0
			42	23	6	13	
92	AA	1	Total	C	N	O	0
			42	23	6	13	
92	AA	1	Total	C	N	O	0
			42	23	6	13	
92	AA	1	Total	C	N	O	0
			42	23	6	13	

- Molecule 93 is VALINE (CCD ID: VAL) (formula: C₅H₁₁NO₂).



Mol	Chain	Residues	Atoms				AltConf
93	e	1	Total	C	N	O	0
			7	5	1	1	

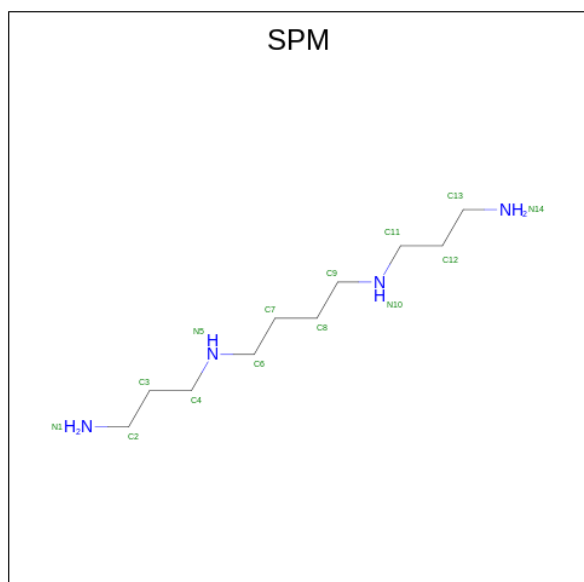
- Molecule 94 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			AltConf
94	r	1	Total	Fe	S	0
			4	2	2	
94	AP	1	Total	Fe	S	0
			4	2	2	
94	AT	1	Total	Fe	S	0
			4	2	2	

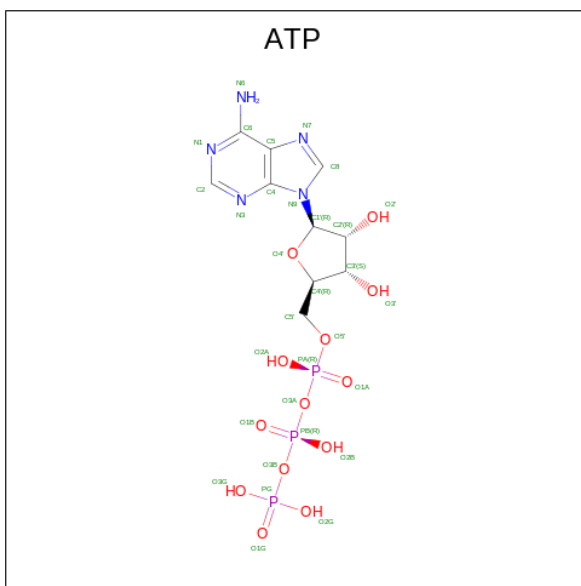
- # NAD

- Molecule 96 is SPERMINE (CCD ID: SPM) (formula: $\text{C}_{10}\text{H}_{26}\text{N}_4$).



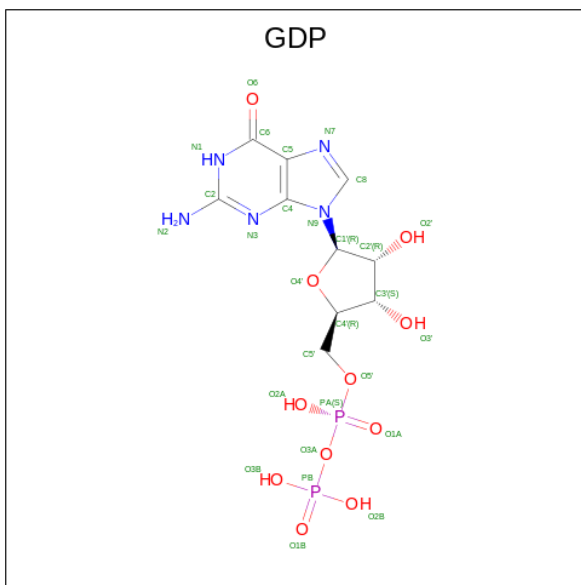
WORLDWIDE
 **PDB**
PROTEIN DATA BANK

- Molecule 97 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
97	AX	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 98 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).

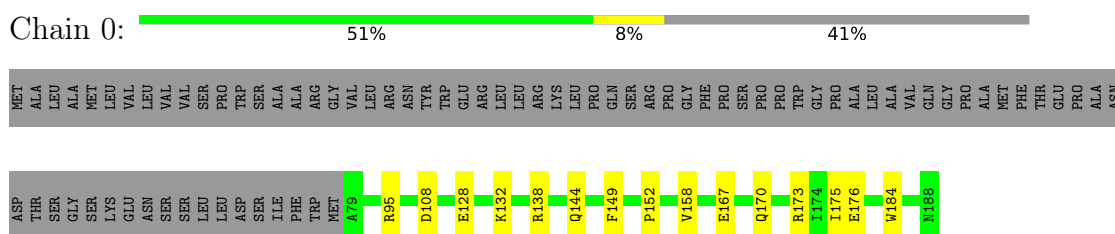


Mol	Chain	Residues	Atoms					AltConf
98	AX	1	Total	C	N	O	P	0
			28	10	5	11	2	

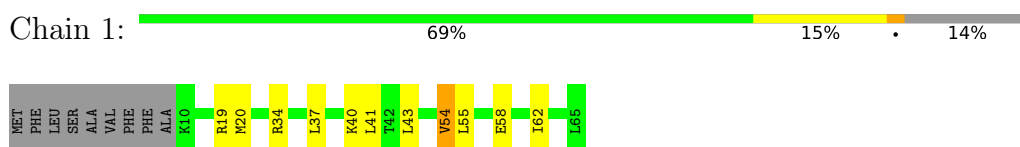
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and 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.

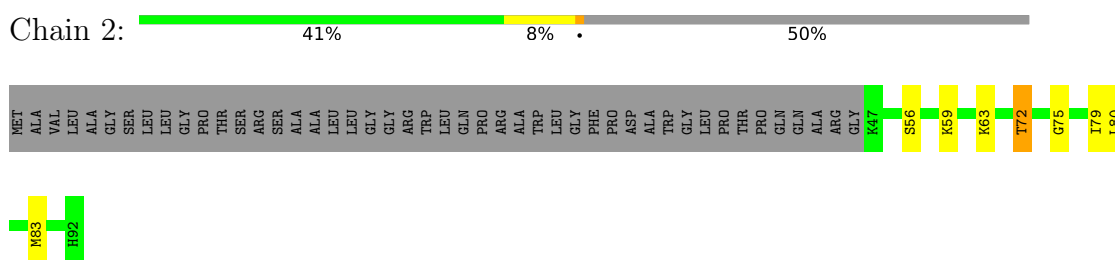
- Molecule 1: Large ribosomal subunit protein bL32m



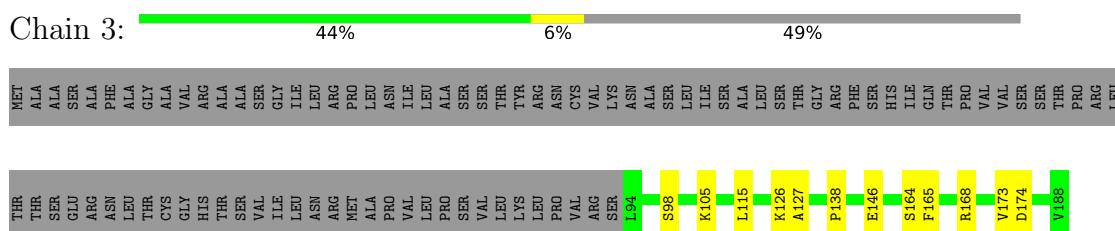
- Molecule 2: Large ribosomal subunit protein bL33m



- Molecule 3: Large ribosomal subunit protein bL34m



- Molecule 4: Large ribosomal subunit protein bL35m



- Molecule 5: Large ribosomal subunit protein bL36m

Chain 4:  35% 63%



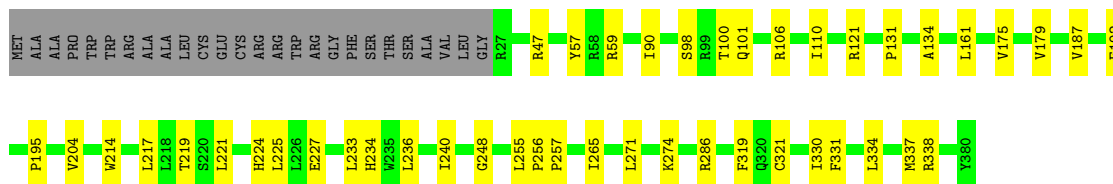
- Molecule 6: Large ribosomal subunit protein mL37

Chain 5:  80% 13% 7%



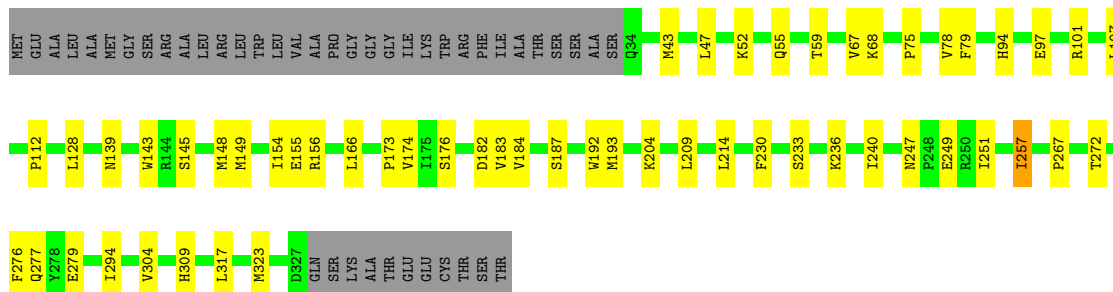
- Molecule 7: Large ribosomal subunit protein mL38

Chain 6:  81% 12% 7%



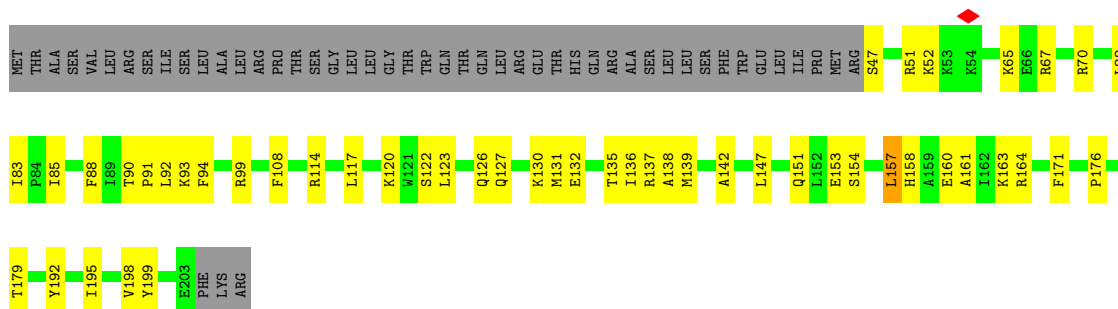
- Molecule 8: Large ribosomal subunit protein mL39

Chain 7:  71% 16% 13%

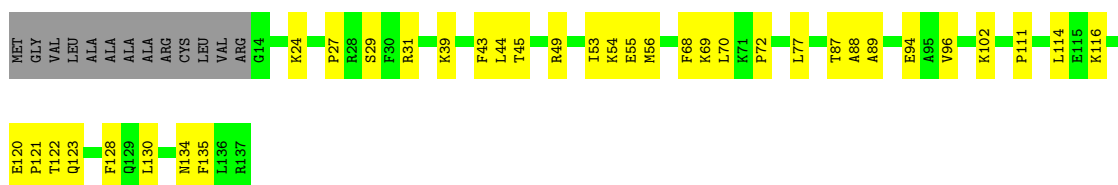


- Molecule 9: Large ribosomal subunit protein mL40

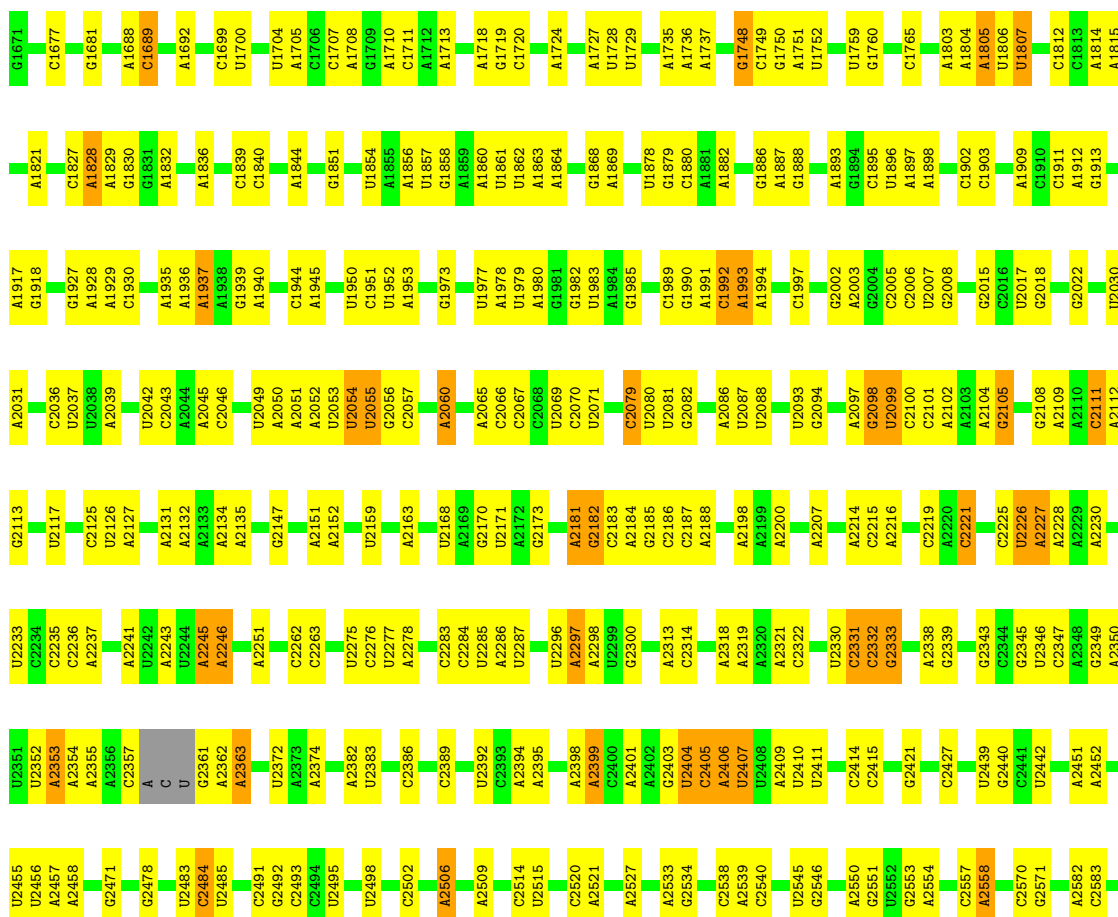
Chain 8:  52% 24% 24%

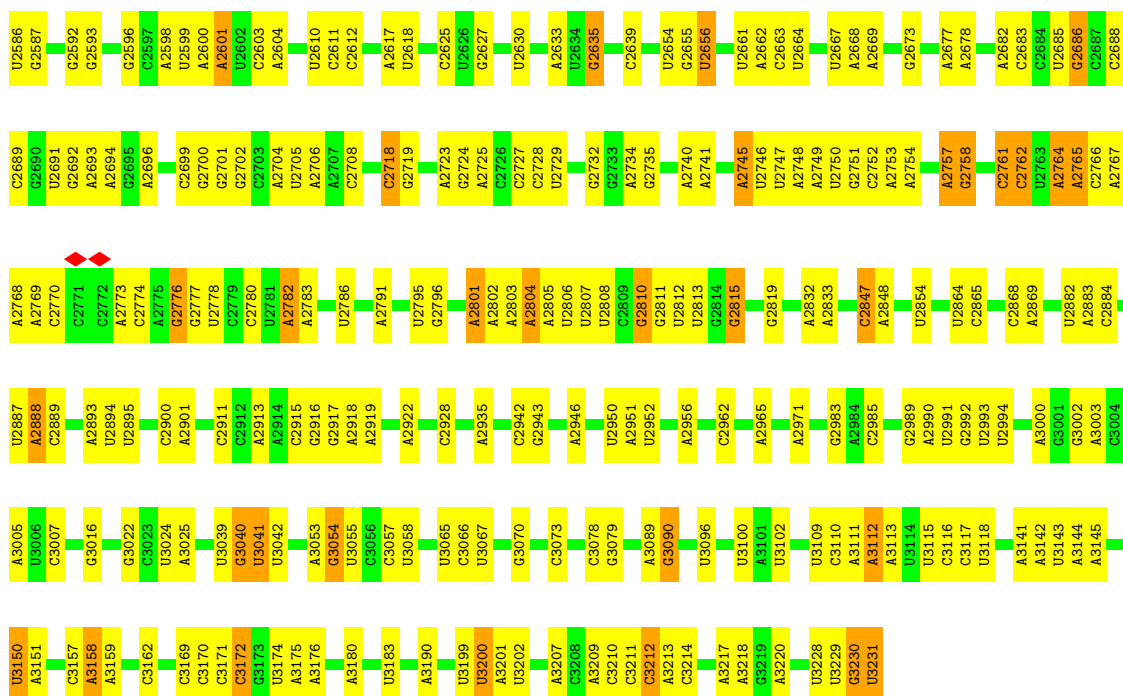


- Molecule 10: Large ribosomal subunit protein mL41



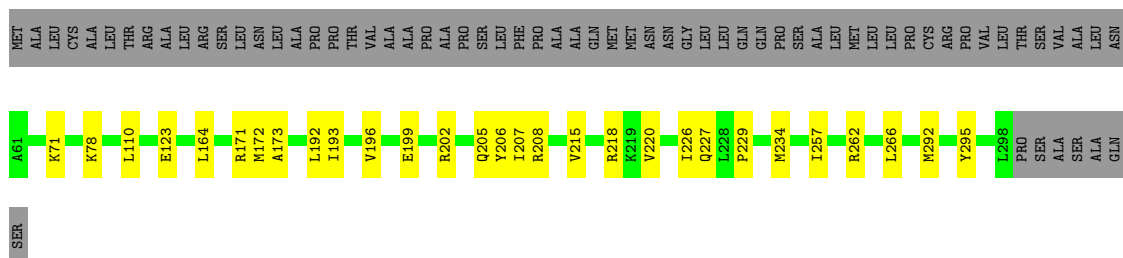
- Molecule 11: 16S mitochondrial rRNA





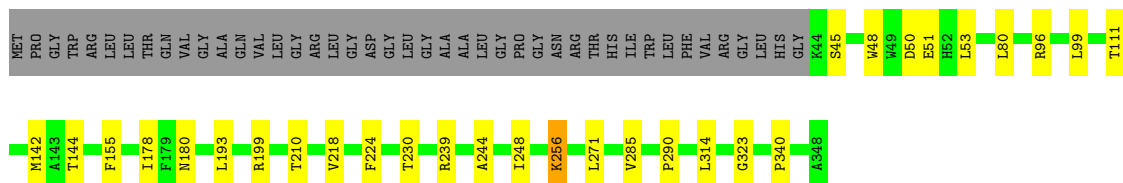
• Molecule 12: Large ribosomal subunit protein uL2m

Chain D: 69% 10% 22%



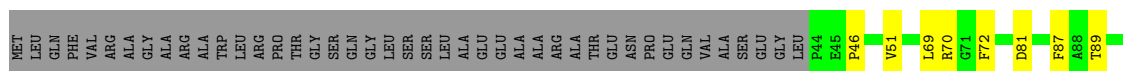
• Molecule 13: Large ribosomal subunit protein uL3m

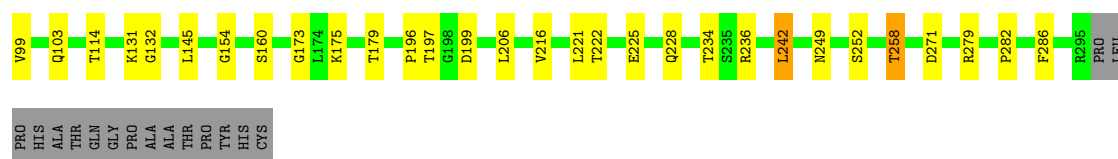
Chain E: 79% 8% 12%



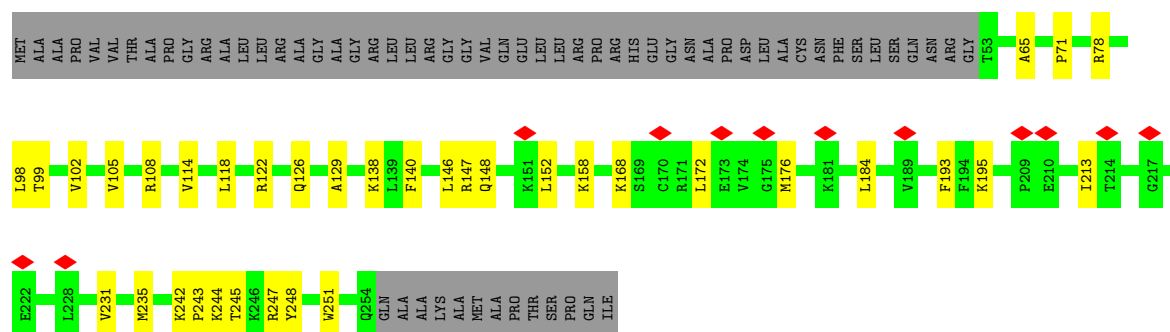
• Molecule 14: Large ribosomal subunit protein uL4m

Chain F: 69% 12% 19%

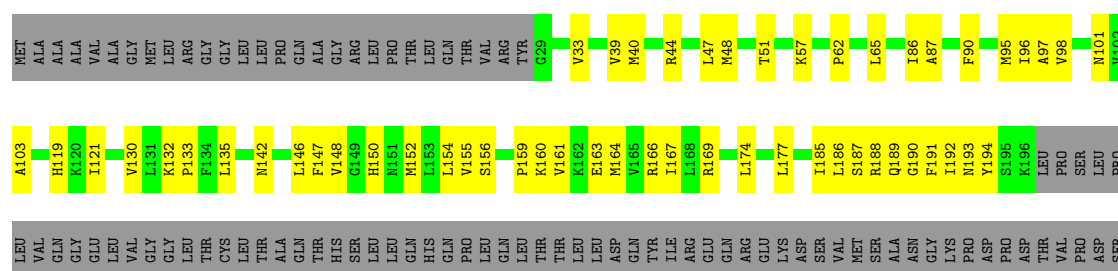




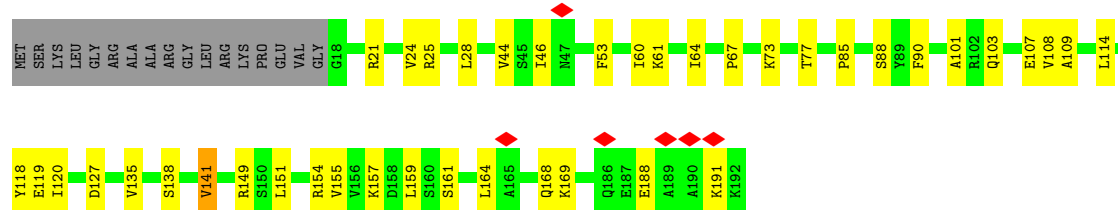
- Molecule 15: Large ribosomal subunit protein bL9m



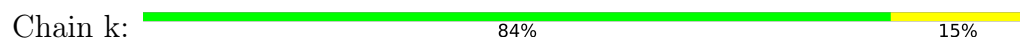
- Molecule 16: Large ribosomal subunit protein uL10m



- Molecule 17: Large ribosomal subunit protein uL11m

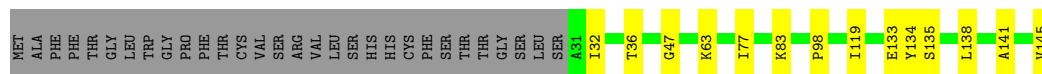


- Molecule 18: Large ribosomal subunit protein uL13m



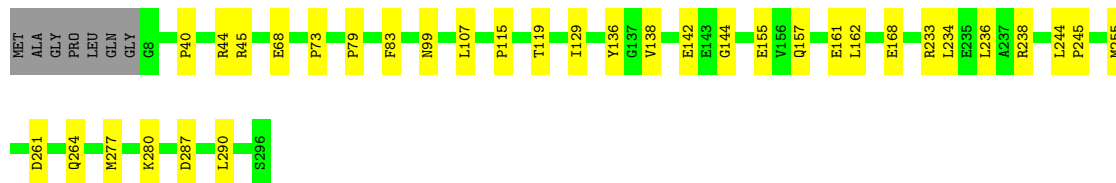
- Molecule 19: Large ribosomal subunit protein uL14m

Chain L:  70% 10% 21%



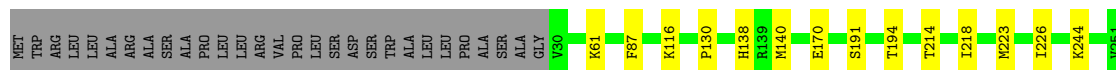
- Molecule 20: Large ribosomal subunit protein uL15m

Chain M:  86% 11%



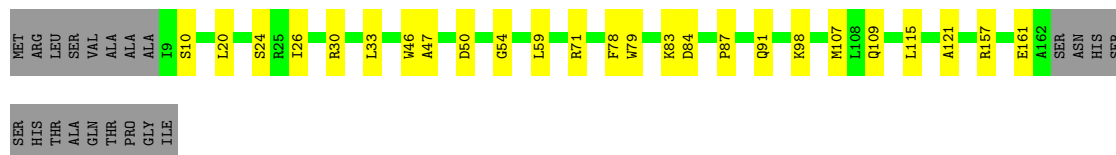
- Molecule 21: Large ribosomal subunit protein uL16m

Chain N:  83% 6% 12%



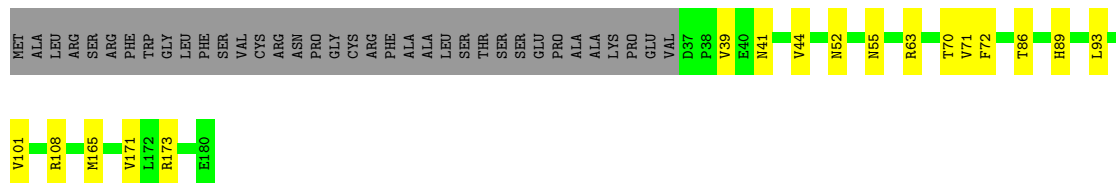
- Molecule 22: Large ribosomal subunit protein bL17m

Chain O:  74% 14% 12%



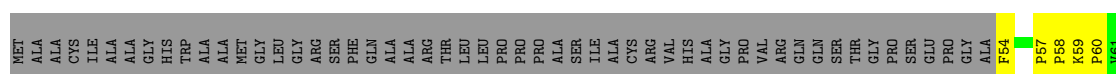
- Molecule 23: Large ribosomal subunit protein uL18m

Chain P:  71% 9% 20%



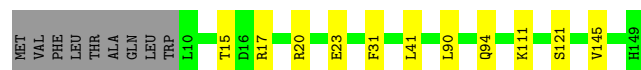
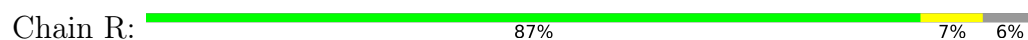
- Molecule 24: Large ribosomal subunit protein bL19m

Chain Q:  70% 12% 18%

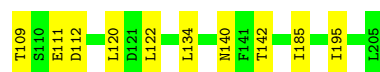
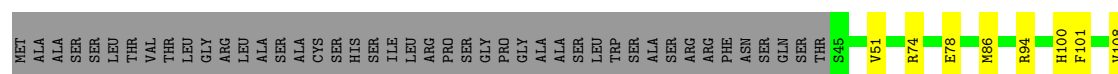




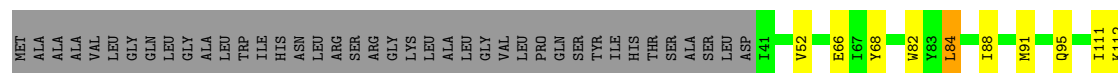
- Molecule 25: Large ribosomal subunit protein bL20m



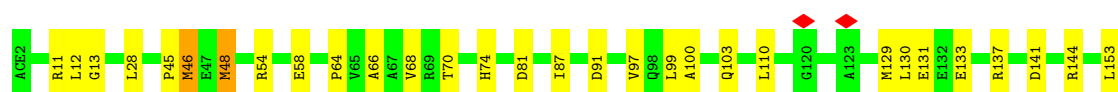
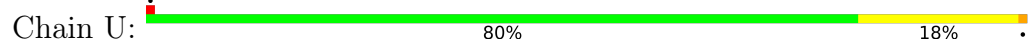
- Molecule 26: Large ribosomal subunit protein bL21m



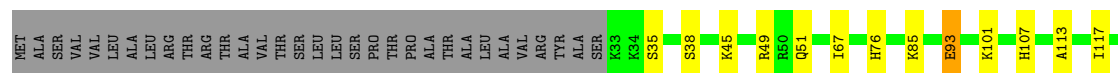
- Molecule 27: Large ribosomal subunit protein uL22m



- Molecule 28: Large ribosomal subunit protein uL23m

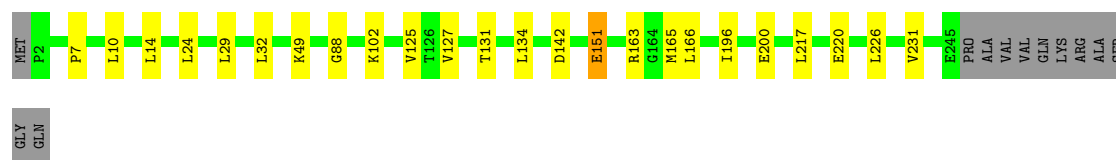


- Molecule 29: Large ribosomal subunit protein bL27m



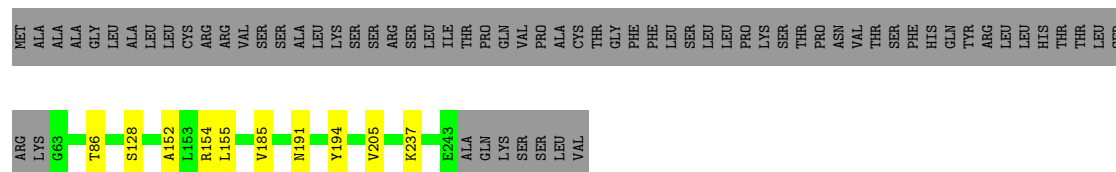
- Molecule 30: Large ribosomal subunit protein bL28m

Chain X: 



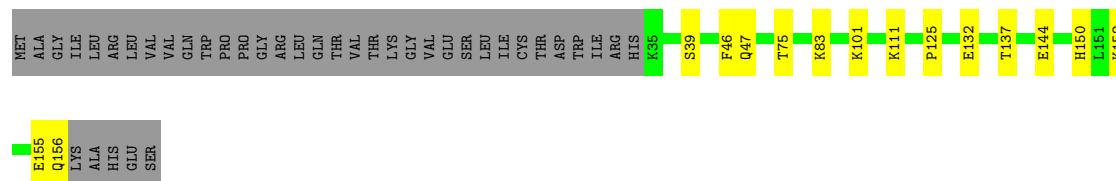
- Molecule 31: Large ribosomal subunit protein uL29m

Chain Y: 



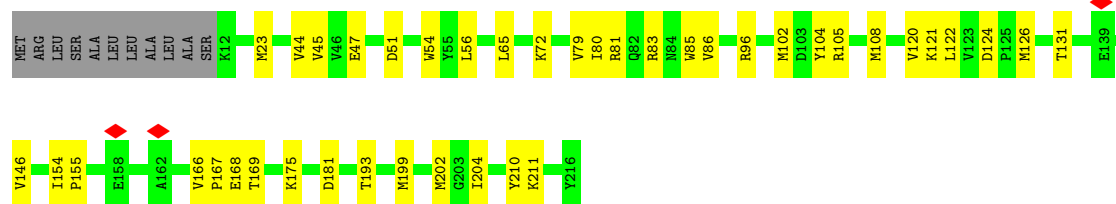
- Molecule 32: Large ribosomal subunit protein uL30m

Chain Z: 



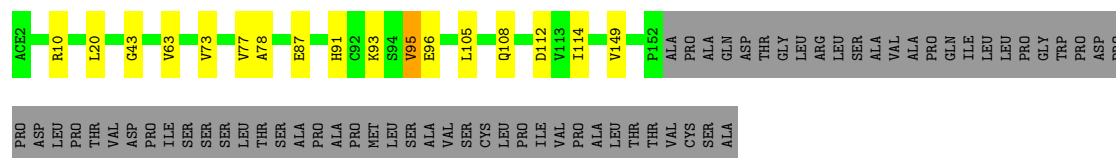
- Molecule 33: Large ribosomal subunit protein uL24m

Chain V: 



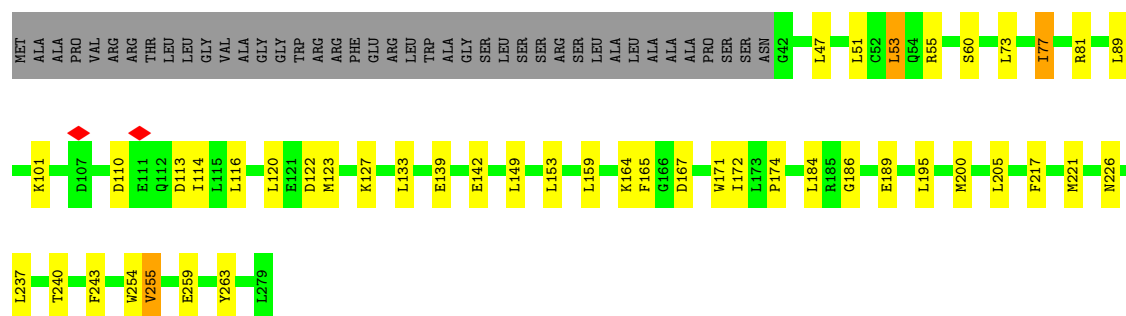
- Molecule 34: Large ribosomal subunit protein mL43

Chain b: 



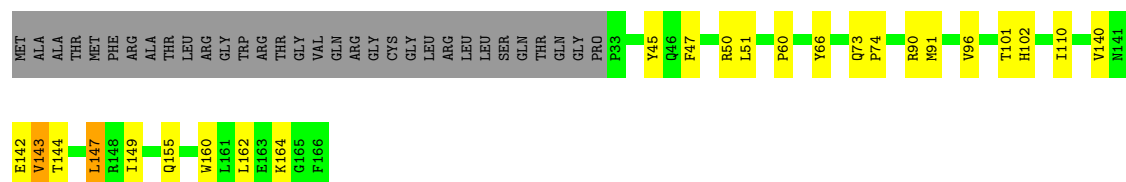
- Molecule 35: Large ribosomal subunit protein mL46

Chain e:  69% 15% 15%



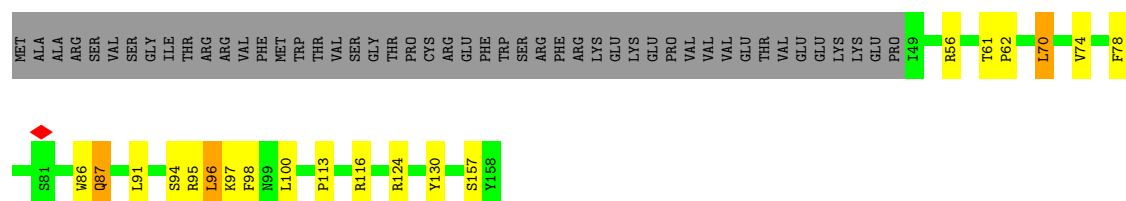
- Molecule 36: Large ribosomal subunit protein mL49

Chain g:  66% 13% 19%



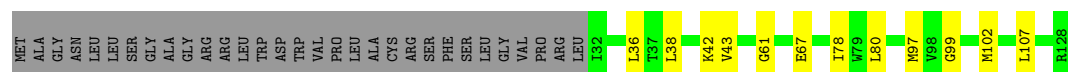
- Molecule 37: Large ribosomal subunit protein mL50

Chain h:  57% 11% 30%



- Molecule 38: Large ribosomal subunit protein mL51

Chain i:  66% 9% 24%



- Molecule 39: Large ribosomal subunit protein mL52

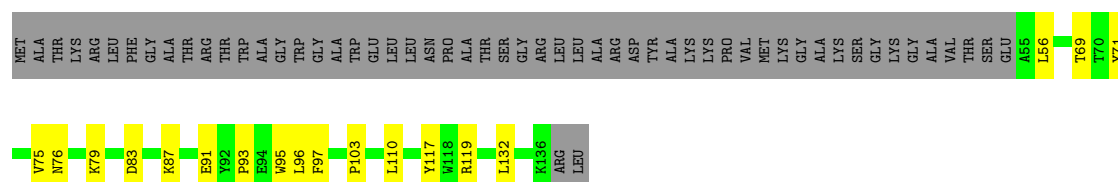
Chain j:  65% 11% 24%



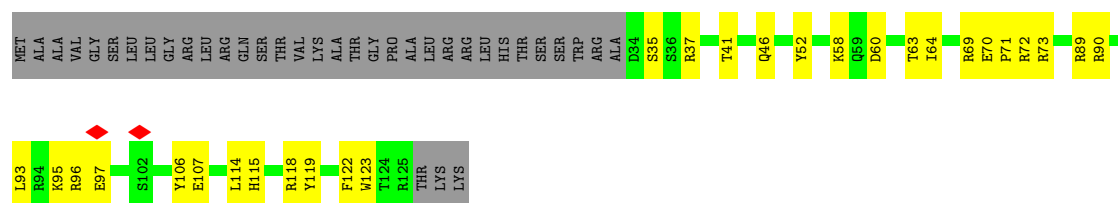
- Molecule 40: Large ribosomal subunit protein mL53



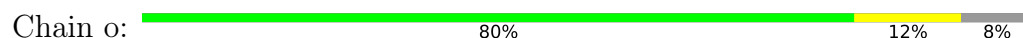
- Molecule 41: Large ribosomal subunit protein mL54



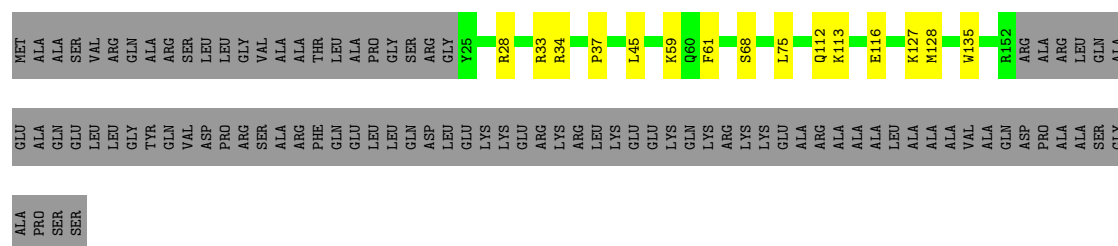
- Molecule 42: Large ribosomal subunit protein mL55



- Molecule 43: Large ribosomal subunit protein mL63

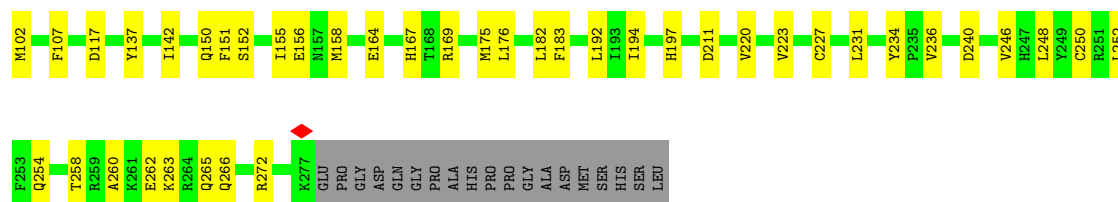


- Molecule 44: Large ribosomal subunit protein mL64

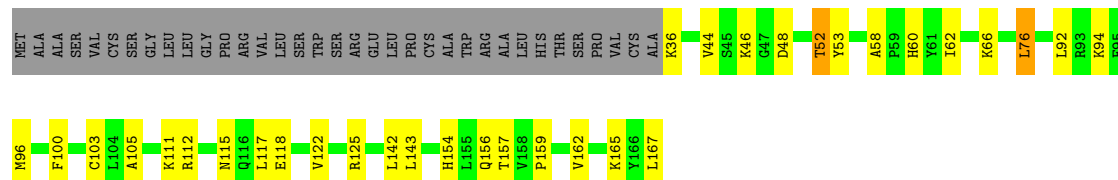


- Molecule 45: Large ribosomal subunit protein mL66

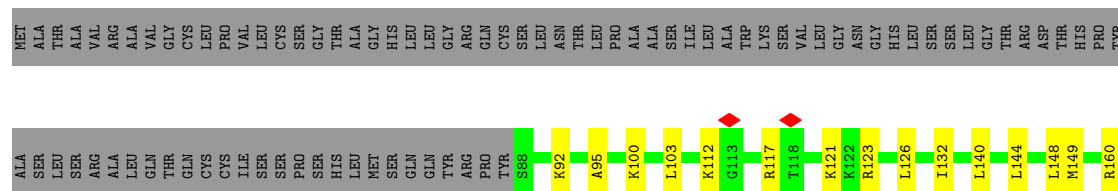




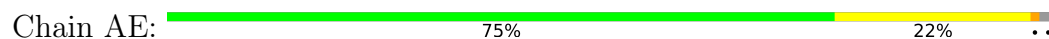
- Molecule 48: Small ribosomal subunit protein uS3m



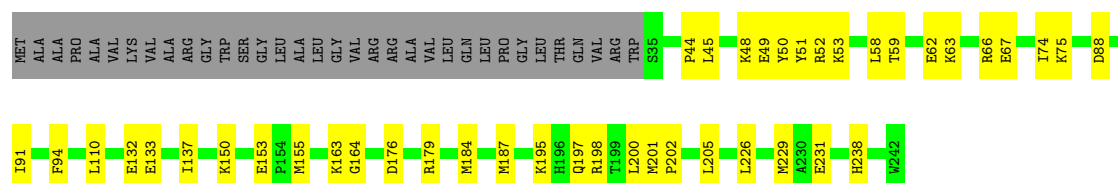
- Molecule 49: Small ribosomal subunit protein uS5m



- Molecule 50: Small ribosomal subunit protein bS6m

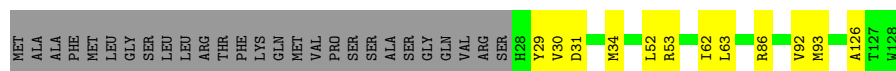


- Molecule 51: Small ribosomal subunit protein uS7m



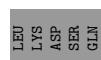
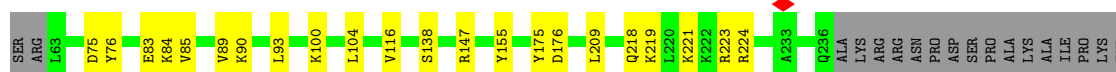
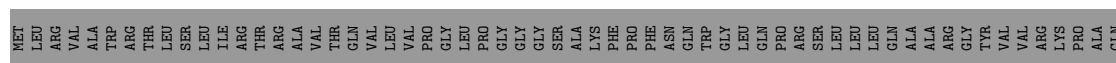
- Molecule 56: Small ribosomal subunit protein uS14m

Chain AK:  70% 9% 21%



- Molecule 57: Small ribosomal subunit protein uS15m

Chain AL:  59% 9% 32%



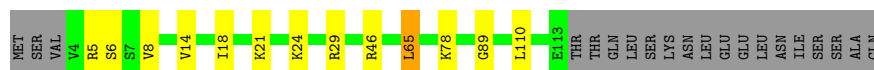
- Molecule 58: Small ribosomal subunit protein bS16m

Chain AM:  71% 16% 13%



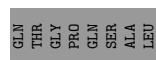
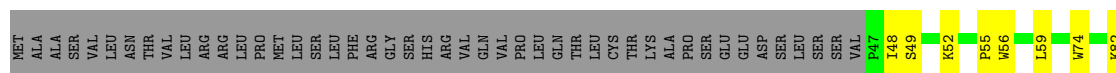
- Molecule 59: Small ribosomal subunit protein uS17m

Chain AN:  75% 9% 15%



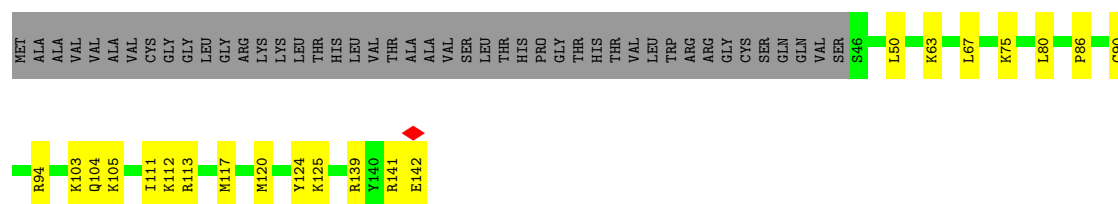
- Molecule 60: Small ribosomal subunit protein mS40

Chain AO:  62% 13% 25%



- Molecule 61: Small ribosomal subunit protein bS18m

Chain AP: 



- Molecule 62: Small ribosomal subunit protein bS21m

Chain C: 



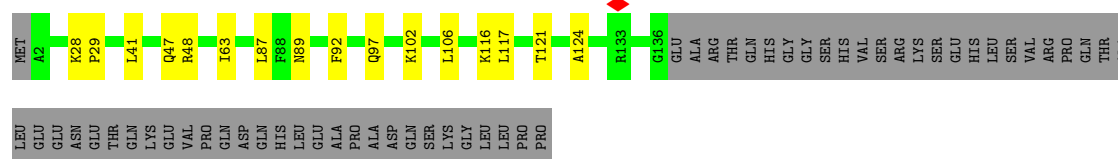
- Molecule 63: Small ribosomal subunit protein mS22

Chain AR: 



- Molecule 64: Small ribosomal subunit protein mS23

Chain AS: 



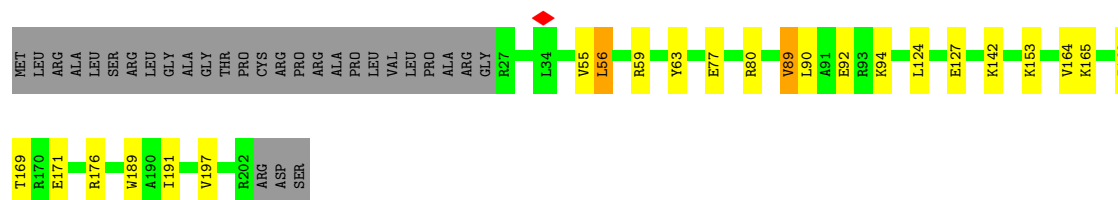
- Molecule 65: Small ribosomal subunit protein mS25

Chain AT: 



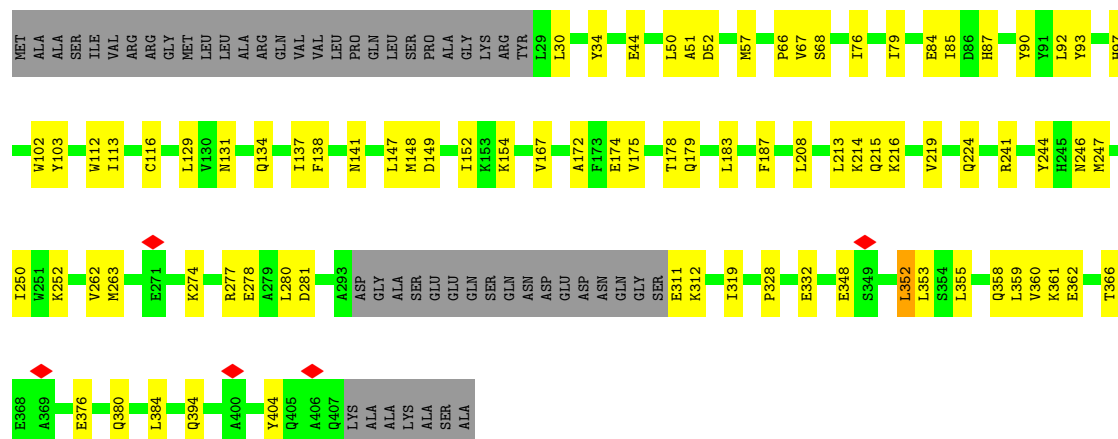
- Molecule 66: Small ribosomal subunit protein mS26

Chain AU: 



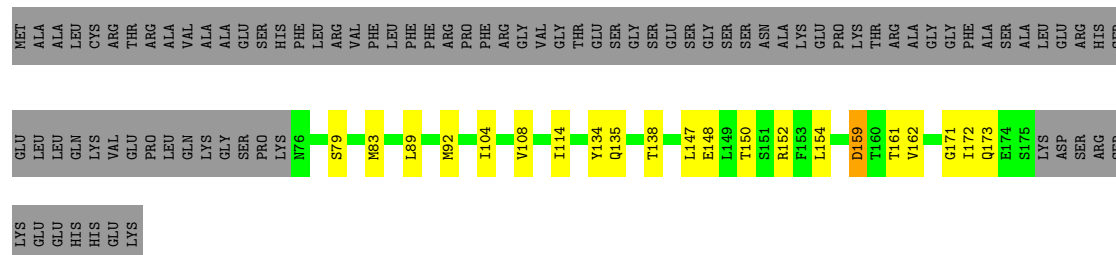
- Molecule 67: Small ribosomal subunit protein mS27

Chain AV: 67% 20% 13%



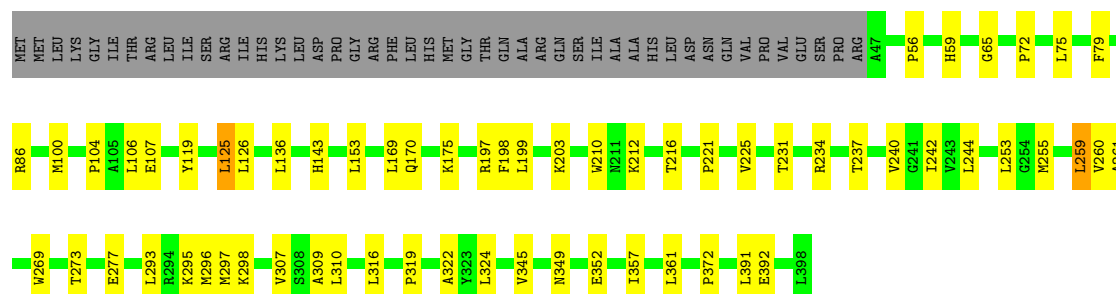
- Molecule 68: Small ribosomal subunit protein bS1m

Chain AW: 42% 11% 47%

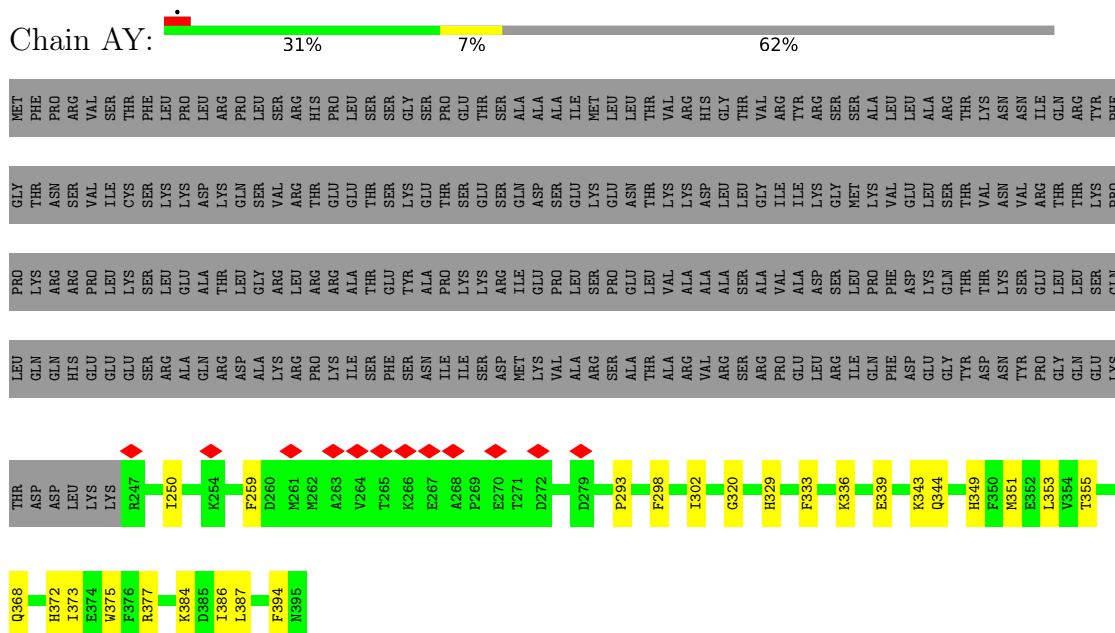


- Molecule 69: Small ribosomal subunit protein mS29

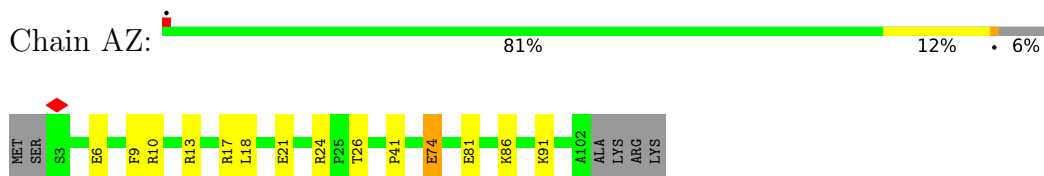
Chain AX: 73% 15% 12%



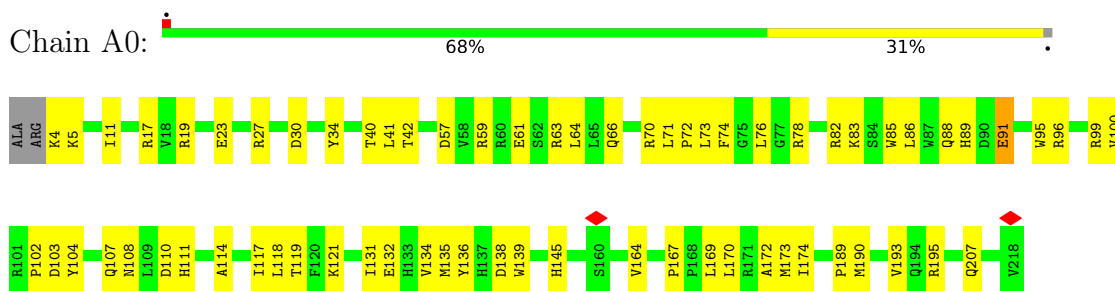
- Molecule 70: Small ribosomal subunit protein mS31



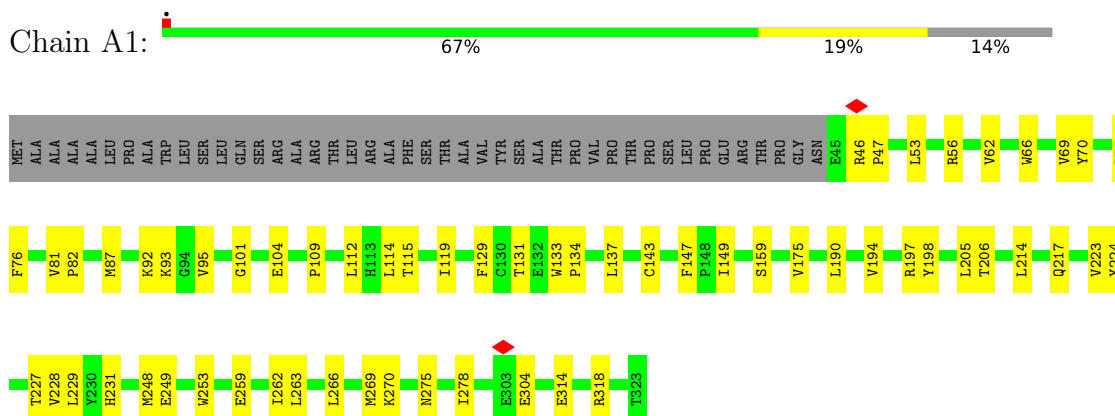
- Molecule 71: Small ribosomal subunit protein mS33



- Molecule 72: Small ribosomal subunit protein mS34



- Molecule 73: Small ribosomal subunit protein mS35



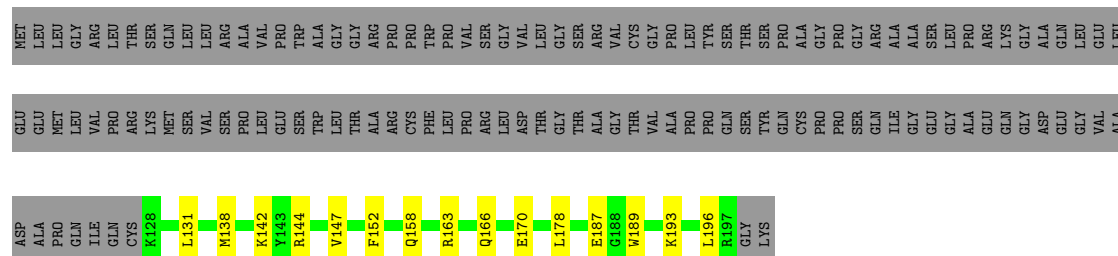
- Molecule 74: Small ribosomal subunit protein mS37

Chain G:  83% 16%



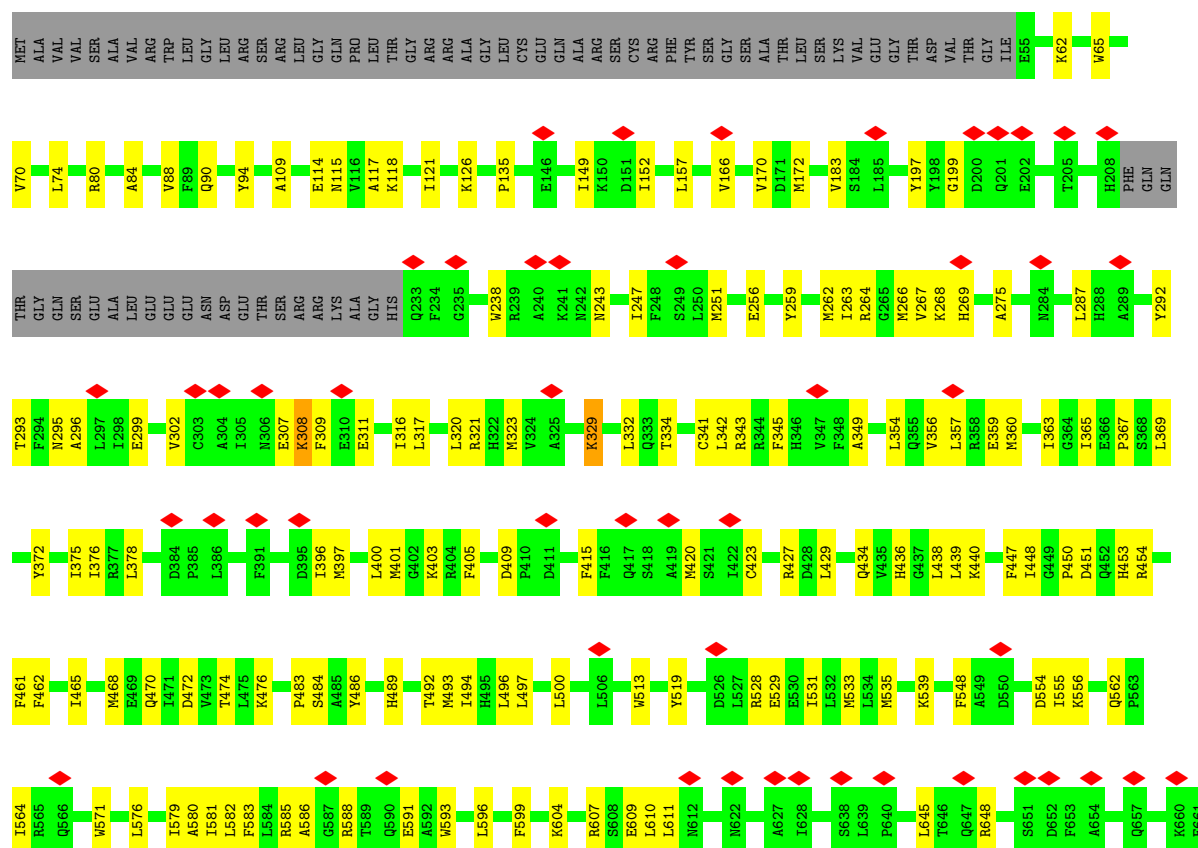
- Molecule 75: Small ribosomal subunit protein mS38

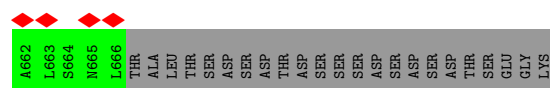
Chain A3:  28% 8% 65%



- Molecule 76: Small ribosomal subunit protein mS39

Chain A4:  8% 63% 22% 15%





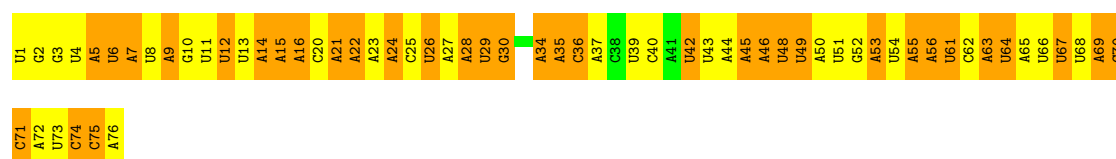
- Molecule 77: mRNA

Chain Az: 38% 9% 50%



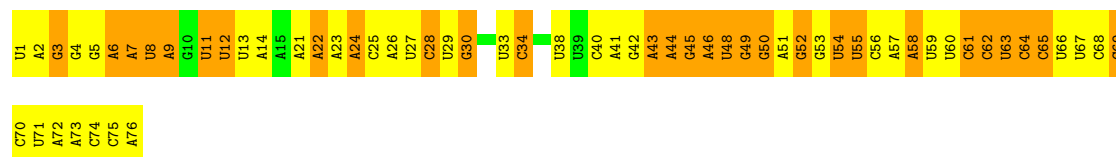
- Molecule 78: A/A-tRNA

Chain Aw: 7% 41% 51%



- Molecule 79: P/P-tRNA

Chain Ax: 11% 47% 41%



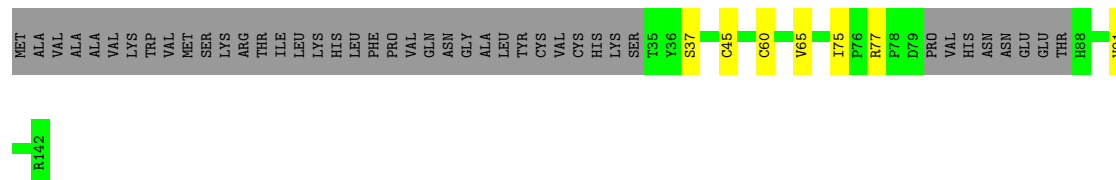
- Molecule 80: mitochondrial tRNAVal

Chain B: 53% 38% 10%



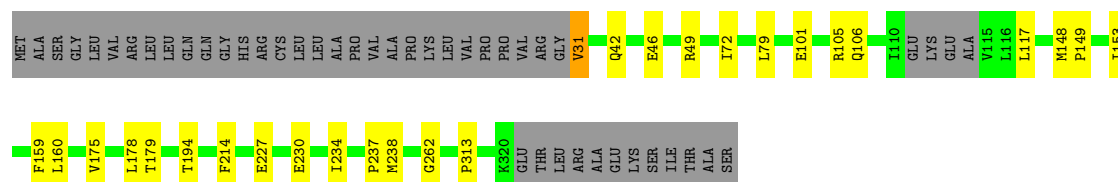
- Molecule 81: Large ribosomal subunit protein mL42

Chain a: 65% 5% 30%



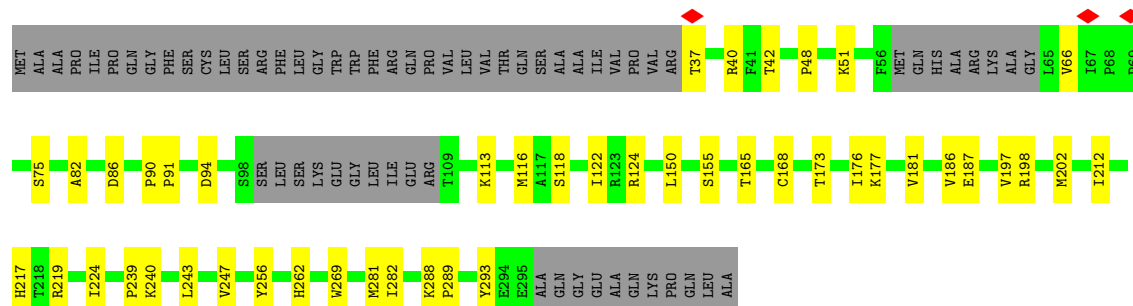
- Molecule 82: Large ribosomal subunit protein mL44

Chain c: 78% 8% 14%



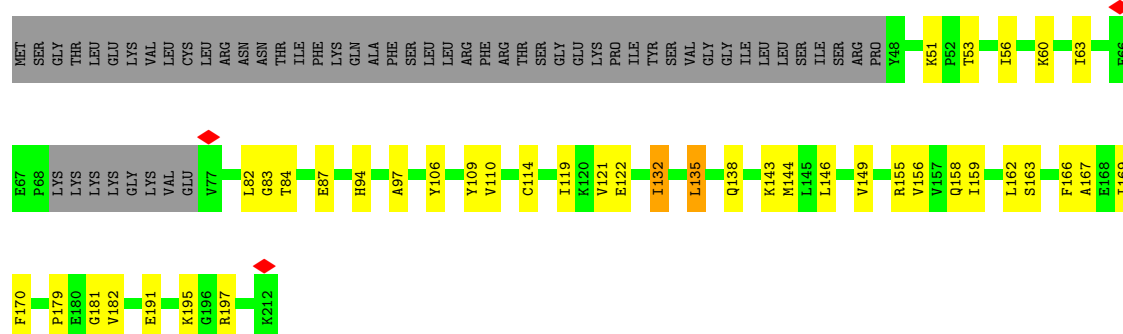
- Molecule 83: Large ribosomal subunit protein mL45

Chain d: 64% 15% 21%



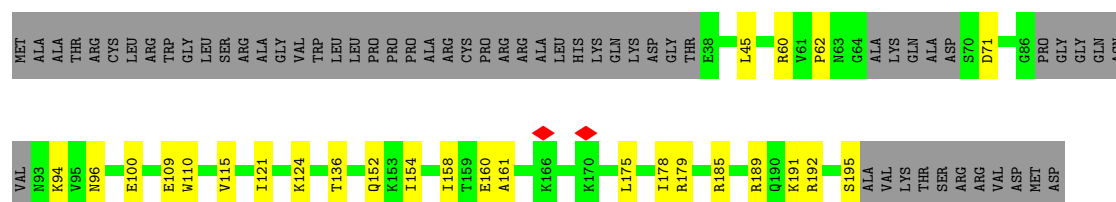
- Molecule 84: Large ribosomal subunit protein mL48

Chain f: 55% 18% 26%



- Molecule 85: Large ribosomal subunit protein mL62

Chain p: 59% 13% 29%



- Molecule 86: Large ribosomal subunit protein mL65

Chain s: 79% 9% 12%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	47726	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	3.946	Depositor
Minimum map value	-2.515	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.130	Depositor
Recommended contour level	0.1	Depositor
Map size ($\text{\AA}$)	552.16, 552.16, 552.16	wwPDB
Map dimensions	680, 680, 680	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.812, 0.812, 0.812	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SPM, 5F0, K, 5MU, PSU, PUT, SPD, NAD, ZN, B8T, 5MC, MA6, 2MG, OMG, MG, OMU, NMY, FES, ATP, 1MA, ACE, GDP

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	0	0.15	0/913	0.32	0/1224
2	1	0.13	0/469	0.32	0/621
3	2	0.14	0/383	0.22	0/507
4	3	0.15	0/853	0.25	0/1136
5	4	0.15	0/350	0.25	0/461
6	5	0.14	0/3305	0.26	0/4502
7	6	0.14	0/3043	0.31	0/4140
8	7	0.14	0/2447	0.32	0/3310
9	8	0.13	0/1354	0.36	0/1819
10	9	0.13	0/1025	0.30	0/1379
11	A	0.16	0/36876	0.26	0/57402
12	D	0.14	0/1896	0.25	0/2549
13	E	0.14	0/2475	0.27	0/3355
14	F	0.15	0/2090	0.29	0/2842
15	H	0.11	0/1698	0.26	0/2292
16	I	0.14	0/1381	0.35	0/1865
17	J	0.12	0/1348	0.32	0/1813
18	k	0.17	0/1497	0.35	0/2031
19	L	0.15	0/905	0.34	0/1218
20	M	0.15	0/2368	0.28	0/3195
21	N	0.15	0/1833	0.31	0/2468
22	O	0.16	0/1283	0.32	0/1727
23	P	0.14	0/1199	0.27	0/1623
24	Q	0.14	0/2039	0.31	0/2750
25	R	0.15	0/1175	0.26	0/1572
26	S	0.15	0/1320	0.31	0/1789
27	T	0.15	0/1403	0.26	0/1886
28	U	0.14	0/1280	0.27	0/1732
29	W	0.16	0/926	0.28	0/1244
30	X	0.13	0/2099	0.26	0/2837
31	Y	0.13	0/1593	0.25	0/2136

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Z	0.17	0/1021	0.36	0/1378
33	V	0.12	0/1721	0.29	0/2333
34	b	0.15	0/1219	0.30	0/1651
35	e	0.11	0/1970	0.34	0/2658
36	g	0.16	0/1151	0.36	0/1569
37	h	0.11	0/918	0.29	0/1249
38	i	0.15	0/850	0.27	0/1135
39	j	0.13	0/760	0.28	0/1023
40	n	0.13	0/783	0.33	0/1057
41	l	0.09	0/707	0.29	0/960
42	m	0.14	0/805	0.38	0/1081
43	o	0.16	0/819	0.33	0/1097
44	q	0.13	0/1107	0.31	0/1498
45	r	0.13	0/1362	0.29	0/1846
46	AA	0.11	0/22537	0.22	0/35085
47	AB	0.14	0/1859	0.36	0/2513
48	AC	0.13	0/1113	0.32	0/1505
49	AD	0.13	0/2783	0.33	0/3724
50	AE	0.15	0/989	0.36	0/1335
51	AF	0.13	0/1767	0.34	0/2373
52	AG	0.12	0/2746	0.33	0/3681
53	AH	0.13	0/1178	0.35	0/1598
54	AI	0.13	0/1030	0.31	0/1386
55	AJ	0.14	0/855	0.37	0/1148
56	AK	0.12	0/880	0.33	0/1182
57	AL	0.13	0/1477	0.35	0/1974
58	AM	0.12	0/963	0.36	0/1295
59	AN	0.11	0/886	0.29	0/1199
60	AO	0.13	0/1648	0.36	0/2243
61	AP	0.12	0/798	0.32	0/1070
62	C	0.12	0/754	0.28	0/1003
63	AR	0.13	0/2456	0.32	0/3317
64	AS	0.13	0/1138	0.34	0/1533
65	AT	0.12	0/1402	0.33	0/1883
66	AU	0.10	0/1510	0.27	0/2025
67	AV	0.10	0/3030	0.32	0/4093
68	AW	0.15	0/801	0.40	0/1079
69	AX	0.10	0/2921	0.32	0/3954
70	AY	0.14	0/1280	0.38	0/1725
71	AZ	0.14	0/857	0.38	0/1141
72	A0	0.15	0/1834	0.40	0/2484
73	A1	0.11	0/2313	0.31	0/3129
74	G	0.16	0/947	0.43	0/1266

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	A3	0.13	0/636	0.34	0/839
76	A4	0.12	0/4877	0.37	0/6598
77	Az	0.41	0/378	0.67	0/586
78	Aw	0.39	0/1603	0.69	0/2488
79	Ax	0.39	0/1655	0.66	0/2569
80	B	0.10	0/1627	0.21	0/2527
81	a	0.13	0/866	0.27	0/1174
82	c	0.13	0/2347	0.30	0/3171
83	d	0.12	0/2039	0.28	0/2759
84	f	0.14	0/1273	0.35	0/1716
85	p	0.13	0/1223	0.34	0/1641
86	s	0.14	0/3239	0.27	0/4400
All	All	0.15	0/184534	0.31	0/262371

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
54	AI	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
54	AI	183	HIS	Peptide,Mainchain
54	AI	184	5F0	Mainchain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	898	0	916	12	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	1	464	0	511	7	0
3	2	377	0	406	4	0
4	3	832	0	883	8	0
5	4	342	0	361	2	0
6	5	3210	0	3206	34	0
7	6	2948	0	2841	31	0
8	7	2390	0	2397	38	0
9	8	1327	0	1368	44	0
10	9	997	0	987	26	0
11	A	33070	0	16793	336	0
12	D	1859	0	1919	31	0
13	E	2406	0	2415	18	0
14	F	2031	0	2065	27	0
15	H	1661	0	1734	27	0
16	I	1351	0	1425	40	0
17	J	1330	0	1407	33	0
18	k	1455	0	1452	19	0
19	L	890	0	941	8	0
20	M	2314	0	2384	21	0
21	N	1786	0	1817	17	0
22	O	1259	0	1294	18	0
23	P	1173	0	1165	12	0
24	Q	1990	0	2031	85	0
25	R	1154	0	1214	7	0
26	S	1293	0	1365	13	0
27	T	1369	0	1410	9	0
28	U	1251	0	1232	18	0
29	W	904	0	934	13	0
30	X	2044	0	2060	20	0
31	Y	1556	0	1597	7	0
32	Z	996	0	1044	10	0
33	V	1676	0	1687	29	0
34	b	1196	0	1195	7	0
35	e	1931	0	1914	46	0
36	g	1113	0	1097	17	0
37	h	895	0	881	14	0
38	i	828	0	857	11	0
39	j	745	0	746	10	0
40	n	774	0	784	20	0
41	l	688	0	674	18	0
42	m	791	0	790	92	0
43	o	798	0	804	9	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	q	1076	0	1049	13	0
45	r	1322	0	1348	19	0
46	AA	20260	0	10286	288	0
47	AB	1818	0	1807	29	0
48	AC	1083	0	1088	23	0
49	AD	2731	0	2804	40	0
50	AE	972	0	999	33	0
51	AF	1725	0	1769	31	0
52	AG	2688	0	2687	41	0
53	AH	1152	0	1183	38	0
54	AI	1020	0	1053	11	0
55	AJ	839	0	887	18	0
56	AK	862	0	885	11	0
57	AL	1453	0	1540	19	0
58	AM	942	0	965	20	0
59	AN	868	0	928	9	0
60	AO	1592	0	1557	22	0
61	AP	781	0	806	22	0
62	C	744	0	758	14	0
63	AR	2409	0	2428	35	0
64	AS	1111	0	1115	10	0
65	AT	1371	0	1393	16	0
66	AU	1488	0	1499	20	0
67	AV	2969	0	2960	115	0
68	AW	789	0	802	12	0
69	AX	2849	0	2841	55	0
70	AY	1246	0	1197	29	0
71	AZ	839	0	855	28	0
72	A0	1787	0	1796	48	0
73	A1	2265	0	2294	69	0
74	G	935	0	971	16	0
75	A3	625	0	699	16	0
76	A4	4768	0	4766	118	0
77	Az	339	0	169	29	0
78	Aw	1434	0	725	138	0
79	Ax	1482	0	752	102	0
80	B	1524	0	779	15	0
81	a	840	0	810	4	0
82	c	2299	0	2320	20	0
83	d	1985	0	1976	32	0
84	f	1252	0	1269	31	0
85	p	1205	0	1223	18	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	s	3155	0	3139	20	0
87	0	1	0	0	0	0
87	4	1	0	0	0	0
87	AO	1	0	0	0	0
88	3	1	0	0	0	0
88	6	1	0	0	0	0
88	A	28	0	0	0	0
88	AA	17	0	0	0	0
88	D	1	0	0	0	0
88	M	1	0	0	0	0
88	N	1	0	0	0	0
88	W	1	0	0	0	0
88	i	1	0	0	0	0
88	o	1	0	0	0	0
89	A	30	0	57	0	0
89	AA	10	0	19	0	0
90	A	6	0	12	0	0
91	A	138	0	0	0	0
91	A3	1	0	0	0	0
91	AA	62	0	0	0	0
91	AB	1	0	0	0	0
91	AX	1	0	0	0	0
91	Az	1	0	0	0	0
91	D	2	0	0	0	0
91	g	1	0	0	0	0
91	o	1	0	0	0	0
92	A	210	0	229	20	0
92	AA	168	0	184	23	0
93	e	7	0	8	1	0
94	AP	4	0	0	0	0
94	AT	4	0	0	0	0
94	r	4	0	0	1	0
95	AA	44	0	26	0	0
96	AA	14	0	26	0	0
97	AX	31	0	12	0	0
98	AX	28	0	12	1	0
All	All	176080	0	148765	2437	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 8.

All (2437) 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)
46:AA:1076:5MU:C5	46:AA:1076:5MU:C4	1.79	1.70
78:Aw:25:C:C2'	78:Aw:26:U:H5''	1.28	1.62
42:m:122:PHE:CD1	53:AH:183:HIS:HD2	1.20	1.59
42:m:122:PHE:HD1	53:AH:183:HIS:CD2	1.20	1.56
42:m:119:TYR:CE2	73:A1:228:VAL:CA	1.84	1.55
42:m:122:PHE:CD1	53:AH:183:HIS:CD2	1.89	1.53
42:m:119:TYR:CE2	73:A1:228:VAL:HA	0.97	1.49
24:Q:54:PHE:CE2	67:AV:134:GLN:CG	2.00	1.45
42:m:90:ARG:HE	46:AA:1396:C:C5'	1.31	1.41
42:m:90:ARG:NH2	46:AA:1396:C:H3'	1.21	1.41
42:m:90:ARG:NE	46:AA:1396:C:H5''	1.38	1.39
78:Aw:25:C:H2'	78:Aw:26:U:C5'	1.53	1.37
24:Q:54:PHE:CE2	67:AV:134:GLN:HG3	1.60	1.30
46:AA:1471:A:OP2	92:AA:1783:NMY:H81	1.31	1.30
24:Q:54:PHE:CD2	67:AV:134:GLN:HG3	1.67	1.30
24:Q:54:PHE:CD1	67:AV:131:ASN:ND2	1.97	1.29
24:Q:54:PHE:CZ	67:AV:134:GLN:CB	2.16	1.29
78:Aw:25:C:C3'	78:Aw:26:U:H5''	1.62	1.29
42:m:90:ARG:NH2	46:AA:1396:C:C3'	2.02	1.21
24:Q:54:PHE:CE2	67:AV:134:GLN:CB	2.22	1.19
42:m:106:TYR:CB	71:AZ:10:ARG:HH12	1.55	1.19
78:Aw:26:U:C6	78:Aw:26:U:H5'	1.77	1.19
42:m:119:TYR:HE2	73:A1:228:VAL:CA	1.36	1.19
46:AA:1220:A:C2	79:Ax:34:C:C4'	2.26	1.19
42:m:119:TYR:CD2	73:A1:228:VAL:HA	1.77	1.18
35:e:101:LYS:CE	69:AX:231:THR:HA	1.75	1.15
69:AX:277:GLU:CG	84:f:138:GLN:OE1	1.94	1.15
24:Q:57:PRO:HG3	67:AV:93:TYR:HB3	1.23	1.14
42:m:90:ARG:CZ	46:AA:1396:C:C3'	2.24	1.14
12:D:172:MET:SD	50:AE:86:ILE:HG23	1.88	1.14
24:Q:54:PHE:CD2	67:AV:134:GLN:CG	2.28	1.13
24:Q:54:PHE:CE2	67:AV:134:GLN:HB3	1.82	1.12
24:Q:54:PHE:CZ	67:AV:134:GLN:HG3	1.83	1.12
42:m:106:TYR:O	71:AZ:13:ARG:NH2	1.82	1.11
24:Q:54:PHE:CD2	67:AV:134:GLN:CD	2.28	1.11
24:Q:64:ASP:HA	67:AV:51:ALA:HB1	1.32	1.11
35:e:101:LYS:HE3	69:AX:231:THR:HA	1.31	1.10
46:AA:1220:A:N3	79:Ax:34:C:H4'	1.64	1.10
42:m:106:TYR:HB2	71:AZ:10:ARG:HH12	1.06	1.10
11:A:2117:U:OP1	92:A:3474:NMY:H81	1.51	1.10
46:AA:1220:A:C2	79:Ax:34:C:H4'	1.85	1.09
11:A:2639:C:O3'	75:A3:163:ARG:NH2	1.86	1.09

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:m:119:TYR:HE2	73:A1:228:VAL:N	1.51	1.07
24:Q:54:PHE:HD1	67:AV:131:ASN:ND2	1.42	1.07
24:Q:57:PRO:HG2	67:AV:93:TYR:CD2	1.89	1.07
46:AA:1556:C:N4	92:AA:1784:NMY:O17	1.88	1.06
78:Aw:25:C:C2'	78:Aw:26:U:C5'	2.22	1.06
46:AA:1473:C:N4	92:AA:1783:NMY:O3	1.87	1.05
78:Aw:26:U:C5'	78:Aw:26:U:H6	1.68	1.05
24:Q:57:PRO:HG3	67:AV:93:TYR:CB	1.86	1.04
24:Q:64:ASP:HA	67:AV:51:ALA:CB	1.87	1.04
42:m:122:PHE:CE1	53:AH:183:HIS:HD2	1.76	1.03
42:m:106:TYR:HB2	71:AZ:10:ARG:NH1	1.73	1.02
11:A:2596:G:C5'	75:A3:152:PHE:CD2	2.44	1.01
78:Aw:4:U:H2'	78:Aw:5:A:O4'	1.60	1.01
77:Az:7:G:N1	78:Aw:36:C:N3	2.09	1.00
42:m:119:TYR:CZ	73:A1:228:VAL:HA	1.97	1.00
46:AA:1471:A:OP2	92:AA:1783:NMY:C8	2.10	1.00
24:Q:54:PHE:CG	67:AV:134:GLN:HG3	1.96	0.99
42:m:115:HIS:ND1	73:A1:224:TYR:OH	1.94	0.99
24:Q:54:PHE:CZ	67:AV:134:GLN:HB2	1.93	0.99
78:Aw:26:U:H5'	78:Aw:26:U:H6	0.85	0.99
42:m:115:HIS:HD1	73:A1:224:TYR:HH	1.01	0.98
11:A:2596:G:H5'	75:A3:152:PHE:CD2	1.97	0.98
42:m:123:TRP:HH2	70:AY:336:LYS:NZ	1.60	0.98
42:m:106:TYR:CD2	71:AZ:10:ARG:NH1	2.31	0.98
24:Q:54:PHE:CE2	67:AV:134:GLN:CD	2.42	0.97
42:m:90:ARG:CZ	46:AA:1396:C:H3'	1.89	0.97
42:m:119:TYR:CD2	73:A1:228:VAL:CA	2.42	0.97
78:Aw:25:C:C3'	78:Aw:26:U:C5'	2.41	0.97
46:AA:902:G:N3	78:Aw:35:A:O2'	1.96	0.97
42:m:123:TRP:HH2	70:AY:336:LYS:HZ3	1.10	0.96
78:Aw:4:U:O5'	78:Aw:4:U:H6	1.48	0.96
77:Az:9:U:H3	78:Aw:34:A:H61	1.12	0.95
42:m:118:ARG:HE	53:AH:189:TRP:HH2	1.02	0.95
42:m:118:ARG:NE	53:AH:189:TRP:CH2	2.31	0.95
69:AX:277:GLU:HG3	84:f:138:GLN:OE1	1.67	0.94
24:Q:54:PHE:CZ	67:AV:134:GLN:CG	2.36	0.94
42:m:122:PHE:HD1	53:AH:183:HIS:NE2	1.64	0.94
42:m:119:TYR:HE2	73:A1:227:THR:C	1.75	0.93
24:Q:57:PRO:CG	67:AV:93:TYR:CD2	2.51	0.93
35:e:101:LYS:HE2	69:AX:231:THR:O	1.69	0.93
77:Az:7:G:N2	78:Aw:36:C:O2	2.03	0.92

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
78:Aw:25:C:H2'	78:Aw:26:U:C4'	1.99	0.91
77:Az:7:G:O6	78:Aw:36:C:N4	2.03	0.91
42:m:107:GLU:HG2	71:AZ:9:PHE:CE2	2.06	0.91
24:Q:66:HIS:HD2	67:AV:52:ASP:OD1	1.55	0.90
46:AA:1220:A:C2	79:Ax:34:C:O4'	2.24	0.90
42:m:119:TYR:CD2	73:A1:228:VAL:CB	2.55	0.89
69:AX:277:GLU:HG2	84:f:138:GLN:OE1	1.71	0.89
24:Q:57:PRO:CG	67:AV:93:TYR:CG	2.56	0.88
11:A:2596:G:H5'	75:A3:152:PHE:CE2	2.08	0.88
24:Q:54:PHE:CE1	67:AV:134:GLN:HG3	2.09	0.88
42:m:90:ARG:HH21	46:AA:1396:C:H3'	1.35	0.88
11:A:2117:U:OP1	92:A:3474:NMY:C8	2.23	0.87
12:D:172:MET:CE	50:AE:86:ILE:HG23	2.02	0.86
92:AA:1785:NMY:H5	92:AA:1785:NMY:H91	1.40	0.86
78:Aw:21:A:H61	78:Aw:46:A:H2'	1.38	0.86
35:e:101:LYS:HE2	69:AX:231:THR:HA	1.58	0.86
24:Q:54:PHE:CZ	67:AV:134:GLN:HB3	1.99	0.85
24:Q:57:PRO:CG	67:AV:93:TYR:HB3	2.05	0.85
78:Aw:25:C:H2'	78:Aw:26:U:H5''	0.86	0.85
14:F:103:GLN:HE22	14:F:249:ASN:HB2	1.39	0.85
79:Ax:63:U:H2'	79:Ax:64:C:C6	2.11	0.84
78:Aw:49:U:H2'	78:Aw:50:A:H8	1.41	0.84
24:Q:57:PRO:CD	67:AV:93:TYR:CG	2.60	0.84
11:A:2404:U:H2'	11:A:2405:C:C5	2.13	0.84
78:Aw:10:G:C2	78:Aw:26:U:H1'	2.13	0.84
42:m:106:TYR:CG	71:AZ:10:ARG:NH1	2.46	0.83
11:A:2404:U:H1'	92:A:3472:NMY:H91	1.43	0.83
24:Q:54:PHE:HD1	67:AV:131:ASN:HD21	1.20	0.83
42:m:90:ARG:NH2	46:AA:1396:C:O5'	2.13	0.82
53:AH:184:ILE:HD11	73:A1:227:THR:HA	1.62	0.82
24:Q:54:PHE:CD1	67:AV:134:GLN:HG3	2.14	0.82
9:8:52:LYS:HG3	78:Aw:39:U:H5''	1.61	0.82
11:A:2404:U:C1'	92:A:3472:NMY:H91	1.92	0.82
42:m:118:ARG:NE	53:AH:189:TRP:HH2	1.63	0.82
76:A4:582:LEU:HA	76:A4:585:ARG:HD2	1.63	0.81
11:A:2583:C:OP1	46:AA:1582:G:C8	2.34	0.81
24:Q:57:PRO:HB2	67:AV:90:TYR:HA	1.62	0.81
42:m:90:ARG:NE	46:AA:1396:C:C5'	2.12	0.81
24:Q:57:PRO:HD2	67:AV:93:TYR:CG	2.15	0.81
24:Q:59:LYS:HA	67:AV:90:TYR:CE1	2.15	0.81
11:A:2112:A:H61	21:N:140:MET:HE2	1.45	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
77:Az:9:U:H3	78:Aw:34:A:N6	1.79	0.80
55:AJ:57:GLN:HB3	55:AJ:109:LEU:HD11	1.64	0.80
11:A:3112:A:N7	11:A:3200:U:O2	2.14	0.80
78:Aw:25:C:H3'	78:Aw:26:U:H5''	1.64	0.79
79:Ax:56:C:H2'	79:Ax:57:A:C8	2.16	0.79
8:7:182:ASP:HB3	8:7:294:ILE:HD11	1.64	0.79
11:A:2352:U:H3	11:A:2361:G:H1	0.81	0.79
24:Q:66:HIS:HD2	67:AV:52:ASP:CG	1.89	0.79
12:D:172:MET:SD	50:AE:86:ILE:CG2	2.69	0.79
46:AA:1078:A:OP1	79:Ax:38:U:O2'	2.01	0.79
78:Aw:4:U:O5'	78:Aw:4:U:C6	2.36	0.79
78:Aw:25:C:H3'	78:Aw:26:U:C5'	2.11	0.79
28:U:45:PRO:HD2	28:U:48:MET:HE3	1.65	0.78
24:Q:57:PRO:CG	67:AV:93:TYR:CB	2.60	0.78
78:Aw:24:A:H2'	78:Aw:25:C:C6	2.18	0.78
12:D:172:MET:HE3	50:AE:84:ARG:O	1.84	0.78
42:m:90:ARG:HE	46:AA:1396:C:C4'	1.97	0.77
11:A:1927:G:H5'	92:A:3472:NMY:H82	1.65	0.77
42:m:119:TYR:CD2	73:A1:228:VAL:HG23	2.19	0.77
83:d:197:VAL:HG22	83:d:212:ILE:HG23	1.67	0.77
53:AH:155:VAL:HG11	73:A1:129:PHE:HB3	1.65	0.76
78:Aw:6:U:H2'	78:Aw:7:A:C8	2.21	0.76
42:m:119:TYR:CZ	73:A1:231:HIS:CD2	2.71	0.76
78:Aw:67:U:H2'	78:Aw:68:U:C6	2.21	0.76
79:Ax:51:A:H2'	79:Ax:52:G:C8	2.21	0.76
67:AV:76:ILE:HD11	67:AV:92:LEU:HD21	1.69	0.75
40:n:30:THR:HG21	40:n:62:PRO:HB2	1.67	0.75
46:AA:1562:G:H1'	46:AA:1583:MA6:H2	1.69	0.75
42:m:90:ARG:HH21	46:AA:1396:C:C5'	1.99	0.74
42:m:119:TYR:CE2	73:A1:227:THR:C	2.61	0.74
76:A4:308:LYS:HD2	76:A4:309:PHE:H	1.51	0.74
78:Aw:21:A:H3'	78:Aw:46:A:H61	1.53	0.74
62:C:78:LYS:HD3	68:AW:162:VAL:HG13	1.70	0.74
42:m:90:ARG:NE	46:AA:1396:C:O3'	2.12	0.74
78:Aw:66:U:H2'	78:Aw:67:U:H5'	1.70	0.74
8:7:155:GLU:HG2	8:7:156:ARG:HD2	1.69	0.74
7:6:47:ARG:HE	7:6:47:ARG:H	1.35	0.74
79:Ax:2:A:H2'	79:Ax:3:G:C8	2.22	0.73
79:Ax:62:C:H2'	79:Ax:63:U:C6	2.23	0.73
79:Ax:61:C:H2'	79:Ax:62:C:C6	2.23	0.73
11:A:2596:G:H5''	75:A3:152:PHE:CD2	2.20	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:m:90:ARG:NE	46:AA:1396:C:C4'	2.51	0.73
78:Aw:4:U:C2'	78:Aw:5:A:O4'	2.34	0.73
70:AY:293:PRO:HB2	76:A4:88:VAL:HG21	1.70	0.73
52:AG:66:ARG:HH21	73:A1:93:LYS:HZ2	1.36	0.73
24:Q:57:PRO:HD2	67:AV:93:TYR:CD2	2.23	0.73
49:AD:95:ALA:HB2	71:AZ:74:GLU:HG2	1.70	0.73
50:AE:92:ASN:HB2	61:AP:117:MET:HE1	1.70	0.73
38:i:99:GLY:HA2	38:i:102:MET:HE2	1.71	0.73
78:Aw:1:U:H2'	78:Aw:2:G:C8	2.24	0.72
21:N:218:ILE:HG23	21:N:223:MET:HB2	1.68	0.72
69:AX:297:MET:HE3	69:AX:297:MET:HA	1.72	0.72
78:Aw:42:U:H2'	78:Aw:43:U:C6	2.24	0.72
42:m:90:ARG:NE	46:AA:1396:C:C3'	2.52	0.72
11:A:2404:U:H1'	92:A:3472:NMY:N9	2.04	0.72
11:A:2404:U:H2'	11:A:2405:C:C6	2.25	0.72
42:m:90:ARG:HE	46:AA:1396:C:H5''	0.57	0.72
42:m:119:TYR:CD2	73:A1:228:VAL:HB	2.25	0.72
73:A1:214:LEU:HB2	73:A1:217:GLN:HE21	1.55	0.72
42:m:119:TYR:CE2	73:A1:227:THR:O	2.43	0.71
24:Q:57:PRO:HG2	67:AV:93:TYR:HD2	1.54	0.71
46:AA:1180:U:O4	92:AA:1783:NMY:C6	2.39	0.71
24:Q:54:PHE:CE1	67:AV:131:ASN:ND2	2.40	0.71
35:e:101:LYS:CE	69:AX:231:THR:CA	2.63	0.71
47:AB:197:HIS:HD2	47:AB:240:ASP:HB2	1.53	0.71
79:Ax:7:A:H61	79:Ax:66:U:H3	1.38	0.71
79:Ax:23:A:H2'	79:Ax:24:A:C8	2.26	0.71
28:U:46:MET:HE1	28:U:91:ASP:HB2	1.72	0.70
24:Q:66:HIS:CD2	67:AV:52:ASP:OD1	2.42	0.70
54:AI:66:ILE:HD12	54:AI:67:PRO:HD2	1.73	0.70
79:Ax:25:C:H3'	79:Ax:26:A:H8	1.54	0.70
49:AD:206:PRO:HA	49:AD:272:LYS:HE2	1.72	0.70
79:Ax:9:A:H1'	79:Ax:45:G:H2'	1.73	0.70
35:e:101:LYS:HE2	69:AX:231:THR:CA	2.20	0.70
11:A:2612:C:H5'	46:AA:1503:G:H21	1.57	0.70
47:AB:107:PHE:HB2	47:AB:117:ASP:HB2	1.72	0.70
46:AA:1423:A:HO2'	79:Ax:40:C:HO2'	1.37	0.69
54:AI:66:ILE:HG13	54:AI:68:GLY:H	1.57	0.69
35:e:101:LYS:HE2	69:AX:231:THR:C	2.17	0.69
53:AH:55:PRO:HA	76:A4:440:LYS:HB3	1.75	0.69
67:AV:57:MET:HE1	67:AV:67:VAL:HG11	1.73	0.69
11:A:1973:G:N7	92:A:3472:NMY:H20	2.06	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:AB:220:VAL:HG22	47:AB:234:TYR:HB2	1.74	0.69
72:A0:30:ASP:HB3	72:A0:111:HIS:HB3	1.74	0.69
76:A4:262:MET:HA	76:A4:262:MET:HE3	1.74	0.69
78:Aw:22:A:H62	78:Aw:46:A:H2	1.41	0.69
35:e:123:MET:HE3	35:e:123:MET:H	1.58	0.69
24:Q:59:LYS:CA	67:AV:90:TYR:CE1	2.76	0.69
37:h:87:GLN:HG3	37:h:124:ARG:HB3	1.74	0.69
24:Q:59:LYS:HA	67:AV:90:TYR:CD1	2.28	0.69
24:Q:64:ASP:CA	67:AV:51:ALA:HB1	2.17	0.69
42:m:119:TYR:HD2	73:A1:228:VAL:HB	1.57	0.69
46:AA:821:U:H2'	46:AA:822:G:H8	1.57	0.69
4:3:138:PRO:HG2	11:A:2854:U:H4'	1.73	0.68
42:m:119:TYR:CE2	73:A1:228:VAL:N	2.38	0.68
67:AV:129:LEU:HA	67:AV:137:ILE:HD11	1.74	0.68
24:Q:57:PRO:CD	67:AV:93:TYR:CD2	2.77	0.68
76:A4:238:TRP:HB2	76:A4:269:HIS:HB3	1.74	0.68
79:Ax:71:U:H2'	79:Ax:72:A:C8	2.28	0.68
42:m:115:HIS:CG	70:AY:333:PHE:CE1	2.81	0.68
79:Ax:11:U:H2'	79:Ax:12:U:C6	2.29	0.68
46:AA:1556:C:H41	92:AA:1784:NMY:C17	2.05	0.68
76:A4:645:LEU:HA	76:A4:648:ARG:HE	1.59	0.68
63:AR:298:THR:HG22	63:AR:328:ILE:HD11	1.76	0.68
85:p:60:ARG:HH22	85:p:62:PRO:HA	1.59	0.68
30:X:226:LEU:HD12	31:Y:155:LEU:HB3	1.75	0.67
35:e:114:ILE:CG2	69:AX:169:LEU:HD11	2.25	0.67
42:m:106:TYR:CE2	71:AZ:9:PHE:HD2	2.11	0.67
92:A:3473:NMY:H5	92:A:3473:NMY:H91	1.59	0.67
12:D:173:ALA:O	50:AE:84:ARG:HD2	1.94	0.67
73:A1:269:MET:HA	73:A1:269:MET:HE3	1.75	0.67
14:F:279:ARG:HH12	14:F:282:PRO:HD3	1.60	0.67
7:6:330:ILE:HG23	7:6:334:LEU:HD12	1.76	0.67
79:Ax:65:C:H2'	79:Ax:66:U:C6	2.29	0.67
42:m:90:ARG:CZ	46:AA:1396:C:C5'	2.73	0.67
42:m:115:HIS:CG	70:AY:333:PHE:HE1	2.12	0.67
50:AE:108:ILE:HD11	61:AP:63:LYS:HE3	1.75	0.67
76:A4:308:LYS:HD2	76:A4:309:PHE:N	2.10	0.67
11:A:2582:A:N1	46:AA:1560:U:O2'	2.25	0.67
65:AT:51:ASN:HB3	65:AT:99:MET:HE3	1.77	0.67
46:AA:1262:C:H4'	49:AD:100:LYS:HG2	1.76	0.67
78:Aw:7:A:H61	78:Aw:66:U:H3	1.42	0.67
65:AT:21:VAL:HG22	65:AT:103:ARG:HB3	1.74	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:D:172:MET:SD	50:AE:86:ILE:CG1	2.83	0.67
42:m:106:TYR:CB	71:AZ:10:ARG:NH1	2.40	0.67
46:AA:1470:A:H2'	46:AA:1471:A:H8	1.59	0.67
42:m:119:TYR:CD2	73:A1:228:VAL:CG2	2.78	0.66
70:AY:250:ILE:HB	76:A4:354:LEU:HD11	1.76	0.66
82:c:179:THR:HG22	82:c:194:THR:HG21	1.78	0.66
2:1:34:ARG:HB3	2:1:41:LEU:HD11	1.76	0.66
78:Aw:24:A:H2'	78:Aw:25:C:H6	1.58	0.66
79:Ax:1:U:H2'	79:Ax:2:A:H8	1.60	0.66
7:6:214:TRP:HB2	7:6:240:ILE:HD11	1.77	0.66
46:AA:1220:A:H2	79:Ax:34:C:C5'	2.08	0.66
37:h:96:LEU:HD23	37:h:96:LEU:H	1.61	0.66
11:A:2545:U:H5''	11:A:2546:G:H5'	1.77	0.66
11:A:3040:OMG:HN1	78:Aw:75:C:H42	1.42	0.66
60:AO:208:PRO:HG2	60:AO:213:LEU:HD21	1.76	0.66
79:Ax:1:U:H2'	79:Ax:2:A:C8	2.31	0.66
9:8:85:ILE:HG22	9:8:88:PHE:H	1.61	0.66
46:AA:1220:A:C2	79:Ax:34:C:C5'	2.79	0.66
76:A4:562:GLN:HG3	76:A4:564:ILE:HB	1.76	0.66
11:A:2587:G:H4'	79:Ax:13:U:H4'	1.78	0.65
44:q:37:PRO:HG2	44:q:68:SER:HA	1.78	0.65
46:AA:1016:U:H1'	61:AP:90:CYS:HB3	1.78	0.65
11:A:2596:G:C5'	75:A3:152:PHE:HD2	2.03	0.65
38:i:78:ILE:H	38:i:78:ILE:HD12	1.62	0.65
46:AA:1470:A:H2'	46:AA:1471:A:C8	2.31	0.65
46:AA:1440:G:H2'	46:AA:1441:A:H8	1.61	0.65
76:A4:576:LEU:HD13	76:A4:579:ILE:HD11	1.78	0.65
24:Q:54:PHE:HE2	67:AV:134:GLN:HB3	1.51	0.65
35:e:114:ILE:HG23	69:AX:169:LEU:HD11	1.78	0.65
11:A:1862:U:H2'	11:A:1863:A:H8	1.61	0.65
45:r:149:ARG:HD3	45:r:152:THR:HG21	1.78	0.65
46:AA:1178:G:O6	92:AA:1783:NYM:N6	2.30	0.65
46:AA:1440:G:H2'	46:AA:1441:A:C8	2.32	0.65
46:AA:1481:C:N4	92:AA:1785:NYM:O17	2.29	0.65
9:8:47:SER:HB3	77:Az:6:G:H1'	1.78	0.65
15:H:172:LEU:HB3	15:H:235:MET:HB3	1.77	0.65
57:AL:175:TYR:HB2	59:AN:89:GLY:HA3	1.77	0.65
60:AO:192:THR:HG21	60:AO:199:TRP:HA	1.79	0.65
9:8:127:GLN:HA	9:8:130:LYS:HB3	1.77	0.65
66:AU:89:VAL:HG13	66:AU:90:LEU:HD22	1.79	0.65
20:M:68:GLU:HG3	20:M:73:PRO:HA	1.77	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
72:A0:167:PRO:HG2	72:A0:170:LEU:HB2	1.79	0.65
86:s:152:GLN:HA	86:s:156:TYR:HB2	1.78	0.65
10:9:53:ILE:HD12	10:9:56:MET:HE3	1.78	0.65
40:n:14:LYS:HD2	40:n:15:GLN:HB2	1.78	0.65
46:AA:1398:U:H2'	46:AA:1399:A:H8	1.61	0.65
65:AT:40:LEU:HD12	65:AT:92:THR:HG22	1.79	0.64
9:8:67:ARG:HA	9:8:70:ARG:HG3	1.78	0.64
15:H:176:MET:HA	15:H:176:MET:HE3	1.78	0.64
42:m:106:TYR:OH	71:AZ:6:GLU:HA	1.98	0.64
78:Aw:52:G:H3'	78:Aw:53:A:H8	1.62	0.64
35:e:255:VAL:HG23	35:e:259:GLU:HG3	1.80	0.64
79:Ax:63:U:H2'	79:Ax:64:C:H6	1.61	0.64
42:m:90:ARG:NH2	46:AA:1396:C:C5'	2.59	0.64
5:4:68:ASN:HB3	5:4:103:MET:HE2	1.78	0.64
11:A:2352:U:O4	11:A:2361:G:O6	2.16	0.64
42:m:123:TRP:CH2	70:AY:336:LYS:NZ	2.52	0.64
24:Q:57:PRO:HD2	67:AV:93:TYR:CD1	2.33	0.64
47:AB:158:MET:HE1	47:AB:250:CYS:HB3	1.79	0.64
72:A0:96:ARG:HB3	72:A0:117:ILE:HB	1.79	0.64
85:p:192:ARG:HB2	85:p:195:SER:HB3	1.79	0.64
6:5:115:GLU:HB2	6:5:119:GLN:HB2	1.79	0.64
13:E:80:LEU:HD12	13:E:323:GLY:HA3	1.79	0.64
16:I:189:GLN:HE22	40:n:56:ARG:HA	1.63	0.64
55:AJ:51:PRO:HG3	55:AJ:122:LYS:HB3	1.80	0.64
86:s:405:ILE:HG12	86:s:410:VAL:HG22	1.80	0.64
7:6:192:GLU:HG2	85:p:185:ARG:HD3	1.79	0.64
61:AP:139:ARG:HH12	61:AP:142:GLU:HB2	1.63	0.64
11:A:3211:C:H4'	11:A:3212:C:H5	1.61	0.63
33:V:202:MET:HE2	33:V:204:ILE:HD11	1.80	0.63
37:h:91:LEU:HD21	37:h:100:LEU:HD23	1.78	0.63
11:A:1857:U:H2'	11:A:1858:G:C8	2.32	0.63
46:AA:1201:A:H2'	46:AA:1202:G:H8	1.63	0.63
42:m:119:TYR:HE2	73:A1:227:THR:O	1.81	0.63
46:AA:1358:A:O2'	79:Ax:30:G:OP1	2.15	0.63
46:AA:1201:A:H2'	46:AA:1202:G:C8	2.34	0.63
79:Ax:2:A:H2'	79:Ax:3:G:H8	1.64	0.63
78:Aw:61:U:H2'	78:Aw:62:C:C6	2.33	0.63
11:A:2740:A:H2'	11:A:2741:A:H8	1.63	0.63
58:AM:100:HIS:HB3	58:AM:103:MET:HG3	1.81	0.63
72:A0:64:LEU:HD13	72:A0:134:VAL:HG22	1.81	0.63
78:Aw:14:A:H3'	78:Aw:15:A:H8	1.64	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:Ax:67:U:H2'	79:Ax:68:C:C6	2.33	0.63
28:U:66:ALA:HB2	28:U:100:ALA:HA	1.80	0.63
33:V:79:VAL:HG22	33:V:86:VAL:HG12	1.81	0.63
46:AA:1555:A:OP2	92:AA:1784:NMY:N19	2.32	0.63
48:AC:111:LYS:HB2	48:AC:118:GLU:HG3	1.80	0.63
65:AT:51:ASN:HA	65:AT:54:GLN:HG3	1.78	0.63
76:A4:489:HIS:HB3	76:A4:492:THR:HG23	1.81	0.63
49:AD:149:MET:HE3	49:AD:149:MET:HA	1.81	0.63
11:A:2740:A:H2'	11:A:2741:A:C8	2.34	0.62
79:Ax:65:C:H2'	79:Ax:66:U:H6	1.64	0.62
11:A:2725:A:H5'	83:d:40:ARG:HH22	1.64	0.62
82:c:148:MET:HG2	82:c:153:ILE:HG12	1.81	0.62
10:9:114:LEU:HD11	30:X:231:VAL:HG21	1.81	0.62
48:AC:92:LEU:HD11	48:AC:117:LEU:HD21	1.81	0.62
63:AR:328:ILE:HD12	63:AR:328:ILE:H	1.64	0.62
78:Aw:49:U:H2'	78:Aw:50:A:C8	2.30	0.62
79:Ax:61:C:H2'	79:Ax:62:C:H6	1.63	0.62
42:m:70:GLU:HG3	42:m:72:ARG:HG3	1.79	0.62
46:AA:1529:A:H1'	67:AV:66:PRO:HD3	1.81	0.62
78:Aw:11:U:H3	78:Aw:24:A:H61	1.48	0.62
9:8:157:LEU:HB2	35:e:184:LEU:HD11	1.82	0.62
63:AR:262:LEU:HD12	63:AR:267:TYR:HB2	1.80	0.62
76:A4:539:LYS:HA	76:A4:585:ARG:HH12	1.63	0.62
86:s:271:LEU:HD23	86:s:273:LEU:HD13	1.82	0.62
11:A:2777:G:H5''	15:H:242:LYS:HG3	1.82	0.62
20:M:234:LEU:HD11	20:M:238:ARG:HH22	1.65	0.62
51:AF:58:LEU:HD12	51:AF:58:LEU:H	1.64	0.62
11:A:2734:A:H2'	11:A:2735:G:H8	1.65	0.62
14:F:89:THR:HG22	14:F:179:THR:HG21	1.81	0.62
42:m:106:TYR:OH	71:AZ:9:PHE:HB3	2.00	0.62
69:AX:269:TRP:HH2	69:AX:297:MET:HG3	1.63	0.62
16:I:95:MET:HB2	16:I:159:PRO:HA	1.82	0.62
78:Aw:43:U:H2'	78:Aw:44:A:C8	2.35	0.62
70:AY:373:ILE:H	70:AY:373:ILE:HD12	1.64	0.61
48:AC:165:LYS:HE2	48:AC:167:LEU:HD13	1.81	0.61
83:d:124:ARG:HH22	83:d:202:MET:HG2	1.65	0.61
67:AV:141:ASN:HD22	67:AV:175:VAL:HB	1.63	0.61
79:Ax:51:A:H2'	79:Ax:52:G:H8	1.65	0.61
46:AA:1180:U:O4	92:AA:1783:NMY:H62	2.01	0.61
69:AX:244:LEU:HD21	69:AX:293:LEU:HD22	1.82	0.61
76:A4:267:VAL:HG11	76:A4:296:ALA:HB1	1.82	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
76:A4:494:ILE:HA	76:A4:497:LEU:HD12	1.81	0.61
79:Ax:22:A:H2'	79:Ax:23:A:C8	2.36	0.61
79:Ax:66:U:H2'	79:Ax:67:U:C6	2.36	0.61
11:A:3150:U:H2'	11:A:3151:A:H8	1.65	0.61
20:M:119:THR:HG21	36:g:51:LEU:HD22	1.82	0.61
24:Q:60:PRO:HB2	67:AV:87:HIS:HD2	1.66	0.61
24:Q:60:PRO:HD3	67:AV:90:TYR:CG	2.36	0.61
12:D:172:MET:CE	50:AE:86:ILE:CG2	2.72	0.61
46:AA:1473:C:N4	92:AA:1783:NMY:HO3	1.98	0.61
78:Aw:13:U:H2'	78:Aw:14:A:C8	2.35	0.61
8:7:112:PRO:HB2	8:7:267:PRO:HG2	1.83	0.61
42:m:106:TYR:HE2	71:AZ:9:PHE:HD2	1.48	0.61
46:AA:1003:A:H2'	46:AA:1004:G:H8	1.66	0.61
46:AA:1175:G:H2'	46:AA:1176:G:H8	1.66	0.61
76:A4:581:ILE:HG22	76:A4:585:ARG:HE	1.65	0.61
14:F:197:THR:HG23	14:F:199:ASP:H	1.64	0.61
11:A:2686:G:OP2	92:A:3473:NMY:H82	2.02	0.60
47:AB:151:PHE:O	47:AB:155:ILE:HD12	2.01	0.60
77:Az:6:G:H1	79:Ax:34:C:H42	1.46	0.60
11:A:2055:U:H2'	11:A:2056:G:H8	1.66	0.60
32:Z:75:THR:HB	32:Z:83:LYS:HG2	1.81	0.60
78:Aw:42:U:H2'	78:Aw:43:U:H6	1.65	0.60
35:e:174:PRO:HB3	35:e:195:LEU:HD21	1.83	0.60
52:AG:229:LEU:HD21	52:AG:241:VAL:HG11	1.83	0.60
65:AT:114:ARG:HH11	65:AT:114:ARG:HG3	1.64	0.60
36:g:142:GLU:HB3	43:o:88:ILE:HG13	1.83	0.60
46:AA:1526:U:H2'	72:A0:99:ARG:HD3	1.83	0.60
49:AD:176:ARG:HH21	49:AD:177:GLU:HG2	1.66	0.60
46:AA:1220:A:H2	79:Ax:34:C:C4'	2.04	0.60
46:AA:663:A:H2'	46:AA:664:G:C8	2.37	0.60
58:AM:114:ARG:HH11	58:AM:114:ARG:HG3	1.65	0.60
78:Aw:66:U:C2'	78:Aw:67:U:H5'	2.32	0.60
53:AH:97:LEU:HD23	73:A1:119:ILE:HD12	1.82	0.60
63:AR:166:PRO:HB2	63:AR:169:GLU:HG3	1.84	0.60
73:A1:53:LEU:HD23	73:A1:53:LEU:H	1.66	0.60
76:A4:149:ILE:O	76:A4:149:ILE:HD12	2.02	0.59
9:8:153:GLU:HG2	35:e:47:LEU:HD21	1.84	0.59
22:O:54:GLY:HA3	24:Q:270:MET:HE2	1.84	0.59
42:m:115:HIS:NE2	71:AZ:17:ARG:O	2.34	0.59
69:AX:210:TRP:HE1	69:AX:216:THR:HG23	1.67	0.59
79:Ax:58:A:C2	79:Ax:61:C:H5''	2.36	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:5:135:LYS:HE3	6:5:239:ILE:HD13	1.83	0.59
11:A:2583:C:OP1	46:AA:1582:G:N9	2.35	0.59
35:e:77:ILE:HG23	35:e:81:ARG:HE	1.66	0.59
36:g:73:GLN:HB3	36:g:162:LEU:HD11	1.83	0.59
42:m:95:LYS:HD3	42:m:95:LYS:N	2.17	0.59
46:AA:899:G:OP1	92:AA:1785:NMY:H9	2.02	0.59
79:Ax:57:A:H2'	79:Ax:58:A:C8	2.37	0.59
9:8:83:ILE:HD12	9:8:83:ILE:H	1.68	0.59
50:AE:11:LYS:HB3	50:AE:13:MET:HE2	1.84	0.59
72:A0:71:LEU:HD11	72:A0:78:ARG:HH11	1.65	0.59
77:Az:9:U:H2'	77:Az:10:G:C8	2.38	0.59
79:Ax:50:G:H2'	79:Ax:51:A:H8	1.67	0.59
78:Aw:9:A:H2'	78:Aw:11:U:O4	2.02	0.59
78:Aw:44:A:H2'	78:Aw:45:A:C8	2.37	0.59
86:s:111:LYS:HG2	86:s:261:ILE:HD13	1.83	0.59
11:A:2718:C:H2'	11:A:2991:U:H4'	1.83	0.59
51:AF:231:GLU:HG2	74:G:53:MET:HG2	1.84	0.59
76:A4:256:GLU:HG2	76:A4:287:LEU:HB3	1.84	0.59
78:Aw:70:C:H2'	78:Aw:71:C:C6	2.38	0.59
46:AA:1578:A:H2'	46:AA:1579:C:C6	2.38	0.59
92:AA:1786:NMY:HN32	92:AA:1786:NMY:H16	1.67	0.59
56:AK:53:ARG:HD3	70:AY:375:TRP:CD2	2.37	0.59
84:f:179:PRO:HD2	84:f:182:VAL:HG21	1.85	0.59
8:7:247:ASN:HD21	8:7:249:GLU:HB3	1.68	0.59
11:A:2086:A:H2'	11:A:2087:U:C6	2.37	0.59
42:m:119:TYR:OH	73:A1:227:THR:O	2.21	0.59
72:A0:17:ARG:H	72:A0:17:ARG:HD2	1.68	0.59
11:A:2111:C:H2'	11:A:2112:A:C8	2.38	0.59
28:U:64:PRO:HB2	28:U:100:ALA:HB3	1.85	0.59
33:V:80:ILE:HB	33:V:85:TRP:HB2	1.85	0.59
76:A4:405:PHE:HB2	76:A4:447:PHE:HE2	1.67	0.59
79:Ax:9:A:H5''	79:Ax:46:A:H1'	1.84	0.59
8:7:94:HIS:HB3	83:d:281:MET:HG3	1.84	0.58
30:X:10:LEU:HD22	44:q:45:LEU:HD13	1.83	0.58
35:e:221:MET:HE2	35:e:221:MET:O	2.02	0.58
61:AP:94:ARG:HB3	61:AP:104:GLN:HG3	1.85	0.58
78:Aw:43:U:H2'	78:Aw:44:A:H8	1.66	0.58
16:I:40:MET:HG2	16:I:44:ARG:HD3	1.85	0.58
46:AA:1175:G:H2'	46:AA:1176:G:C8	2.37	0.58
11:A:3073:C:HO2'	83:d:37:THR:N	2.01	0.58
17:J:108:VAL:HG22	17:J:154:ARG:HD3	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:m:69:ARG:HG2	42:m:69:ARG:HH11	1.68	0.58
15:H:114:VAL:HB	15:H:118:LEU:HD23	1.85	0.58
21:N:218:ILE:HA	21:N:223:MET:HG3	1.84	0.58
46:AA:1413:U:OP1	84:f:143:LYS:HG2	2.03	0.58
49:AD:112:LYS:HE2	77:Az:11:U:O4'	2.02	0.58
11:A:2339:G:H21	11:A:2427:C:H5'	1.68	0.58
26:S:100:HIS:HB2	26:S:134:LEU:HD11	1.83	0.58
40:n:8:LEU:HD11	40:n:95:ARG:HG3	1.85	0.58
35:e:186:GLY:HA2	35:e:189:GLU:HG2	1.85	0.58
46:AA:1559:G:N7	92:AA:1784:NMY:H82	2.17	0.58
9:8:93:LYS:H	9:8:93:LYS:HE2	1.66	0.58
11:A:2099:U:H2'	11:A:2100:C:C6	2.37	0.58
18:k:172:PRO:HG2	45:r:56:THR:HG23	1.86	0.58
26:S:120:LEU:HB3	26:S:122:LEU:HD12	1.85	0.58
78:Aw:4:U:H2'	78:Aw:5:A:C8	2.38	0.58
78:Aw:74:C:H3'	78:Aw:75:C:C6	2.39	0.58
46:AA:1264:C:H1'	53:AH:124:VAL:HG23	1.86	0.58
60:AO:94:CYS:HB2	60:AO:108:CYS:SG	2.43	0.58
66:AU:169:THR:HG23	66:AU:171:GLU:H	1.69	0.58
78:Aw:9:A:O2'	78:Aw:45:A:H2'	2.04	0.58
78:Aw:23:A:H3'	78:Aw:24:A:H8	1.68	0.58
7:6:233:LEU:HD23	7:6:286:ARG:HE	1.69	0.58
13:E:340:PRO:HB2	24:Q:101:GLU:HB3	1.86	0.58
46:AA:715:G:H1'	46:AA:817:G:H5'	1.86	0.58
52:AG:85:LYS:HG3	52:AG:104:ILE:HD11	1.84	0.58
67:AV:179:GLN:HB2	67:AV:215:GLN:HE21	1.68	0.58
37:h:74:VAL:HG11	37:h:86:TRP:HE3	1.69	0.58
46:AA:1308:U:H2'	46:AA:1309:A:H8	1.69	0.58
42:m:119:TYR:CZ	73:A1:231:HIS:HD2	2.18	0.57
42:m:119:TYR:CG	73:A1:228:VAL:HG23	2.39	0.57
49:AD:221:ARG:HG3	49:AD:326:LEU:HD21	1.84	0.57
80:B:68:C:H2'	80:B:69:U:C6	2.39	0.57
86:s:145:VAL:HG21	86:s:187:LEU:HD11	1.85	0.57
14:F:99:VAL:HG21	14:F:173:GLY:HA3	1.87	0.57
46:AA:1365:A:H4'	46:AA:1389:G:H4'	1.86	0.57
79:Ax:22:A:H2'	79:Ax:23:A:H8	1.68	0.57
11:A:2586:U:O4	92:AA:1786:NMY:O4	2.19	0.57
24:Q:57:PRO:O	67:AV:90:TYR:HD1	1.86	0.57
48:AC:100:PHE:HB3	48:AC:103:CYS:HB2	1.86	0.57
62:C:72:ILE:HD12	74:G:104:LEU:HD21	1.85	0.57
23:P:93:LEU:HD21	23:P:101:VAL:HG22	1.85	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:U:129:MET:HG2	83:d:82:ALA:HB2	1.84	0.57
84:f:122:GLU:HB2	84:f:158:GLN:HG2	1.86	0.57
6:5:355:LEU:HD12	6:5:376:VAL:HG12	1.86	0.57
52:AG:320:VAL:HG23	52:AG:322:ARG:HG2	1.86	0.57
63:AR:155:LYS:HB3	63:AR:177:PRO:HD3	1.86	0.57
70:AY:377:ARG:HG2	70:AY:377:ARG:HH11	1.70	0.57
10:9:116:LYS:H	10:9:116:LYS:HD2	1.69	0.57
13:E:244:ALA:HB1	13:E:248:ILE:HD11	1.87	0.57
18:k:20:LEU:HD11	18:k:60:MET:HG2	1.87	0.57
23:P:89:HIS:CD2	23:P:108:ARG:HG3	2.39	0.57
33:V:80:ILE:HD13	33:V:85:TRP:HE3	1.70	0.57
69:AX:277:GLU:CD	84:f:138:GLN:OE1	2.45	0.57
78:Aw:16:A:H61	78:Aw:61:U:H5	1.52	0.57
82:c:105:ARG:HH22	82:c:117:LEU:HG	1.70	0.57
84:f:121:VAL:HG12	84:f:159:ILE:HG22	1.87	0.57
11:A:2782:A:H5'	15:H:247:ARG:HH22	1.67	0.57
56:AK:53:ARG:HH21	70:AY:372:HIS:CE1	2.22	0.57
77:Az:15:U:H2'	77:Az:16:A:C8	2.40	0.57
78:Aw:54:U:H2'	78:Aw:55:A:H4'	1.85	0.57
11:A:3024:U:H2'	11:A:3025:A:H8	1.70	0.57
32:Z:101:LYS:HD3	39:j:84:MET:HG3	1.86	0.57
43:o:15:ARG:HB3	43:o:18:ILE:HG12	1.87	0.57
46:AA:1025:A:H2'	46:AA:1026:A:C8	2.40	0.57
61:AP:80:LEU:HB3	61:AP:120:MET:HE1	1.86	0.57
70:AY:320:GLY:HA3	76:A4:135:PRO:HB3	1.86	0.57
83:d:186:VAL:HG12	83:d:187:GLU:HG3	1.87	0.57
1:0:149:PHE:HA	22:O:84:ASP:OD2	2.04	0.57
9:8:147:LEU:O	9:8:158:HIS:HE1	1.88	0.57
35:e:55:ARG:HG3	35:e:149:LEU:HD22	1.86	0.57
58:AM:32:TYR:HE1	58:AM:56:PRO:HG3	1.70	0.57
80:B:30:A:H2'	80:B:31:A:H8	1.69	0.57
9:8:92:LEU:HD12	9:8:92:LEU:H	1.68	0.57
34:b:77:VAL:HG22	34:b:87:GLU:HG3	1.87	0.57
76:A4:360:MET:HG2	76:A4:367:PRO:HB3	1.86	0.57
11:A:3201:A:H2'	11:A:3202:U:O4'	2.04	0.56
72:A0:174:ILE:H	72:A0:174:ILE:HD12	1.70	0.56
80:B:23:A:H2'	80:B:24:G:C8	2.40	0.56
85:p:94:LYS:HE2	85:p:96:ASN:HB2	1.85	0.56
3:2:72:THR:HG23	3:2:75:GLY:H	1.71	0.56
8:7:276:PHE:HB2	8:7:304:VAL:HG22	1.87	0.56
11:A:1911:C:H2'	11:A:1912:A:H8	1.70	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:2355:A:H5'	11:A:2673:G:H21	1.69	0.56
17:J:159:LEU:HD11	17:J:164:LEU:HD23	1.86	0.56
35:e:116:LEU:O	35:e:120:LEU:HD12	2.06	0.56
46:AA:900:C:H41	55:AJ:74:ASN:ND2	2.03	0.56
46:AA:970:A:H2'	46:AA:971:A:H8	1.71	0.56
46:AA:1006:U:H2'	46:AA:1007:G:H8	1.70	0.56
48:AC:125:ARG:HD2	48:AC:159:PRO:HA	1.86	0.56
56:AK:52:LEU:HD22	71:AZ:41:PRO:HG3	1.87	0.56
58:AM:87:MET:HE2	58:AM:87:MET:HA	1.86	0.56
78:Aw:26:U:C6	78:Aw:26:U:C4'	2.89	0.56
79:Ax:58:A:H2'	79:Ax:61:C:C5	2.40	0.56
11:A:2727:C:H2'	11:A:2728:C:C6	2.40	0.56
49:AD:132:ILE:HG12	49:AD:144:LEU:HD11	1.87	0.56
52:AG:108:ILE:HG13	52:AG:125:MET:HB2	1.85	0.56
69:AX:319:PRO:HG2	69:AX:322:ALA:HB2	1.86	0.56
79:Ax:4:G:H1	79:Ax:69:C:H42	1.52	0.56
7:6:225:LEU:HB3	23:P:44:VAL:HG13	1.88	0.56
23:P:70:THR:HG21	29:W:76:HIS:HB3	1.88	0.56
34:b:73:VAL:HG13	34:b:91:HIS:HB2	1.87	0.56
8:7:107:LEU:HD22	8:7:128:LEU:HD21	1.87	0.56
72:A0:64:LEU:HD12	72:A0:139:TRP:CE2	2.40	0.56
76:A4:513:TRP:HE1	76:A4:554:ASP:HB3	1.70	0.56
15:H:147:ARG:HA	15:H:152:LEU:HB2	1.88	0.56
17:J:90:PHE:HD2	17:J:120:ILE:HG23	1.71	0.56
46:AA:1239:C:H2'	46:AA:1240:A:H8	1.69	0.56
50:AE:26:ILE:HA	50:AE:29:LEU:HD23	1.86	0.56
79:Ax:43:A:H3'	79:Ax:44:A:H8	1.69	0.56
83:d:113:LYS:HA	83:d:116:MET:HE3	1.87	0.56
11:A:2803:A:H2'	11:A:2804:A:O4'	2.06	0.56
35:e:122:ASP:OD2	69:AX:212:LYS:NZ	2.25	0.56
39:j:97:LYS:HZ2	39:j:97:LYS:C	2.14	0.56
50:AE:47:LEU:HD13	50:AE:51:ILE:HD12	1.87	0.56
77:Az:14:A:H2'	77:Az:14:A:N3	2.20	0.56
78:Aw:1:U:H2'	78:Aw:2:G:H8	1.71	0.56
11:A:2081:U:H2'	11:A:2082:G:C8	2.40	0.56
27:T:151:ARG:HB2	27:T:161:MET:HG3	1.87	0.56
57:AL:209:LEU:HD23	75:A3:189:TRP:CE2	2.41	0.56
46:AA:970:A:H2'	46:AA:971:A:C8	2.40	0.56
72:A0:164:VAL:HG13	72:A0:193:VAL:HG21	1.88	0.56
78:Aw:52:G:H3'	78:Aw:53:A:C8	2.40	0.56
11:A:1862:U:H2'	11:A:1863:A:C8	2.41	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:2727:C:H2'	11:A:2728:C:H6	1.71	0.55
11:A:2782:A:H62	15:H:242:LYS:HE3	1.69	0.55
28:U:68:VAL:HG22	28:U:97:VAL:HG22	1.86	0.55
52:AG:317:PHE:HE2	52:AG:348:MET:HE3	1.70	0.55
48:AC:105:ALA:HB3	48:AC:122:VAL:HG12	1.87	0.55
78:Aw:4:U:H2'	78:Aw:5:A:C1'	2.36	0.55
78:Aw:10:G:N3	78:Aw:10:G:H2'	2.20	0.55
78:Aw:49:U:H3	78:Aw:65:A:H61	1.53	0.55
35:e:205:LEU:HD21	35:e:237:LEU:HD23	1.88	0.55
57:AL:147:ARG:NH1	57:AL:147:ARG:HB2	2.21	0.55
70:AY:384:LYS:O	70:AY:384:LYS:HD3	2.07	0.55
11:A:2583:C:OP1	46:AA:1582:G:C4	2.60	0.55
67:AV:380:GLN:O	67:AV:384:LEU:HD12	2.06	0.55
14:F:69:LEU:HD22	14:F:206:LEU:HD21	1.89	0.55
19:L:145:VAL:HG21	24:Q:160:VAL:HG11	1.89	0.55
30:X:14:LEU:HD13	44:q:45:LEU:HD12	1.88	0.55
69:AX:273:THR:HG23	69:AX:316:LEU:HD13	1.89	0.55
78:Aw:21:A:N6	78:Aw:46:A:H2'	2.17	0.55
11:A:2331:C:H3'	11:A:2332:C:O4'	2.06	0.55
46:AA:1239:C:H2'	46:AA:1240:A:C8	2.41	0.55
46:AA:1523:A:H5''	67:AV:68:SER:N	2.22	0.55
67:AV:213:LEU:HD12	67:AV:224:GLN:HE22	1.71	0.55
12:D:172:MET:SD	50:AE:86:ILE:HG13	2.47	0.55
42:m:106:TYR:HD2	71:AZ:10:ARG:NH1	2.02	0.55
46:AA:985:U:H2'	46:AA:986:G:H8	1.72	0.55
76:A4:535:MET:HE3	76:A4:548:PHE:CD2	2.42	0.55
77:Az:7:G:C6	78:Aw:36:C:N3	2.73	0.55
79:Ax:28:C:H2'	79:Ax:29:U:C6	2.42	0.55
11:A:1868:G:H2'	20:M:40:PRO:HG3	1.89	0.55
13:E:50:ASP:HA	13:E:53:LEU:HG	1.89	0.55
46:AA:881:A:N6	60:AO:82:LYS:HB3	2.22	0.55
46:AA:892:A:OP1	55:AJ:77:ASN:HB2	2.07	0.55
46:AA:1467:C:H2'	46:AA:1468:U:H6	1.72	0.55
42:m:90:ARG:NH2	46:AA:1396:C:C4'	2.69	0.55
53:AH:78:VAL:HB	53:AH:143:LEU:HB2	1.88	0.55
54:AI:150:VAL:HG22	54:AI:176:THR:HB	1.89	0.55
66:AU:77:GLU:HG2	66:AU:80:ARG:HH12	1.71	0.55
79:Ax:50:G:H2'	79:Ax:51:A:C8	2.41	0.55
7:6:98:SER:HB3	7:6:101:GLN:HB2	1.89	0.54
11:A:3143:U:H2'	11:A:3144:A:H8	1.73	0.54
35:e:51:LEU:HD21	35:e:53:LEU:HD23	1.88	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:AE:117:LEU:HD13	74:G:10:LEU:HD22	1.88	0.54
72:A0:107:GLN:HG2	72:A0:108:ASN:OD1	2.06	0.54
8:7:148:MET:HE2	8:7:257:ILE:HG22	1.89	0.54
15:H:244:LYS:HA	15:H:247:ARG:HH21	1.72	0.54
35:e:123:MET:HG2	35:e:127:LYS:NZ	2.22	0.54
46:AA:909:G:H2'	46:AA:910:A:H8	1.73	0.54
51:AF:110:LEU:HD22	51:AF:201:MET:HB3	1.87	0.54
67:AV:167:VAL:HG13	67:AV:172:ALA:HB3	1.89	0.54
6:5:112:ARG:HH11	11:A:2406:A:H61	1.56	0.54
11:A:2353:A:H61	11:A:2357:C:H5	1.54	0.54
46:AA:1552:G:H2'	46:AA:1553:A:H8	1.73	0.54
47:AB:88:ARG:HB3	47:AB:91:LEU:HD12	1.89	0.54
56:AK:92:VAL:HG23	56:AK:93:MET:HG2	1.88	0.54
73:A1:259:GLU:O	73:A1:263:LEU:HG	2.08	0.54
30:X:142:ASP:HA	30:X:165:MET:HE1	1.88	0.54
51:AF:201:MET:HE2	51:AF:201:MET:HA	1.89	0.54
58:AM:102:MET:HE1	66:AU:56:LEU:HD21	1.90	0.54
67:AV:57:MET:HA	67:AV:57:MET:HE3	1.90	0.54
67:AV:246:ASN:HB3	72:A0:70:ARG:HH22	1.73	0.54
73:A1:92:LYS:O	73:A1:93:LYS:HG2	2.07	0.54
11:A:2277:U:H2'	11:A:2278:A:H8	1.73	0.54
60:AO:94:CYS:SG	60:AO:105:CYS:HB3	2.47	0.54
69:AX:199:LEU:H	69:AX:199:LEU:HD23	1.72	0.54
76:A4:582:LEU:HG	76:A4:588:ARG:HH22	1.72	0.54
1:0:138:ARG:HB3	11:A:2321:A:C8	2.42	0.54
11:A:1863:A:H2'	11:A:1864:A:C8	2.43	0.54
11:A:2514:C:H2'	11:A:2515:U:H6	1.72	0.54
15:H:146:LEU:HB3	15:H:152:LEU:HD12	1.89	0.54
46:AA:1133:C:H2'	46:AA:1134:G:H8	1.73	0.54
66:AU:168:ILE:HG12	66:AU:176:ARG:HG3	1.90	0.54
17:J:149:ARG:HH22	41:l:103:PRO:HA	1.73	0.54
42:m:96:ARG:NH1	42:m:97:GLU:HG3	2.23	0.54
63:AR:327:LEU:HD12	63:AR:328:ILE:HD12	1.89	0.54
6:5:201:ARG:HB3	6:5:232:THR:HG22	1.90	0.54
9:8:179:THR:HG21	35:e:133:LEU:HD22	1.90	0.54
33:V:65:LEU:HD21	33:V:121:LYS:HG3	1.89	0.54
46:AA:832:U:H2'	46:AA:833:A:H8	1.71	0.54
67:AV:250:ILE:HG23	67:AV:252:LYS:H	1.73	0.54
78:Aw:28:A:H2'	78:Aw:28:A:N3	2.22	0.54
2:1:40:LYS:HE2	2:1:58:GLU:HG2	1.90	0.54
11:A:1911:C:H2'	11:A:1912:A:C8	2.42	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:L:32:ILE:HG23	19:L:36:THR:HG21	1.89	0.54
26:S:86:MET:HE1	26:S:140:ASN:HB2	1.89	0.54
46:AA:740:G:H2'	46:AA:741:A:H8	1.73	0.54
74:G:11:ALA:HB2	74:G:19:PRO:HB3	1.90	0.54
76:A4:591:GLU:CD	76:A4:591:GLU:H	2.15	0.54
78:Aw:7:A:N6	78:Aw:66:U:H3	2.06	0.54
10:9:24:LYS:HG2	11:A:2421:G:H5''	1.89	0.54
24:Q:57:PRO:O	67:AV:90:TYR:CD1	2.61	0.54
46:AA:1470:A:OP2	92:AA:1783:NMY:O12	2.26	0.54
47:AB:164:GLU:HA	47:AB:164:GLU:OE2	2.07	0.54
24:Q:268:ASP:HB3	24:Q:271:ARG:HG3	1.90	0.53
53:AH:157:LEU:O	53:AH:161:GLN:HG3	2.08	0.53
64:AS:102:LYS:HZ2	64:AS:124:ALA:HB1	1.72	0.53
46:AA:872:G:H2'	46:AA:873:G:H8	1.73	0.53
57:AL:76:TYR:CE2	57:AL:93:LEU:HD22	2.44	0.53
76:A4:586:ALA:HB3	76:A4:588:ARG:NH1	2.24	0.53
46:AA:969:A:H2'	46:AA:970:A:H8	1.73	0.53
58:AM:34:ILE:HG22	58:AM:51:LEU:HB2	1.90	0.53
8:7:154:ILE:HG21	8:7:183:VAL:HG21	1.90	0.53
35:e:127:LYS:H	35:e:127:LYS:HD2	1.72	0.53
40:n:16:VAL:HG23	40:n:51:VAL:HG13	1.91	0.53
49:AD:291:PHE:CE2	49:AD:358:THR:HG22	2.43	0.53
52:AG:78:ILE:HD11	52:AG:127:HIS:HE1	1.73	0.53
73:A1:262:ILE:O	73:A1:266:LEU:HD22	2.08	0.53
76:A4:157:LEU:HD21	76:A4:172:MET:HB3	1.90	0.53
20:M:287:ASP:HB3	20:M:290:LEU:HB2	1.89	0.53
23:P:70:THR:HG23	23:P:71:VAL:HG13	1.88	0.53
26:S:108:VAL:HB	26:S:195:ILE:HG13	1.89	0.53
46:AA:1452:U:H2'	46:AA:1453:A:H8	1.74	0.53
51:AF:238:HIS:HE1	74:G:46:ILE:HG21	1.73	0.53
67:AV:311:GLU:HG2	67:AV:312:LYS:HG3	1.90	0.53
76:A4:403:LYS:HB3	76:A4:405:PHE:HE1	1.73	0.53
78:Aw:12:U:H3	78:Aw:23:A:H61	1.55	0.53
79:Ax:70:C:H2'	79:Ax:71:U:H6	1.73	0.53
11:A:1952:U:H2'	11:A:1953:A:C8	2.44	0.53
16:I:90:PHE:HE1	16:I:96:ILE:HG21	1.73	0.53
61:AP:124:TYR:HB3	62:C:9:ALA:HB2	1.91	0.53
79:Ax:70:C:H2'	79:Ax:71:U:C6	2.43	0.53
8:7:173:PRO:HG2	8:7:176:SER:HB3	1.90	0.53
11:A:3002:G:H2'	11:A:3003:A:H8	1.74	0.53
11:A:3089:A:H3'	11:A:3090:G:H5''	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:m:63:THR:O	42:m:64:ILE:HD13	2.09	0.53
46:AA:871:A:H4'	46:AA:872:G:H5'	1.90	0.53
50:AE:96:HIS:HB3	50:AE:99:THR:HG23	1.90	0.53
79:Ax:7:A:N6	79:Ax:66:U:H3	2.04	0.53
10:9:72:PRO:HD2	33:V:175:LYS:HG3	1.91	0.53
15:H:105:VAL:HG22	15:H:158:LYS:HD2	1.90	0.53
16:I:132:LYS:NZ	16:I:148:VAL:HG22	2.23	0.53
46:AA:727:U:H5''	59:AN:5:ARG:HH11	1.73	0.53
65:AT:39:GLU:HG2	65:AT:40:LEU:HD22	1.90	0.53
83:d:48:PRO:HD2	83:d:51:LYS:HE3	1.90	0.53
11:A:1977:U:H2'	11:A:1978:A:H8	1.74	0.53
11:A:2067:C:H5''	84:f:60:LYS:HB2	1.91	0.53
11:A:2598:A:H3'	11:A:2625:C:H42	1.74	0.53
35:e:123:MET:HG2	35:e:127:LYS:HZ1	1.73	0.53
77:Az:1:U:P	77:Az:1:U:H6	2.32	0.53
11:A:1829:A:H2'	11:A:1830:G:H8	1.74	0.53
11:A:3150:U:H2'	11:A:3151:A:C8	2.44	0.53
46:AA:1575:U:H2'	46:AA:1576:G:H8	1.74	0.53
52:AG:200:LEU:HD22	52:AG:244:PHE:HB3	1.90	0.53
58:AM:64:LYS:HE2	63:AR:154:THR:HB	1.91	0.53
76:A4:372:TYR:O	76:A4:375:ILE:HG13	2.09	0.53
76:A4:427:ARG:HA	76:A4:468:MET:HE1	1.91	0.53
76:A4:461:PHE:CE1	76:A4:465:ILE:HD11	2.44	0.53
78:Aw:62:C:H2'	78:Aw:63:A:O4'	2.09	0.53
11:A:1886:G:H1	38:i:61:GLY:HA3	1.74	0.52
11:A:2151:A:H2'	11:A:2152:A:C8	2.44	0.52
11:A:2330:U:H4'	11:A:2331:C:C2	2.45	0.52
36:g:101:THR:HG22	36:g:102:HIS:ND1	2.24	0.52
42:m:90:ARG:HH21	46:AA:1396:C:C4'	2.21	0.52
63:AR:126:LEU:HA	63:AR:266:ARG:HG2	1.91	0.52
79:Ax:72:A:H2'	79:Ax:73:A:C8	2.44	0.52
82:c:46:GLU:HA	82:c:49:ARG:HD2	1.91	0.52
84:f:162:LEU:HD11	84:f:167:ALA:HA	1.91	0.52
85:p:109:GLU:CD	85:p:109:GLU:H	2.18	0.52
3:2:80:LEU:HD11	31:Y:205:VAL:HG22	1.91	0.52
9:8:151:GLN:HB2	9:8:158:HIS:CE1	2.43	0.52
11:A:2728:C:H2'	11:A:2729:U:H6	1.73	0.52
16:I:33:VAL:HG13	21:N:244:LYS:HB3	1.92	0.52
27:T:88:ILE:HA	27:T:91:MET:SD	2.49	0.52
30:X:196:ILE:HD12	30:X:200:GLU:HG2	1.91	0.52
40:n:23:PHE:CD1	40:n:57:HIS:CE1	2.97	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:AE:3:ARG:HD2	50:AE:69:TYR:CZ	2.44	0.52
11:A:1719:G:H2'	11:A:1720:C:H6	1.74	0.52
26:S:51:VAL:HG12	45:r:76:ASN:HB2	1.90	0.52
70:AY:384:LYS:HZ1	70:AY:394:PHE:H	1.56	0.52
83:d:217:HIS:HD2	83:d:243:LEU:HD13	1.75	0.52
11:A:3065:U:H4'	13:E:239:ARG:HH21	1.74	0.52
16:I:121:ILE:HG23	16:I:156:SER:HB3	1.91	0.52
17:J:114:LEU:HD12	17:J:155:VAL:HG12	1.90	0.52
64:AS:97:GLN:OE1	64:AS:97:GLN:HA	2.10	0.52
73:A1:198:TYR:HB2	73:A1:205:LEU:HD23	1.90	0.52
11:A:2053:U:HO2'	11:A:2054:U:H6	1.58	0.52
24:Q:66:HIS:CD2	67:AV:52:ASP:CG	2.79	0.52
34:b:95:VAL:HG13	34:b:96:GLU:OE1	2.09	0.52
37:h:94:SER:HA	37:h:97:LYS:HB3	1.92	0.52
44:q:59:LYS:HD2	44:q:59:LYS:O	2.10	0.52
52:AG:224:LEU:HD11	62:C:86:GLY:HA3	1.92	0.52
60:AO:146:GLN:OE1	60:AO:146:GLN:HA	2.10	0.52
68:AW:79:SER:O	68:AW:83:MET:HG3	2.10	0.52
76:A4:420:MET:HA	76:A4:423:CYS:HB2	1.90	0.52
11:A:2596:G:C5'	75:A3:152:PHE:CE2	2.84	0.52
30:X:217:LEU:HA	30:X:220:GLU:HG2	1.92	0.52
46:AA:1488:5MC:H2'	46:AA:1489:G:C8	2.45	0.52
51:AF:49:GLU:CD	51:AF:49:GLU:H	2.18	0.52
7:6:175:VAL:HG22	7:6:204:VAL:HG22	1.92	0.52
11:A:2405:C:H5'	12:D:78:LYS:NZ	2.25	0.52
17:J:164:LEU:O	17:J:168:GLN:HG3	2.10	0.52
30:X:7:PRO:HD2	30:X:10:LEU:HD12	1.92	0.52
37:h:74:VAL:HG11	37:h:86:TRP:CE3	2.45	0.52
46:AA:649:A:H3'	49:AD:335:LYS:HE2	1.91	0.52
49:AD:126:LEU:HD21	71:AZ:81:GLU:HG2	1.92	0.52
83:d:219:ARG:HH21	83:d:239:PRO:HG2	1.75	0.52
21:N:223:MET:HE3	43:o:42:GLU:HG2	1.92	0.52
27:T:122:ALA:HB1	27:T:128:VAL:HG21	1.91	0.52
46:AA:1468:U:C2	46:AA:1469:G:C8	2.98	0.52
72:A0:189:PRO:O	72:A0:190:MET:HE2	2.10	0.52
76:A4:309:PHE:HB2	76:A4:345:PHE:CG	2.45	0.52
76:A4:343:ARG:HA	76:A4:378:LEU:HD13	1.91	0.52
78:Aw:43:U:C2	78:Aw:44:A:C8	2.98	0.52
9:8:82:LEU:HD12	84:f:197:ARG:HG2	1.92	0.52
16:I:47:LEU:HD22	21:N:226:ILE:HG12	1.92	0.52
17:J:61:LYS:HA	41:l:79:LYS:HE3	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:M:244:LEU:HD12	20:M:245:PRO:HD2	1.92	0.52
46:AA:1472:G:H2'	46:AA:1473:C:C6	2.45	0.52
46:AA:1595:G:H2'	46:AA:1596:A:C8	2.45	0.52
47:AB:223:VAL:HG23	47:AB:227:CYS:HB2	1.92	0.52
49:AD:117:ARG:CZ	77:Az:13:U:H4'	2.40	0.52
78:Aw:70:C:H2'	78:Aw:71:C:H6	1.74	0.52
7:6:57:TYR:CD2	29:W:117:ILE:HD12	2.45	0.51
7:6:131:PRO:HG2	7:6:134:ALA:HB3	1.91	0.51
7:6:255:LEU:HD12	7:6:256:PRO:HD2	1.93	0.51
11:A:3115:U:H2'	11:A:3116:C:H6	1.75	0.51
17:J:85:PRO:HG2	17:J:90:PHE:CE1	2.45	0.51
20:M:261:ASP:HB3	20:M:264:GLN:HB2	1.92	0.51
52:AG:360:GLU:HA	52:AG:363:TRP:CE3	2.45	0.51
67:AV:278:GLU:HB2	67:AV:352:LEU:HD23	1.92	0.51
22:O:157:ARG:O	22:O:161:GLU:HG3	2.10	0.51
63:AR:355:ARG:HH21	63:AR:356:HIS:HD2	1.58	0.51
1:0:167:GLU:HA	1:0:170:GLN:HG2	1.92	0.51
78:Aw:68:U:H2'	78:Aw:69:A:C8	2.46	0.51
80:B:56:U:H5''	80:B:58:A:N7	2.26	0.51
11:A:1863:A:H2'	11:A:1864:A:H8	1.75	0.51
11:A:2127:A:H4'	11:A:2251:A:C5	2.45	0.51
24:Q:259:LYS:HE2	24:Q:259:LYS:N	2.24	0.51
46:AA:916:C:H2'	46:AA:917:C:C6	2.46	0.51
47:AB:272:ARG:NE	47:AB:272:ARG:HA	2.25	0.51
53:AH:133:GLN:HB3	56:AK:126:ALA:HB3	1.93	0.51
76:A4:607:ARG:HD2	76:A4:609:GLU:HG2	1.92	0.51
78:Aw:29:U:H2'	78:Aw:30:G:O4'	2.10	0.51
79:Ax:64:C:H2'	79:Ax:65:C:C6	2.45	0.51
16:I:163:GLU:HB3	16:I:166:ARG:HH22	1.75	0.51
59:AN:8:VAL:HG21	59:AN:78:LYS:HB3	1.92	0.51
67:AV:360:VAL:HG13	67:AV:361:LYS:HD3	1.93	0.51
4:3:98:SER:HB3	4:3:105:LYS:HE3	1.93	0.51
6:5:155:LEU:HD12	6:5:403:PRO:HG2	1.92	0.51
11:A:2455:U:H2'	11:A:2456:U:C6	2.45	0.51
11:A:3078:C:H2'	11:A:3079:G:C8	2.46	0.51
17:J:103:GLN:OE1	17:J:103:GLN:HA	2.10	0.51
25:R:94:GLN:HE22	25:R:145:VAL:HG13	1.76	0.51
44:q:112:GLN:O	44:q:116:GLU:HG2	2.10	0.51
46:AA:661:C:H2'	46:AA:662:U:C6	2.45	0.51
48:AC:125:ARG:HG2	76:A4:94:TYR:CD1	2.45	0.51
51:AF:153:GLU:HB3	51:AF:179:ARG:HG2	1.91	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:AP:86:PRO:HA	61:AP:125:LYS:HB3	1.91	0.51
86:s:149:CYS:SG	86:s:179:GLN:HB3	2.51	0.51
6:5:136:VAL:HG11	6:5:417:LEU:HD23	1.91	0.51
6:5:385:HIS:HB2	11:A:2395:A:H1'	1.92	0.51
11:A:2245:A:H4'	11:A:2246:A:OP1	2.11	0.51
14:F:132:GLY:HA3	83:d:42:THR:HG21	1.92	0.51
22:O:26:ILE:HG13	24:Q:264:TRP:CD1	2.45	0.51
41:l:119:ARG:HG2	41:l:119:ARG:HH11	1.76	0.51
58:AM:37:ALA:HA	58:AM:48:VAL:HG23	1.92	0.51
58:AM:101:PRO:HD3	66:AU:63:TYR:CD2	2.45	0.51
77:Az:6:G:H1	79:Ax:34:C:N4	2.07	0.51
78:Aw:10:G:N1	78:Aw:26:U:H1'	2.25	0.51
24:Q:54:PHE:HZ	67:AV:134:GLN:HB2	1.70	0.51
47:AB:258:THR:O	47:AB:262:GLU:HG3	2.11	0.51
53:AH:166:GLU:OE1	73:A1:109:PRO:HB3	2.11	0.51
76:A4:583:PHE:HA	76:A4:588:ARG:CZ	2.40	0.51
11:A:2006:C:H2'	11:A:2007:U:C6	2.46	0.51
14:F:72:PHE:HA	14:F:206:LEU:HD13	1.93	0.51
16:I:98:VAL:HG12	16:I:177:LEU:HD12	1.92	0.51
16:I:186:LEU:HG	16:I:190:GLY:HA3	1.93	0.51
17:J:60:ILE:HD11	17:J:64:ILE:HG12	1.91	0.51
17:J:154:ARG:HD2	17:J:154:ARG:N	2.26	0.51
28:U:129:MET:O	28:U:133:GLU:HG2	2.10	0.51
52:AG:201:ILE:HG23	52:AG:203:GLU:H	1.75	0.51
60:AO:105:CYS:HB2	60:AO:142:VAL:HA	1.93	0.51
65:AT:47:PHE:HE1	65:AT:99:MET:HE2	1.75	0.51
7:6:47:ARG:HE	7:6:47:ARG:N	2.07	0.51
11:A:1927:G:H5'	92:A:3472:NMY:C8	2.39	0.51
11:A:1939:G:O2'	11:A:1973:G:H4'	2.11	0.51
24:Q:54:PHE:CD2	67:AV:134:GLN:NE2	2.77	0.51
32:Z:150:HIS:HB3	32:Z:152:LYS:HE2	1.92	0.51
46:AA:1006:U:H2'	46:AA:1007:G:C8	2.46	0.51
49:AD:265:MET:HE1	52:AG:56:ILE:HG12	1.93	0.51
50:AE:9:ILE:HG22	50:AE:89:ILE:HB	1.92	0.51
51:AF:197:GLN:H	51:AF:197:GLN:CD	2.19	0.51
72:A0:91:GLU:HG3	72:A0:121:LYS:HA	1.92	0.51
79:Ax:27:U:H2'	79:Ax:28:C:C6	2.46	0.51
11:A:2748:A:H2'	11:A:2749:A:C8	2.46	0.50
11:A:3041:U:O2	78:Aw:74:C:H5	1.94	0.50
16:I:142:ASN:HB2	16:I:185:ILE:HD13	1.93	0.50
24:Q:54:PHE:CE2	67:AV:134:GLN:OE1	2.62	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:AA:1220:A:N1	79:Ax:34:C:O4'	2.43	0.50
68:AW:104:ILE:HG12	68:AW:114:ILE:HG12	1.93	0.50
76:A4:450:PRO:HD2	76:A4:453:HIS:CG	2.47	0.50
50:AE:6:LEU:HB3	50:AE:66:VAL:HB	1.93	0.50
55:AJ:100:HIS:ND1	55:AJ:102:LEU:HB2	2.26	0.50
72:A0:132:GLU:HA	72:A0:207:GLN:HG3	1.93	0.50
4:3:165:PHE:O	4:3:168:ARG:HG2	2.11	0.50
11:A:2702:G:H5'	18:k:114:LYS:HE2	1.93	0.50
11:A:2748:A:H2'	11:A:2749:A:H8	1.75	0.50
16:I:86:ILE:HD12	16:I:87:ALA:N	2.25	0.50
25:R:17:ARG:HA	25:R:20:ARG:HD2	1.92	0.50
32:Z:155:GLU:HG2	32:Z:156:GLN:HG3	1.92	0.50
46:AA:832:U:H2'	46:AA:833:A:C8	2.46	0.50
61:AP:67:LEU:HD23	66:AU:191:ILE:HD13	1.93	0.50
67:AV:361:LYS:HD3	67:AV:361:LYS:N	2.27	0.50
70:AY:353:LEU:HD21	71:AZ:26:THR:HG21	1.93	0.50
46:AA:1233:C:O2	56:AK:86:ARG:HD2	2.12	0.50
46:AA:1561:C:H2'	46:AA:1562:G:C8	2.47	0.50
48:AC:125:ARG:HG3	48:AC:157:THR:HG22	1.92	0.50
51:AF:94:PHE:HD1	51:AF:184:MET:HB3	1.76	0.50
52:AG:92:MET:HE2	52:AG:107:ALA:HA	1.93	0.50
71:AZ:21:GLU:OE1	71:AZ:21:GLU:HA	2.11	0.50
79:Ax:25:C:H3'	79:Ax:26:A:C8	2.41	0.50
1:0:170:GLN:OE1	1:0:170:GLN:HA	2.12	0.50
11:A:2409:A:H2'	11:A:2410:U:C6	2.46	0.50
46:AA:985:U:H2'	46:AA:986:G:C8	2.46	0.50
47:AB:194:ILE:HD12	47:AB:220:VAL:HB	1.92	0.50
68:AW:92:MET:O	68:AW:92:MET:HE3	2.12	0.50
76:A4:427:ARG:C	76:A4:468:MET:HE1	2.37	0.50
79:Ax:58:A:H2'	79:Ax:61:C:H5	1.75	0.50
84:f:163:SER:HB3	84:f:166:PHE:HB2	1.94	0.50
85:p:179:ARG:HH11	85:p:179:ARG:HG3	1.75	0.50
7:6:121:ARG:HH12	9:8:108:PHE:HE1	1.60	0.50
8:7:139:ASN:HB3	8:7:174:VAL:HG21	1.93	0.50
11:A:2042:U:H2'	11:A:2043:C:H6	1.77	0.50
11:A:2455:U:H5''	22:O:47:ALA:HB3	1.94	0.50
17:J:149:ARG:HG2	17:J:154:ARG:HH22	1.76	0.50
46:AA:1575:U:H2'	46:AA:1576:G:C8	2.46	0.50
51:AF:187:MET:HE2	51:AF:187:MET:HA	1.93	0.50
78:Aw:29:U:C2	78:Aw:30:G:C8	2.99	0.50
79:Ax:54:U:H3'	79:Ax:55:U:C6	2.46	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:6:90:ILE:HA	39:j:112:LYS:HB2	1.92	0.50
9:8:114:ARG:HG2	35:e:73:LEU:HD21	1.94	0.50
17:J:157:LYS:HZ1	41:l:97:PHE:HB3	1.76	0.50
23:P:52:ASN:HB3	23:P:55:ASN:HB2	1.94	0.50
60:AO:169:GLN:HE22	63:AR:266:ARG:HD3	1.76	0.50
66:AU:142:LYS:N	66:AU:142:LYS:HE2	2.27	0.50
79:Ax:68:C:H2'	79:Ax:69:C:C6	2.47	0.50
7:6:217:LEU:HB3	7:6:236:LEU:HD13	1.94	0.50
11:A:2275:U:H2'	11:A:2276:C:C6	2.47	0.50
17:J:24:VAL:HB	17:J:53:PHE:HE2	1.76	0.50
37:h:70:LEU:O	37:h:74:VAL:HG12	2.12	0.50
84:f:135:LEU:HB2	84:f:144:MET:HE3	1.94	0.50
11:A:1839:C:H2'	11:A:1840:C:C6	2.47	0.50
11:A:2819:G:H21	29:W:38:SER:HB3	1.76	0.50
27:T:84:LEU:HB3	27:T:111:ILE:HD12	1.94	0.50
28:U:99:LEU:HB3	28:U:103:GLN:HG3	1.93	0.50
46:AA:1200:G:C2	46:AA:1201:A:C8	3.00	0.50
65:AT:34:TYR:HA	65:AT:74:PRO:HB3	1.94	0.50
68:AW:89:LEU:O	68:AW:92:MET:HB3	2.12	0.50
78:Aw:21:A:H3'	78:Aw:46:A:N6	2.24	0.50
11:A:1935:A:C2	11:A:1936:A:H1'	2.47	0.49
11:A:2685:U:OP1	92:A:3473:NMY:H81	2.12	0.49
46:AA:872:G:H2'	46:AA:873:G:C8	2.46	0.49
70:AY:259:PHE:HZ	76:A4:320:LEU:HD22	1.77	0.49
84:f:94:HIS:HA	84:f:156:VAL:HG22	1.93	0.49
11:A:2318:A:H2'	11:A:2319:A:C8	2.48	0.49
11:A:2804:A:H2'	11:A:2805:A:H8	1.77	0.49
11:A:3040:OMG:H2'	11:A:3041:U:H4'	1.94	0.49
11:A:3230:G:H4'	11:A:3231:U:H5''	1.94	0.49
42:m:64:ILE:HG21	84:f:181:GLY:HA3	1.93	0.49
55:AJ:52:THR:HG22	55:AJ:58:LEU:HD12	1.94	0.49
76:A4:372:TYR:O	76:A4:376:ILE:HD12	2.12	0.49
76:A4:513:TRP:CE2	76:A4:555:ILE:HG13	2.47	0.49
78:Aw:16:A:N6	78:Aw:56:A:H2'	2.27	0.49
6:5:30:ALA:HB2	12:D:110:LEU:HD22	1.94	0.49
11:A:2900:C:H2'	11:A:2901:A:H8	1.77	0.49
18:k:27:PRO:HG2	18:k:30:LYS:HB2	1.94	0.49
22:O:46:TRP:CD1	22:O:121:ALA:HB2	2.47	0.49
42:m:90:ARG:HH21	46:AA:1396:C:C3'	1.99	0.49
46:AA:1552:G:H2'	46:AA:1553:A:C8	2.47	0.49
52:AG:237:GLU:HA	52:AG:237:GLU:OE2	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:AJ:102:LEU:HD11	55:AJ:108:VAL:HG11	1.93	0.49
76:A4:295:ASN:OD1	76:A4:334:THR:HG22	2.11	0.49
85:p:178:ILE:HD12	85:p:179:ARG:N	2.27	0.49
9:8:192:TYR:HB3	84:f:132:ILE:HD11	1.93	0.49
11:A:1750:G:H2'	11:A:1751:A:C8	2.47	0.49
11:A:2704:A:H2'	11:A:2705:U:C6	2.48	0.49
19:L:134:TYR:O	19:L:138:LEU:HD12	2.13	0.49
29:W:67:ILE:HG21	29:W:131:VAL:HG11	1.93	0.49
46:AA:777:G:H5''	59:AN:21:LYS:HB3	1.93	0.49
48:AC:62:ILE:HD13	48:AC:66:LYS:HE2	1.94	0.49
71:AZ:86:LYS:HG3	71:AZ:91:LYS:HB2	1.95	0.49
76:A4:405:PHE:HB2	76:A4:447:PHE:CE2	2.45	0.49
76:A4:599:PHE:HA	76:A4:604:LYS:HE3	1.94	0.49
11:A:2405:C:OP1	12:D:78:LYS:NZ	2.46	0.49
11:A:2728:C:H2'	11:A:2729:U:C6	2.48	0.49
17:J:90:PHE:HB3	17:J:120:ILE:HG12	1.94	0.49
30:X:151:GLU:CD	30:X:151:GLU:H	2.20	0.49
36:g:96:VAL:HG22	36:g:110:ILE:HG12	1.94	0.49
46:AA:675:A:H2'	46:AA:676:G:H8	1.77	0.49
46:AA:1042:U:H2'	46:AA:1043:C:H6	1.77	0.49
46:AA:1174:U:H2'	46:AA:1175:G:H8	1.77	0.49
81:a:75:ILE:HG22	81:a:77:ARG:HG2	1.94	0.49
85:p:110:TRP:H	85:p:110:TRP:CD1	2.30	0.49
10:9:128:PHE:HD1	10:9:135:PHE:HB3	1.77	0.49
11:A:2049:U:H2'	11:A:2050:A:H8	1.76	0.49
11:A:2661:U:H2'	11:A:2662:A:C8	2.47	0.49
50:AE:26:ILE:HG23	50:AE:36:VAL:HG21	1.94	0.49
52:AG:364:MET:HG2	52:AG:369:LEU:HD12	1.94	0.49
60:AO:48:ILE:HA	60:AO:52:LYS:HZ1	1.78	0.49
67:AV:376:GLU:O	67:AV:380:GLN:HG2	2.12	0.49
82:c:238:MET:HA	82:c:238:MET:HE3	1.95	0.49
7:6:47:ARG:H	7:6:47:ARG:NE	2.07	0.49
11:A:1829:A:H2'	11:A:1830:G:C8	2.47	0.49
11:A:2060:A:C8	11:A:2079:C:C4	3.00	0.49
46:AA:1056:A:H4'	46:AA:1588:G:N2	2.27	0.49
46:AA:1069:A:H5''	46:AA:1070:C:H5	1.77	0.49
49:AD:121:LYS:HA	49:AD:121:LYS:HE3	1.95	0.49
54:AI:92:HIS:HA	54:AI:156:PRO:HD3	1.93	0.49
59:AN:110:LEU:HD21	66:AU:124:LEU:HB2	1.94	0.49
69:AX:324:LEU:HD13	73:A1:304:GLU:HG2	1.93	0.49
76:A4:369:LEU:HD23	76:A4:415:PHE:HD2	1.77	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:5:113:LEU:HD12	6:5:311:ALA:HB1	1.94	0.49
8:7:230:PHE:HD2	8:7:240:ILE:HD11	1.75	0.49
11:A:1814:A:H2'	11:A:1815:A:H8	1.77	0.49
11:A:2403:G:O3'	11:A:2404:U:O2	2.31	0.49
16:I:119:HIS:CD2	16:I:163:GLU:HG3	2.47	0.49
24:Q:60:PRO:HD2	67:AV:90:TYR:CD2	2.48	0.49
28:U:137:ARG:HH11	33:V:104:TYR:HE1	1.61	0.49
33:V:124:ASP:OD1	33:V:126:MET:HG2	2.13	0.49
50:AE:115:GLU:OE1	50:AE:115:GLU:N	2.46	0.49
61:AP:113:ARG:O	61:AP:117:MET:HG2	2.13	0.49
63:AR:128:MET:HE1	63:AR:269:GLY:HA3	1.93	0.49
65:AT:32:VAL:HB	65:AT:66:MET:HG3	1.95	0.49
11:A:2099:U:H2'	11:A:2100:C:H6	1.78	0.49
11:A:3174:U:H2'	11:A:3175:A:C8	2.48	0.49
46:AA:1408:A:H2'	46:AA:1409:A:H8	1.77	0.49
47:AB:263:LYS:HA	47:AB:266:GLN:HG2	1.94	0.49
73:A1:214:LEU:HB2	73:A1:217:GLN:HG3	1.94	0.49
79:Ax:28:C:H2'	79:Ax:29:U:H6	1.77	0.49
80:B:29:C:H2'	80:B:30:A:H8	1.78	0.49
82:c:234:ILE:HD11	82:c:237:PRO:HB3	1.95	0.49
85:p:115:VAL:HG13	85:p:161:ALA:HB3	1.94	0.49
11:A:1735:A:H2'	11:A:1735:A:N3	2.27	0.49
17:J:159:LEU:HD21	17:J:164:LEU:HD23	1.93	0.49
33:V:154:ILE:HD12	33:V:155:PRO:HD2	1.94	0.49
35:e:114:ILE:HG23	69:AX:169:LEU:CD1	2.43	0.49
46:AA:1173:C:H2'	46:AA:1174:U:C6	2.48	0.49
67:AV:113:ILE:HG23	67:AV:147:LEU:HD12	1.94	0.49
69:AX:244:LEU:HG	69:AX:296:MET:SD	2.52	0.49
77:Az:15:U:H6	77:Az:15:U:H5''	1.77	0.49
79:Ax:29:U:H3	79:Ax:41:A:H61	1.61	0.49
8:7:209:LEU:HD12	8:7:257:ILE:HD11	1.95	0.48
11:A:2051:A:H2'	11:A:2052:A:C8	2.48	0.48
11:A:2455:U:H2'	11:A:2456:U:H6	1.78	0.48
17:J:88:SER:HA	17:J:151:LEU:HD11	1.94	0.48
24:Q:59:LYS:HA	67:AV:90:TYR:CZ	2.47	0.48
31:Y:191:ASN:HB3	31:Y:194:TYR:HB3	1.95	0.48
35:e:101:LYS:HE3	69:AX:231:THR:CA	2.21	0.48
43:o:12:ILE:HG21	43:o:16:GLN:HA	1.94	0.48
46:AA:1004:G:H5'	54:AI:96:GLN:HE22	1.77	0.48
47:AB:197:HIS:CD2	47:AB:240:ASP:HB2	2.42	0.48
51:AF:50:TYR:HD1	51:AF:51:TYR:CD1	2.31	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:AX:126:LEU:HB2	69:AX:309:ALA:HA	1.94	0.48
6:5:215:ARG:HD2	6:5:364:LEU:O	2.14	0.48
11:A:2558:A:C4	46:AA:1001:C:N4	2.81	0.48
11:A:3115:U:H2'	11:A:3116:C:C6	2.48	0.48
15:H:138:LYS:HE3	15:H:138:LYS:HB3	1.56	0.48
25:R:94:GLN:NE2	25:R:145:VAL:HG13	2.26	0.48
32:Z:137:THR:HG21	39:j:74:ALA:HB2	1.93	0.48
42:m:119:TYR:CZ	73:A1:227:THR:O	2.66	0.48
51:AF:51:TYR:HA	51:AF:66:ARG:HH12	1.78	0.48
53:AH:177:LEU:HB3	73:A1:147:PHE:HB3	1.94	0.48
60:AO:59:LEU:HD22	60:AO:121:LYS:HB3	1.95	0.48
70:AY:339:GLU:OE1	70:AY:339:GLU:HA	2.12	0.48
2:1:54:VAL:HG22	44:q:128:MET:HE3	1.95	0.48
14:F:175:LYS:O	14:F:179:THR:HG23	2.13	0.48
18:k:36:SER:O	18:k:40:GLN:HG3	2.13	0.48
23:P:165:MET:HE3	23:P:165:MET:HB3	1.76	0.48
24:Q:58:PRO:C	67:AV:90:TYR:CD1	2.91	0.48
27:T:112:LYS:NZ	27:T:116:LEU:HD11	2.28	0.48
46:AA:931:C:C2	55:AJ:42:PRO:HD3	2.48	0.48
49:AD:409:GLU:OE1	49:AD:409:GLU:HA	2.14	0.48
57:AL:104:LEU:HD21	57:AL:138:SER:HB2	1.95	0.48
63:AR:338:LYS:HE2	63:AR:341:TYR:HB3	1.94	0.48
69:AX:72:PRO:HA	69:AX:75:LEU:HD23	1.95	0.48
78:Aw:26:U:C5'	78:Aw:26:U:C6	2.60	0.48
79:Ax:57:A:H2'	79:Ax:58:A:H8	1.77	0.48
4:3:173:VAL:HG22	4:3:174:ASP:OD2	2.12	0.48
46:AA:659:U:H2'	46:AA:660:C:C6	2.49	0.48
46:AA:799:A:H2'	46:AA:800:C:C6	2.49	0.48
46:AA:1195:U:H2'	46:AA:1196:A:C8	2.48	0.48
67:AV:219:VAL:HG22	67:AV:355:LEU:HG	1.95	0.48
69:AX:170:GLN:HE22	69:AX:175:LYS:HG3	1.78	0.48
76:A4:465:ILE:HG22	76:A4:474:THR:HG23	1.94	0.48
86:s:365:LYS:HG3	86:s:402:TYR:CZ	2.48	0.48
6:5:66:PHE:HE1	6:5:72:ARG:HH21	1.60	0.48
7:6:161:LEU:HD13	7:6:271:LEU:HD11	1.94	0.48
8:7:107:LEU:HD13	8:7:128:LEU:HD11	1.96	0.48
9:8:137:ARG:HD3	9:8:138:ALA:N	2.28	0.48
11:A:1728:U:H2'	11:A:1729:U:O4'	2.13	0.48
11:A:1929:A:H2'	11:A:1930:C:C6	2.48	0.48
11:A:2245:A:H5''	45:r:189:ARG:HH21	1.79	0.48
11:A:2699:C:H2'	11:A:2700:G:H8	1.79	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:V:199:MET:HE3	33:V:199:MET:HB3	1.75	0.48
46:AA:659:U:H2'	46:AA:660:C:H6	1.77	0.48
67:AV:79:ILE:HG23	67:AV:84:GLU:HB2	1.96	0.48
69:AX:153:LEU:HD12	69:AX:260:VAL:HG13	1.95	0.48
78:Aw:21:A:C2	78:Aw:48:U:C2	3.01	0.48
6:5:181:VAL:HG21	6:5:294:LEU:HD21	1.95	0.48
17:J:67:PRO:HD3	17:J:85:PRO:HA	1.95	0.48
45:r:69:GLN:HB2	94:r:201:FES:S2	2.53	0.48
52:AG:256:LEU:H	52:AG:256:LEU:HD12	1.79	0.48
72:A0:57:ASP:OD1	72:A0:83:LYS:HE2	2.14	0.48
75:A3:166:GLN:NE2	75:A3:193:LYS:HA	2.29	0.48
11:A:2101:C:H2'	11:A:2102:A:H8	1.79	0.48
11:A:2746:U:H2'	11:A:2747:U:C6	2.48	0.48
11:A:2751:G:H2'	11:A:2752:C:C6	2.49	0.48
46:AA:701:G:H2'	46:AA:702:C:C6	2.48	0.48
46:AA:839:A:H2'	46:AA:840:A:H8	1.78	0.48
46:AA:1362:G:H2'	46:AA:1363:C:C6	2.49	0.48
67:AV:224:GLN:HB3	67:AV:262:VAL:HG21	1.95	0.48
78:Aw:67:U:H3'	78:Aw:67:U:OP2	2.14	0.48
82:c:227:GLU:HG3	82:c:230:GLU:HG3	1.96	0.48
85:p:100:GLU:HB2	85:p:136:THR:HG22	1.96	0.48
11:A:2108:G:H2'	11:A:2109:A:H2'	1.95	0.48
11:A:2275:U:H2'	11:A:2276:C:H6	1.79	0.48
11:A:2298:A:N6	14:F:145:LEU:HD22	2.29	0.48
11:A:3144:A:H2'	11:A:3145:A:H8	1.78	0.48
22:O:71:ARG:HG2	22:O:71:ARG:HH11	1.79	0.48
29:W:113:ALA:O	29:W:117:ILE:HG23	2.14	0.48
35:e:114:ILE:HG21	69:AX:169:LEU:HD11	1.94	0.48
38:i:67:GLU:HA	38:i:67:GLU:OE2	2.14	0.48
46:AA:852:A:H3'	46:AA:853:C:H6	1.79	0.48
68:AW:154:LEU:HB3	74:G:29:LEU:HG	1.96	0.48
11:A:1803:A:H4'	11:A:1804:A:H3'	1.95	0.48
11:A:2404:U:C6	92:A:3472:NMY:H10	2.49	0.48
18:k:74:GLN:HB3	45:r:162:ILE:HD12	1.95	0.48
24:Q:100:LEU:HD21	24:Q:286:ILE:HG12	1.96	0.48
37:h:78:PHE:CE2	37:h:96:LEU:HD12	2.48	0.48
46:AA:969:A:H2'	46:AA:970:A:C8	2.48	0.48
46:AA:1467:C:H2'	46:AA:1468:U:C6	2.48	0.48
47:AB:169:ARG:HG3	52:AG:159:TYR:CE1	2.49	0.48
47:AB:265:GLN:OE1	47:AB:265:GLN:HA	2.13	0.48
50:AE:6:LEU:HD13	50:AE:93:ILE:HG13	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
76:A4:247:ILE:H	76:A4:247:ILE:HD12	1.78	0.48
76:A4:436:HIS:HE1	76:A4:440:LYS:HE3	1.78	0.48
83:d:86:ASP:HB3	83:d:198:ARG:HG3	1.96	0.48
84:f:114:CYS:HB3	84:f:119:ILE:HB	1.95	0.48
6:5:128:LEU:HD11	6:5:376:VAL:HG22	1.95	0.48
9:8:117:LEU:HA	9:8:120:LYS:HE2	1.96	0.48
11:A:3143:U:H2'	11:A:3144:A:C8	2.49	0.48
14:F:70:ARG:HA	14:F:196:PRO:HD3	1.95	0.48
16:I:135:LEU:HD11	16:I:147:PHE:CD2	2.49	0.48
22:O:20:LEU:H	22:O:24:SER:HB3	1.79	0.48
39:j:65:ARG:O	39:j:69:GLU:HG3	2.13	0.48
46:AA:1165:C:H2'	46:AA:1166:A:C8	2.48	0.48
46:AA:1174:U:H2'	46:AA:1175:G:C8	2.49	0.48
46:AA:1422:G:N3	79:Ax:41:A:O2'	2.46	0.48
46:AA:1572:A:H2'	46:AA:1573:A:C8	2.48	0.48
63:AR:294:ILE:O	63:AR:298:THR:HG23	2.14	0.48
65:AT:110:GLU:O	65:AT:114:ARG:HG2	2.14	0.48
76:A4:266:MET:HB2	76:A4:275:ALA:HB2	1.95	0.48
13:E:96:ARG:NH2	13:E:314:LEU:HD13	2.29	0.47
16:I:90:PHE:CD1	16:I:96:ILE:HD13	2.49	0.47
24:Q:154:VAL:HB	24:Q:199:THR:HG22	1.95	0.47
49:AD:316:CYS:HB2	49:AD:334:ALA:HB3	1.96	0.47
4:3:115:LEU:HB2	20:M:83:PHE:HB3	1.96	0.47
92:A:3472:NMY:H9	92:A:3472:NMY:H1	1.46	0.47
12:D:257:ILE:O	12:D:262:ARG:HD2	2.14	0.47
18:k:117:HIS:HB3	18:k:121:MET:HE3	1.96	0.47
38:i:97:MET:HE2	38:i:97:MET:HB3	1.79	0.47
38:i:102:MET:HE3	38:i:107:LEU:HD23	1.95	0.47
46:AA:806:C:C2	72:A0:11:ILE:HB	2.49	0.47
46:AA:1042:U:H2'	46:AA:1043:C:C6	2.49	0.47
49:AD:172:MET:HA	49:AD:175:GLN:HG3	1.97	0.47
50:AE:115:GLU:HG2	50:AE:116:LYS:HG3	1.95	0.47
52:AG:87:HIS:ND1	73:A1:82:PRO:HB2	2.29	0.47
57:AL:223:ARG:HB3	57:AL:224:ARG:NH1	2.29	0.47
62:C:51:ARG:O	62:C:55:GLU:HG3	2.14	0.47
67:AV:154:LYS:HE2	67:AV:154:LYS:N	2.28	0.47
72:A0:88:GLN:HG2	72:A0:89:HIS:CE1	2.49	0.47
78:Aw:28:A:C6	78:Aw:29:U:C4	3.02	0.47
81:a:45:CYS:HA	81:a:65:VAL:HG13	1.95	0.47
11:A:2404:U:H2'	11:A:2405:C:C4	2.49	0.47
11:A:2691:U:H2'	11:A:2692:G:C8	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:2747:U:H2'	11:A:2748:A:H8	1.78	0.47
18:k:59:ILE:HG22	18:k:62:THR:HG22	1.96	0.47
35:e:55:ARG:HH22	35:e:153:LEU:HD23	1.79	0.47
55:AJ:128:GLY:HA3	55:AJ:134:HIS:CE1	2.49	0.47
58:AM:89:LYS:HG3	58:AM:103:MET:SD	2.55	0.47
73:A1:76:PHE:CE1	73:A1:81:VAL:HG21	2.49	0.47
79:Ax:71:U:H2'	79:Ax:72:A:H8	1.77	0.47
80:B:28:C:H2'	80:B:29:C:H6	1.79	0.47
85:p:160:GLU:OE1	85:p:160:GLU:HA	2.14	0.47
9:8:52:LYS:HE3	78:Aw:25:C:OP1	2.14	0.47
11:A:2596:G:H5'	75:A3:152:PHE:HD2	1.63	0.47
26:S:142:THR:HG23	81:a:60:CYS:HB2	1.96	0.47
45:r:78:LYS:HE3	45:r:79:HIS:CE1	2.49	0.47
46:AA:1033:U:H4'	50:AE:94:VAL:HG12	1.95	0.47
46:AA:1191:C:H2'	46:AA:1192:C:C6	2.49	0.47
46:AA:1383:A:H2'	51:AF:198:ARG:HD2	1.96	0.47
48:AC:76:LEU:HD13	53:AH:83:HIS:CE1	2.50	0.47
49:AD:196:ASN:C	77:Az:14:A:H62	2.23	0.47
51:AF:58:LEU:HD23	51:AF:62:GLU:OE1	2.14	0.47
63:AR:213:GLU:HA	63:AR:216:ARG:HH21	1.80	0.47
67:AV:187:PHE:CD2	67:AV:352:LEU:HD13	2.49	0.47
79:Ax:48:U:H5''	79:Ax:48:U:H6	1.79	0.47
28:U:153:LEU:HD21	83:d:240:LYS:HD2	1.96	0.47
51:AF:88:ASP:HB3	51:AF:91:ILE:HB	1.95	0.47
63:AR:170:ARG:HD2	63:AR:193:ILE:HD11	1.95	0.47
74:G:43:ALA:HB1	74:G:46:ILE:HD11	1.95	0.47
76:A4:307:GLU:OE1	76:A4:311:GLU:HB2	2.14	0.47
78:Aw:2:G:C6	78:Aw:72:A:C6	3.02	0.47
83:d:165:THR:HG23	83:d:168:CYS:H	1.79	0.47
86:s:403:GLU:HG2	86:s:412:GLY:HA3	1.97	0.47
3:2:79:ILE:O	3:2:83:MET:HG3	2.14	0.47
8:7:279:GLU:HB3	8:7:317:LEU:HD21	1.97	0.47
9:8:132:GLU:O	9:8:136:ILE:HD12	2.15	0.47
11:A:2049:U:H2'	11:A:2050:A:C8	2.48	0.47
11:A:2098:G:OP1	92:A:3474:NMY:H61	2.13	0.47
11:A:3089:A:OP2	79:Ax:74:C:H4'	2.14	0.47
16:I:163:GLU:H	16:I:163:GLU:CD	2.23	0.47
24:Q:255:LYS:HB3	24:Q:255:LYS:NZ	2.30	0.47
28:U:130:LEU:HD13	83:d:66:VAL:HG13	1.95	0.47
46:AA:1455:U:O3'	52:AG:336:GLY:HA3	2.14	0.47
67:AV:44:GLU:CD	67:AV:44:GLU:H	2.22	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:AV:183:LEU:O	67:AV:187:PHE:HB2	2.15	0.47
78:Aw:10:G:C6	78:Aw:26:U:O2	2.66	0.47
78:Aw:13:U:H1'	78:Aw:23:A:N1	2.30	0.47
78:Aw:14:A:C6	78:Aw:22:A:C5	3.02	0.47
4:3:127:ALA:HA	20:M:79:PRO:HD3	1.97	0.47
10:9:54:LYS:HG3	10:9:55:GLU:OE1	2.15	0.47
11:A:2553:G:H2'	11:A:2554:A:H8	1.79	0.47
11:A:2734:A:H2'	11:A:2735:G:C8	2.46	0.47
13:E:142:MET:HE2	13:E:180:ASN:HB3	1.97	0.47
14:F:87:PHE:C	14:F:179:THR:HG22	2.40	0.47
18:k:140:ASN:HB2	82:c:262:GLY:HA2	1.95	0.47
20:M:115:PRO:HD3	20:M:255:MET:HG2	1.97	0.47
21:N:61:LYS:HE2	21:N:61:LYS:HB3	1.68	0.47
24:Q:182:ARG:HG3	24:Q:187:LEU:HD11	1.96	0.47
31:Y:237:LYS:HG3	33:V:45:VAL:HG11	1.96	0.47
46:AA:657:G:OP2	92:AA:1785:NMY:N6	2.47	0.47
46:AA:1132:U:H2'	46:AA:1133:C:C6	2.50	0.47
48:AC:52:THR:HG22	48:AC:53:TYR:H	1.79	0.47
51:AF:59:THR:O	51:AF:63:LYS:HG2	2.15	0.47
51:AF:164:GLY:HA2	77:Az:1:U:P	2.54	0.47
55:AJ:71:LYS:HE2	55:AJ:119:PRO:HG3	1.96	0.47
58:AM:73:ILE:O	58:AM:77:ILE:HG12	2.15	0.47
60:AO:95:ILE:HD12	60:AO:95:ILE:O	2.13	0.47
62:C:54:ARG:O	62:C:58:GLU:HG3	2.15	0.47
65:AT:46:LYS:HD3	65:AT:46:LYS:HA	1.67	0.47
69:AX:295:LYS:NZ	98:AX:503:GDP:H5''	2.30	0.47
73:A1:223:VAL:O	73:A1:227:THR:HG23	2.15	0.47
76:A4:342:LEU:HD13	76:A4:349:ALA:HB1	1.96	0.47
77:Az:2:A:H3'	77:Az:3:A:H8	1.80	0.47
78:Aw:50:A:H2'	78:Aw:50:A:N3	2.29	0.47
18:k:100:PRO:HB2	18:k:129:PRO:HB3	1.96	0.47
19:L:98:PRO:HA	24:Q:162:ILE:HG12	1.96	0.47
22:O:98:LYS:HB3	22:O:98:LYS:NZ	2.30	0.47
24:Q:62:ILE:HD11	67:AV:50:LEU:HD23	1.97	0.47
46:AA:1427:A:H2'	46:AA:1428:G:C8	2.50	0.47
46:AA:1553:A:H2'	46:AA:1554:G:C8	2.50	0.47
47:AB:158:MET:HE3	47:AB:158:MET:HB2	1.74	0.47
72:A0:95:TRP:CH2	72:A0:118:LEU:HB2	2.50	0.47
76:A4:263:ILE:HD11	76:A4:293:THR:HA	1.95	0.47
7:6:195:PRO:HG3	7:6:321:CYS:SG	2.55	0.47
11:A:3144:A:H2'	11:A:3145:A:C8	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:F:234:THR:HG21	14:F:242:LEU:HB2	1.96	0.47
46:AA:1004:G:H5'	54:AI:96:GLN:NE2	2.30	0.47
46:AA:1220:A:H2	79:Ax:34:C:H5'	1.79	0.47
63:AR:72:ASP:HB2	63:AR:75:VAL:HG12	1.97	0.47
76:A4:593:TRP:HA	76:A4:596:LEU:HD13	1.96	0.47
78:Aw:11:U:H3	78:Aw:24:A:N6	2.11	0.47
78:Aw:23:A:C3'	78:Aw:24:A:H8	2.27	0.47
78:Aw:54:U:C4	78:Aw:55:A:H1'	2.50	0.47
79:Ax:6:A:H61	79:Ax:67:U:H3	1.63	0.47
82:c:159:PHE:HD2	82:c:160:LEU:HD22	1.79	0.47
85:p:175:LEU:HA	85:p:178:ILE:HG13	1.97	0.47
9:8:139:MET:HA	9:8:142:ALA:HB3	1.95	0.47
11:A:1861:U:H2'	11:A:1862:U:C6	2.49	0.47
11:A:2776:G:H2'	11:A:2777:G:C8	2.50	0.47
17:J:188:GLU:HA	17:J:191:LYS:HD2	1.97	0.47
23:P:171:VAL:HG12	23:P:173:ARG:H	1.80	0.47
28:U:141:ASP:HB3	28:U:144:ARG:HG2	1.96	0.47
32:Z:47:GLN:HA	32:Z:47:GLN:OE1	2.15	0.47
42:m:106:TYR:CE2	71:AZ:9:PHE:CD2	2.99	0.47
42:m:123:TRP:CE3	70:AY:329:HIS:CG	3.03	0.47
45:r:174:MET:HE3	45:r:174:MET:HB2	1.87	0.47
46:AA:684:U:H2'	46:AA:685:A:H8	1.79	0.47
46:AA:821:U:H2'	46:AA:822:G:C8	2.45	0.47
68:AW:152:ARG:HB2	68:AW:159:ASP:OD1	2.14	0.47
78:Aw:3:G:N3	78:Aw:3:G:H2'	2.29	0.47
82:c:101:GLU:OE1	82:c:101:GLU:HA	2.14	0.47
6:5:55:LEU:HD21	30:X:163:ARG:HG2	1.97	0.46
7:6:224:HIS:CE1	7:6:227:GLU:H	2.33	0.46
11:A:2065:A:C4	11:A:2066:C:C5	3.04	0.46
11:A:2677:A:H2'	11:A:2678:A:C8	2.49	0.46
17:J:119:GLU:HB3	41:I:75:VAL:HG21	1.96	0.46
42:m:63:THR:C	42:m:64:ILE:HD13	2.40	0.46
46:AA:1473:C:C4	92:AA:1783:NMY:O3	2.64	0.46
49:AD:253:ALA:HB1	49:AD:279:LEU:HD12	1.96	0.46
51:AF:229:MET:HE3	51:AF:229:MET:HB3	1.73	0.46
61:AP:103:LYS:HD3	61:AP:103:LYS:HA	1.75	0.46
63:AR:297:ALA:O	63:AR:301:VAL:HG22	2.15	0.46
84:f:135:LEU:HD12	84:f:146:LEU:HA	1.97	0.46
6:5:193:LEU:HD11	86:s:190:PRO:HA	1.96	0.46
6:5:393:LYS:HE2	11:A:1936:A:N6	2.30	0.46
9:8:160:GLU:HA	9:8:163:LYS:HD2	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:1828:A:H4'	11:A:1829:A:C8	2.50	0.46
11:A:2286:A:H2'	11:A:2287:U:C6	2.50	0.46
24:Q:57:PRO:HD2	67:AV:93:TYR:CE2	2.50	0.46
46:AA:1416:A:H2'	46:AA:1417:A:C8	2.50	0.46
48:AC:96:MET:HE1	48:AC:143:LEU:HD11	1.98	0.46
55:AJ:136:GLN:OE1	55:AJ:136:GLN:HA	2.14	0.46
57:AL:219:LYS:HB2	57:AL:219:LYS:NZ	2.31	0.46
69:AX:119:TYR:CG	73:A1:269:MET:HE1	2.51	0.46
76:A4:199:GLY:HA3	76:A4:269:HIS:CE1	2.50	0.46
85:p:121:ILE:O	85:p:124:LYS:HG2	2.15	0.46
7:6:234:HIS:CE1	7:6:257:PRO:HA	2.50	0.46
8:7:323:MET:HA	8:7:323:MET:HE2	1.97	0.46
9:8:122:SER:OG	80:B:29:C:H1'	2.14	0.46
11:A:2656:U:H4'	13:E:230:THR:OG1	2.16	0.46
11:A:3142:A:H2'	11:A:3143:U:C6	2.51	0.46
35:e:217:PHE:HE2	35:e:226:ASN:HB3	1.80	0.46
46:AA:1151:C:H5'	46:AA:1152:A:C8	2.50	0.46
51:AF:150:LYS:HE2	51:AF:150:LYS:HB2	1.80	0.46
76:A4:436:HIS:CE1	76:A4:440:LYS:HE3	2.51	0.46
78:Aw:23:A:H2'	78:Aw:24:A:C8	2.50	0.46
11:A:1688:A:H2'	11:A:1689:C:H4'	1.97	0.46
35:e:110:ASP:HB3	35:e:113:ASP:HB2	1.97	0.46
11:A:2596:G:H5''	75:A3:152:PHE:HD2	1.68	0.46
11:A:2942:C:H2'	11:A:2943:G:H8	1.81	0.46
43:o:51:MET:HE3	43:o:51:MET:HB2	1.86	0.46
63:AR:159:THR:HB	63:AR:172:ILE:HG23	1.97	0.46
67:AV:174:GLU:HA	67:AV:214:LYS:NZ	2.31	0.46
71:AZ:6:GLU:HA	71:AZ:6:GLU:OE2	2.15	0.46
76:A4:529:GLU:O	76:A4:533:MET:HG2	2.15	0.46
76:A4:571:TRP:HB3	76:A4:576:LEU:HD21	1.96	0.46
85:p:152:GLN:OE1	85:p:152:GLN:HA	2.15	0.46
7:6:330:ILE:H	7:6:330:ILE:HD12	1.80	0.46
9:8:70:ARG:NH1	79:Ax:50:G:H5''	2.30	0.46
11:A:1814:A:H2'	11:A:1815:A:C8	2.50	0.46
11:A:1829:A:H5''	25:R:31:PHE:CD1	2.51	0.46
11:A:2663:C:H2'	11:A:2664:U:H6	1.81	0.46
11:A:2668:A:H2'	11:A:2669:A:C8	2.51	0.46
11:A:2795:U:H2'	11:A:2796:G:H8	1.81	0.46
11:A:3141:A:H2'	11:A:3142:A:C8	2.50	0.46
11:A:3171:C:H4'	11:A:3172:C:C5	2.51	0.46
14:F:103:GLN:NE2	14:F:249:ASN:HD22	2.14	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:J:53:PHE:C	17:J:53:PHE:CD1	2.94	0.46
28:U:12:LEU:HD12	28:U:13:GLY:N	2.30	0.46
36:g:90:ARG:HG3	36:g:91:MET:SD	2.55	0.46
49:AD:388:ARG:NH1	49:AD:388:ARG:HB3	2.31	0.46
54:AI:172:VAL:HG12	62:C:14:VAL:HG11	1.96	0.46
58:AM:102:MET:HE2	58:AM:102:MET:HA	1.96	0.46
63:AR:75:VAL:HG23	63:AR:303:LEU:HD11	1.97	0.46
70:AY:349:HIS:CD2	71:AZ:24:ARG:HD2	2.50	0.46
76:A4:329:LYS:HD2	76:A4:329:LYS:HA	1.64	0.46
78:Aw:52:G:N2	78:Aw:63:A:H1'	2.30	0.46
7:6:265:ILE:HD12	7:6:265:ILE:N	2.30	0.46
11:A:2170:G:H2'	11:A:2171:U:C5	2.51	0.46
11:A:2782:A:C4	15:H:243:PRO:HD2	2.51	0.46
22:O:79:TRP:CE2	24:Q:269:MET:HE2	2.51	0.46
24:Q:54:PHE:HZ	67:AV:134:GLN:CB	2.12	0.46
46:AA:1171:A:H2'	46:AA:1172:C:O4'	2.15	0.46
48:AC:76:LEU:HD12	53:AH:138:THR:HG23	1.97	0.46
50:AE:21:THR:O	50:AE:25:THR:HG22	2.15	0.46
52:AG:57:PRO:HD3	77:Az:15:U:O2	2.15	0.46
8:7:68:LYS:HG3	8:7:78:VAL:HG12	1.98	0.46
11:A:2888:A:O2'	29:W:85:LYS:HD3	2.16	0.46
11:A:3169:C:H2'	11:A:3170:C:C6	2.50	0.46
15:H:242:LYS:HB2	15:H:245:THR:HG23	1.97	0.46
17:J:103:GLN:O	17:J:107:GLU:HG3	2.16	0.46
19:L:133:GLU:OE1	19:L:133:GLU:N	2.48	0.46
44:q:127:LYS:HE2	44:q:127:LYS:HB2	1.74	0.46
46:AA:911:U:H2'	46:AA:912:U:C6	2.51	0.46
58:AM:51:LEU:HD13	58:AM:73:ILE:HG12	1.97	0.46
58:AM:100:HIS:HA	66:AU:63:TYR:CE2	2.51	0.46
70:AY:336:LYS:H	70:AY:336:LYS:HD2	1.80	0.46
73:A1:249:GLU:CD	73:A1:249:GLU:H	2.24	0.46
76:A4:470:GLN:HE22	76:A4:472:ASP:HB3	1.81	0.46
9:8:176:PRO:HG2	42:m:35:SER:HB2	1.98	0.46
10:9:102:LYS:HB2	10:9:102:LYS:HE3	1.55	0.46
11:A:1952:U:H2'	11:A:1953:A:H8	1.80	0.46
29:W:49:ARG:HB3	29:W:51:GLN:HG3	1.97	0.46
46:AA:871:A:H1'	46:AA:872:G:C8	2.51	0.46
49:AD:380:LEU:HD12	49:AD:381:PRO:HD2	1.98	0.46
56:AK:62:ILE:HG21	70:AY:349:HIS:ND1	2.30	0.46
70:AY:351:MET:O	70:AY:355:THR:HG23	2.16	0.46
76:A4:263:ILE:HA	76:A4:266:MET:HG2	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
78:Aw:14:A:H3'	78:Aw:15:A:C8	2.46	0.46
84:f:106:TYR:O	84:f:110:VAL:HG22	2.16	0.46
1:0:184:TRP:CD1	1:0:184:TRP:H	2.34	0.46
9:8:52:LYS:HE2	78:Aw:39:U:OP1	2.16	0.46
11:A:2182:G:H2'	11:A:2183:C:C6	2.51	0.46
11:A:2221:C:H5	45:r:102:ARG:HH22	1.64	0.46
11:A:2514:C:H2'	11:A:2515:U:C6	2.51	0.46
16:I:161:VAL:HG21	16:I:194:TYR:HD2	1.80	0.46
22:O:83:LYS:HA	22:O:83:LYS:HD3	1.79	0.46
46:AA:1499:U:H2'	46:AA:1500:C:H6	1.80	0.46
51:AF:74:ILE:HG13	52:AG:366:GLN:HA	1.98	0.46
80:B:3:G:H2'	80:B:4:A:C8	2.51	0.46
84:f:191:GLU:O	84:f:195:LYS:HG2	2.15	0.46
11:A:2056:G:H2'	11:A:2057:C:H6	1.81	0.45
11:A:2751:G:H2'	11:A:2752:C:H6	1.81	0.45
11:A:3150:U:C2	11:A:3151:A:C8	3.04	0.45
13:E:99:LEU:HD23	13:E:193:LEU:HB3	1.99	0.45
15:H:184:LEU:HD12	15:H:213:ILE:HG21	1.98	0.45
40:n:16:VAL:HG12	40:n:66:VAL:HG22	1.97	0.45
46:AA:1038:C:H4'	57:AL:155:TYR:CE2	2.51	0.45
46:AA:1452:U:H2'	46:AA:1453:A:C8	2.51	0.45
49:AD:103:LEU:HD11	49:AD:123:ARG:HB2	1.98	0.45
55:AJ:137:LYS:HD2	55:AJ:138:LYS:HB2	1.97	0.45
59:AN:18:ILE:HD13	59:AN:29:ARG:HB2	1.96	0.45
79:Ax:23:A:H2'	79:Ax:24:A:H8	1.77	0.45
11:A:1936:A:H4'	11:A:1937:A:N7	2.31	0.45
16:I:39:VAL:HG11	43:o:22:ARG:HD2	1.98	0.45
18:k:150:LYS:HB3	18:k:150:LYS:HE2	1.64	0.45
20:M:238:ARG:HD3	85:p:71:ASP:OD2	2.16	0.45
26:S:94:ARG:HA	82:c:313:PRO:HD3	1.97	0.45
28:U:144:ARG:HD2	28:U:144:ARG:HA	1.75	0.45
40:n:97:ARG:HD3	40:n:97:ARG:HA	1.57	0.45
46:AA:1002:C:H2'	46:AA:1003:A:C8	2.51	0.45
46:AA:1347:G:H2'	46:AA:1348:G:H8	1.82	0.45
46:AA:1429:C:H4'	46:AA:1430:A:H5'	1.97	0.45
53:AH:63:VAL:HG22	76:A4:65:TRP:HB3	1.97	0.45
53:AH:163:ASN:HB3	73:A1:114:LEU:HD11	1.99	0.45
57:AL:89:VAL:O	57:AL:93:LEU:HG	2.16	0.45
61:AP:124:TYR:HE2	62:C:4:HIS:HB3	1.81	0.45
69:AX:104:PRO:HG2	69:AX:345:VAL:HG13	1.97	0.45
73:A1:87:MET:HE2	73:A1:104:GLU:HB3	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:D:171:ARG:NH2	50:AE:86:ILE:HD11	2.32	0.45
36:g:50:ARG:HG2	36:g:50:ARG:HH11	1.80	0.45
39:j:91:TRP:CD2	43:o:58:GLN:HG2	2.51	0.45
46:AA:1348:G:H2'	46:AA:1349:U:C6	2.51	0.45
46:AA:1462:G:H2'	46:AA:1463:G:C8	2.52	0.45
47:AB:142:ILE:HG13	47:AB:192:LEU:HD23	1.99	0.45
52:AG:111:LEU:HD22	73:A1:112:LEU:HD23	1.98	0.45
62:C:20:GLU:OE1	62:C:20:GLU:HA	2.16	0.45
67:AV:138:PHE:CG	72:A0:72:PRO:HA	2.52	0.45
79:Ax:8:U:O2	79:Ax:21:A:H2	1.99	0.45
83:d:124:ARG:HH12	83:d:202:MET:HG3	1.81	0.45
83:d:173:THR:HA	83:d:176:ILE:HD11	1.97	0.45
84:f:97:ALA:HB2	84:f:182:VAL:HG12	1.98	0.45
11:A:1806:U:H4'	11:A:1807:U:H5'	1.99	0.45
13:E:199:ARG:HD3	13:E:199:ARG:HA	1.84	0.45
24:Q:60:PRO:HB2	67:AV:87:HIS:CD2	2.48	0.45
37:h:113:PRO:HG2	37:h:116:ARG:HG3	1.99	0.45
46:AA:981:C:H2'	46:AA:982:A:H8	1.81	0.45
63:AR:194:GLN:HE22	63:AR:199:LYS:H	1.63	0.45
76:A4:451:ASP:HA	76:A4:454:ARG:HE	1.82	0.45
10:9:134:ASN:HB2	33:V:210:TYR:HE2	1.80	0.45
11:A:2868:C:H2'	11:A:2869:A:O4'	2.15	0.45
92:A:3474:NMY:O3	92:A:3474:NMY:H62	2.16	0.45
12:D:234:MET:HG3	12:D:295:TYR:HE1	1.81	0.45
24:Q:176:VAL:HG11	24:Q:179:LEU:HB2	1.98	0.45
40:n:77:ARG:O	40:n:81:LEU:HD23	2.16	0.45
45:r:70:CYS:HB2	45:r:107:LEU:HA	1.98	0.45
46:AA:1066:C:H2'	46:AA:1067:A:C8	2.52	0.45
47:AB:182:LEU:HD12	47:AB:182:LEU:H	1.81	0.45
53:AH:72:LEU:HB3	53:AH:177:LEU:HD23	1.98	0.45
65:AT:91:GLU:HG2	65:AT:92:THR:HG23	1.98	0.45
67:AV:394:GLN:OE1	67:AV:394:GLN:HA	2.16	0.45
69:AX:65:GLY:HA2	69:AX:100:MET:HE3	1.98	0.45
76:A4:197:TYR:CE1	76:A4:268:LYS:HE2	2.52	0.45
76:A4:436:HIS:CE1	76:A4:439:LEU:HD23	2.51	0.45
80:B:69:U:H2'	80:B:70:C:C6	2.51	0.45
86:s:105:TRP:CG	86:s:271:LEU:HD13	2.51	0.45
10:9:68:PHE:CE2	10:9:70:LEU:HB2	2.51	0.45
11:A:1936:A:H4'	11:A:1937:A:C8	2.52	0.45
11:A:2802:A:H2'	11:A:2803:A:O4'	2.16	0.45
20:M:107:LEU:HD13	36:g:60:PRO:HG3	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:W:117:ILE:HA	29:W:120:LEU:HG	1.97	0.45
36:g:140:VAL:HG22	36:g:147:LEU:HD23	1.98	0.45
42:m:52:TYR:CZ	42:m:71:PRO:HG3	2.52	0.45
42:m:107:GLU:HG2	71:AZ:9:PHE:CZ	2.51	0.45
46:AA:824:U:H2'	46:AA:825:U:C6	2.52	0.45
46:AA:1286:A:OP1	49:AD:260:LYS:HD2	2.16	0.45
52:AG:201:ILE:HG22	52:AG:204:GLU:HG2	1.99	0.45
53:AH:126:ILE:HB	53:AH:127:TYR:H	1.57	0.45
55:AJ:127:ARG:HD3	55:AJ:127:ARG:HA	1.75	0.45
76:A4:199:GLY:HA3	76:A4:269:HIS:HE1	1.82	0.45
76:A4:610:LEU:H	76:A4:610:LEU:HD23	1.81	0.45
11:A:3054:G:H2'	11:A:3055:U:C6	2.52	0.45
11:A:3200:U:H2'	11:A:3201:A:C2	2.52	0.45
16:I:40:MET:HE1	16:I:48:MET:HE2	1.99	0.45
20:M:44:ARG:HG3	20:M:45:ARG:HG2	1.98	0.45
46:AA:686:A:H2'	46:AA:687:G:C8	2.51	0.45
46:AA:1195:U:H2'	46:AA:1196:A:H8	1.81	0.45
46:AA:1441:A:H61	46:AA:1449:G:H1	1.64	0.45
46:AA:1578:A:H2'	46:AA:1579:C:H6	1.80	0.45
51:AF:195:LYS:HD3	51:AF:195:LYS:HA	1.78	0.45
63:AR:260:ASP:HB2	63:AR:291:ARG:NH1	2.32	0.45
69:AX:261:ALA:HA	69:AX:307:VAL:O	2.15	0.45
72:A0:100:VAL:HG12	72:A0:102:PRO:HD3	1.99	0.45
78:Aw:52:G:C3'	78:Aw:53:A:H8	2.28	0.45
78:Aw:72:A:H2'	78:Aw:73:U:C6	2.52	0.45
79:Ax:54:U:H2'	79:Ax:55:U:O4'	2.17	0.45
3:2:59:LYS:HG2	3:2:63:LYS:HE2	1.99	0.45
7:6:106:ARG:O	7:6:110:ILE:HG12	2.16	0.45
8:7:101:ARG:HG3	8:7:101:ARG:HH11	1.81	0.45
10:9:134:ASN:HB2	33:V:210:TYR:CE2	2.52	0.45
11:A:2392:U:H2'	11:A:2394:A:H62	1.82	0.45
11:A:3112:A:N7	11:A:3200:U:C2	2.84	0.45
16:I:192:ILE:HD12	16:I:193:ASN:N	2.31	0.45
46:AA:1439:A:H2'	46:AA:1440:G:H8	1.81	0.45
46:AA:1509:U:H2'	46:AA:1510:U:C6	2.52	0.45
60:AO:136:TYR:CE1	60:AO:139:TYR:HB2	2.52	0.45
76:A4:369:LEU:HD23	76:A4:415:PHE:CD2	2.51	0.45
79:Ax:24:A:H2'	79:Ax:25:C:H6	1.81	0.45
83:d:91:PRO:HG2	83:d:94:ASP:HB2	1.98	0.45
83:d:113:LYS:H	83:d:113:LYS:HG2	1.55	0.45
1:0:152:PRO:HG3	1:0:173:ARG:CZ	2.47	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:146:GLU:OE1	4:3:146:GLU:HA	2.17	0.45
11:A:1737:A:H61	11:A:1760:G:H1'	1.81	0.45
11:A:2801:A:H2'	11:A:2802:A:C8	2.52	0.45
39:j:71:GLU:O	39:j:75:ARG:HG3	2.17	0.45
46:AA:1035:U:H5''	50:AE:72:THR:HB	1.99	0.45
92:AA:1786:NMY:H16	92:AA:1786:NMY:N23	2.31	0.45
48:AC:58:ALA:HB3	48:AC:60:HIS:CE1	2.52	0.45
49:AD:140:LEU:HD11	49:AD:160:ARG:HG2	1.98	0.45
55:AJ:98:GLU:N	55:AJ:98:GLU:OE1	2.50	0.45
61:AP:80:LEU:HG	61:AP:111:ILE:HG13	1.99	0.45
64:AS:87:LEU:HD13	68:AW:89:LEU:HD13	1.99	0.45
72:A0:83:LYS:HA	72:A0:86:LEU:HD12	1.99	0.45
72:A0:108:ASN:HB2	72:A0:110:ASP:OD1	2.16	0.45
78:Aw:63:A:C2	78:Aw:64:U:C1'	3.00	0.45
1:0:158:VAL:HG22	1:0:175:ILE:HB	1.99	0.45
6:5:177:CYS:HB3	6:5:178:PRO:HD3	1.99	0.45
9:8:161:ALA:HB2	35:e:184:LEU:HD12	1.99	0.45
11:A:2795:U:H2'	11:A:2796:G:C8	2.52	0.45
13:E:48:TRP:CE2	13:E:51:GLU:HB2	2.52	0.45
41:l:87:LYS:HD3	41:l:91:GLU:HB3	1.99	0.45
46:AA:838:U:O3'	58:AM:21:LEU:HB2	2.17	0.45
46:AA:1572:A:H2'	46:AA:1573:A:H8	1.82	0.45
58:AM:115:ALA:O	58:AM:118:VAL:HG22	2.17	0.45
60:AO:115:VAL:HG13	60:AO:150:LEU:HD23	1.99	0.45
67:AV:278:GLU:HA	67:AV:281:ASP:OD2	2.17	0.45
69:AX:298:LYS:HB2	69:AX:298:LYS:HE2	1.67	0.45
72:A0:34:TYR:CZ	72:A0:135:MET:HE2	2.52	0.45
78:Aw:14:A:C5	78:Aw:22:A:C6	3.05	0.45
79:Ax:3:G:H2'	79:Ax:4:G:C8	2.52	0.45
79:Ax:21:A:C2	79:Ax:48:U:C2	3.05	0.45
85:p:154:ILE:O	85:p:158:ILE:HG12	2.17	0.45
2:1:20:MET:HE1	2:1:43:LEU:CD2	2.46	0.44
8:7:75:PRO:HB2	83:d:293:TYR:CZ	2.52	0.44
11:A:2227:A:H2'	11:A:2227:A:N3	2.32	0.44
11:A:2553:G:H2'	11:A:2554:A:C8	2.52	0.44
11:A:2639:C:H4'	75:A3:163:ARG:NH2	2.32	0.44
11:A:2757:A:H2'	11:A:2758:G:O4'	2.18	0.44
18:k:7:ALA:HB3	18:k:8:PRO:HD3	1.99	0.44
28:U:54:ARG:O	28:U:58:GLU:HG3	2.17	0.44
42:m:37:ARG:HE	84:f:109:TYR:HE2	1.63	0.44
46:AA:1400:U:H2'	46:AA:1401:G:C8	2.51	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:AA:1455:U:H2'	46:AA:1456:U:C6	2.52	0.44
49:AD:172:MET:HG2	49:AD:175:GLN:HE21	1.82	0.44
49:AD:183:LYS:HA	49:AD:183:LYS:HD2	1.82	0.44
54:AI:62:ILE:HD11	62:C:12:VAL:HB	1.99	0.44
69:AX:269:TRP:CH2	69:AX:297:MET:HG3	2.48	0.44
70:AY:259:PHE:HB2	76:A4:363:ILE:HD11	1.99	0.44
72:A0:82:ARG:HD3	72:A0:85:TRP:CE2	2.52	0.44
79:Ax:55:U:O2	79:Ax:57:A:H3'	2.17	0.44
11:A:1979:U:H2'	11:A:1980:A:C8	2.52	0.44
11:A:2007:U:H2'	11:A:2008:G:C8	2.52	0.44
11:A:2483:U:H2'	11:A:2484:C:O4'	2.16	0.44
12:D:205:GLN:HA	12:D:208:ARG:HH11	1.81	0.44
15:H:98:LEU:HD23	15:H:129:ALA:HB2	2.00	0.44
16:I:146:LEU:HD12	16:I:146:LEU:HA	1.74	0.44
46:AA:1036:A:H5''	57:AL:100:LYS:HB2	1.98	0.44
46:AA:1144:U:H2'	46:AA:1145:A:C8	2.52	0.44
46:AA:1194:C:H2'	46:AA:1195:U:C6	2.52	0.44
46:AA:1339:G:C2	46:AA:1340:C:C5	3.06	0.44
46:AA:1399:A:H2'	46:AA:1400:U:C6	2.53	0.44
46:AA:1478:A:C4	75:A3:131:LEU:HD21	2.52	0.44
46:AA:1527:A:H2'	46:AA:1528:A:O4'	2.16	0.44
48:AC:46:LYS:HA	48:AC:46:LYS:HD3	1.79	0.44
69:AX:210:TRP:CH2	69:AX:225:VAL:HG23	2.51	0.44
72:A0:114:ALA:C	72:A0:131:ILE:HD12	2.43	0.44
76:A4:152:ILE:HA	76:A4:172:MET:HE3	1.99	0.44
76:A4:448:ILE:HD13	76:A4:448:ILE:HA	1.82	0.44
78:Aw:12:U:H3	78:Aw:23:A:N6	2.15	0.44
10:9:39:LYS:HG3	11:A:1705:A:C8	2.52	0.44
11:A:2045:A:H2'	11:A:2046:C:H6	1.82	0.44
11:A:2051:A:H2'	11:A:2052:A:H8	1.82	0.44
11:A:2187:C:H2'	11:A:2188:A:C8	2.53	0.44
11:A:2346:U:H2'	11:A:2347:C:C6	2.52	0.44
13:E:271:LEU:HB3	13:E:285:VAL:HG13	1.99	0.44
14:F:221:LEU:HG	14:F:222:THR:HG23	2.00	0.44
20:M:136:TYR:O	20:M:157:GLN:HG2	2.18	0.44
35:e:159:LEU:HD23	35:e:254:TRP:CE2	2.52	0.44
35:e:165:PHE:HD1	93:e:301:VAL:HB	1.81	0.44
35:e:200:MET:HE1	35:e:243:PHE:HE1	1.82	0.44
52:AG:92:MET:HB2	52:AG:94:GLU:HG3	1.97	0.44
53:AH:81:LYS:HE2	53:AH:171:GLU:OE1	2.17	0.44
60:AO:235:MET:HE3	63:AR:149:GLU:O	2.16	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
76:A4:332:LEU:HD22	76:A4:365:ILE:HG23	1.99	0.44
79:Ax:50:G:C4	79:Ax:51:A:C8	3.05	0.44
9:8:83:ILE:HG23	9:8:199:TYR:HB2	2.00	0.44
9:8:91:PRO:HD2	9:8:94:PHE:CD2	2.52	0.44
11:A:2097:A:H3'	11:A:2098:G:H5''	1.99	0.44
11:A:3158:A:H2'	11:A:3159:A:C8	2.52	0.44
16:I:97:ALA:HB3	16:I:154:LEU:HB2	1.99	0.44
22:O:87:PRO:O	22:O:91:GLN:HG3	2.17	0.44
27:T:91:MET:HE2	27:T:95:GLN:OE1	2.17	0.44
30:X:14:LEU:HD12	30:X:14:LEU:HA	1.82	0.44
33:V:122:LEU:HD23	33:V:122:LEU:HA	1.84	0.44
38:i:42:LYS:HD3	38:i:42:LYS:HA	1.65	0.44
46:AA:659:U:OP1	49:AD:226:ARG:HD3	2.17	0.44
46:AA:798:C:H2'	46:AA:799:A:C8	2.53	0.44
51:AF:132:GLU:CD	51:AF:132:GLU:H	2.26	0.44
52:AG:78:ILE:HD11	52:AG:127:HIS:CE1	2.52	0.44
62:C:20:GLU:HB3	62:C:24:ARG:HH21	1.82	0.44
67:AV:213:LEU:HD22	72:A0:145:HIS:HB2	2.00	0.44
74:G:46:ILE:O	74:G:49:MET:HB3	2.18	0.44
74:G:48:GLU:H	74:G:48:GLU:CD	2.25	0.44
76:A4:243:ASN:O	76:A4:247:ILE:HD12	2.18	0.44
76:A4:610:LEU:HG	76:A4:611:LEU:HD22	1.98	0.44
78:Aw:63:A:C2	78:Aw:64:U:H1'	2.53	0.44
8:7:145:SER:O	8:7:149:MET:HG3	2.18	0.44
9:8:139:MET:HG3	84:f:169:ILE:HD11	1.98	0.44
11:A:2533:A:H2'	11:A:2534:G:C8	2.53	0.44
11:A:3174:U:H2'	11:A:3175:A:H8	1.82	0.44
22:O:79:TRP:NE1	24:Q:269:MET:HE2	2.32	0.44
24:Q:60:PRO:HD3	67:AV:90:TYR:CB	2.48	0.44
33:V:124:ASP:HB2	33:V:131:THR:HG21	1.99	0.44
36:g:47:PHE:HA	36:g:50:ARG:HH11	1.83	0.44
38:i:78:ILE:HD12	38:i:78:ILE:N	2.31	0.44
46:AA:826:A:C6	55:AJ:56:PRO:HD2	2.51	0.44
47:AB:137:TYR:HB2	47:AB:260:ALA:HB1	1.99	0.44
47:AB:175:MET:HE2	47:AB:183:PHE:CZ	2.52	0.44
62:C:21:SER:O	62:C:25:THR:HG23	2.17	0.44
65:AT:114:ARG:HG3	65:AT:114:ARG:NH1	2.33	0.44
67:AV:358:GLN:O	67:AV:362:GLU:HG2	2.18	0.44
76:A4:493:MET:O	76:A4:496:LEU:HG	2.18	0.44
79:Ax:56:C:C4	79:Ax:57:A:C6	3.06	0.44
10:9:87:THR:HG22	10:9:89:ALA:H	1.82	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:1991:A:H5''	11:A:1992:C:OP1	2.18	0.44
24:Q:244:ARG:NH2	24:Q:247:LEU:HD11	2.33	0.44
32:Z:101:LYS:HE2	39:j:80:LEU:HD22	1.99	0.44
33:V:104:TYR:HD1	33:V:105:ARG:N	2.15	0.44
38:i:38:LEU:HD23	38:i:38:LEU:HA	1.86	0.44
41:l:93:PRO:HB2	41:l:95:TRP:CD1	2.51	0.44
46:AA:786:G:H2'	46:AA:787:C:H6	1.83	0.44
46:AA:1525:C:H5	67:AV:103:TYR:HA	1.82	0.44
53:AH:129:LYS:HB3	53:AH:129:LYS:HE2	1.75	0.44
62:C:83:PRO:HA	68:AW:108:VAL:HG21	1.99	0.44
64:AS:117:LEU:O	64:AS:121:THR:HG22	2.18	0.44
69:AX:357:ILE:HD11	69:AX:391:LEU:HD11	2.00	0.44
78:Aw:50:A:C4	78:Aw:65:A:C2	3.05	0.44
79:Ax:21:A:H2'	79:Ax:46:A:N6	2.33	0.44
7:6:179:VAL:HG21	85:p:189:ARG:HH12	1.82	0.44
8:7:214:LEU:O	8:7:272:THR:HG23	2.18	0.44
11:A:2087:U:H2'	11:A:2088:U:C6	2.52	0.44
11:A:2491:C:H2'	11:A:2492:G:C8	2.52	0.44
11:A:3089:A:O5'	79:Ax:74:C:H5''	2.17	0.44
19:L:119:ILE:HB	19:L:141:ALA:HA	2.00	0.44
45:r:58:LYS:HE2	45:r:58:LYS:HB2	1.70	0.44
46:AA:1055:U:C2	46:AA:1056:A:C8	3.06	0.44
47:AB:175:MET:HE3	47:AB:175:MET:HA	2.00	0.44
69:AX:259:LEU:HD21	69:AX:261:ALA:HB2	2.00	0.44
70:AY:343:LYS:HE3	70:AY:344:GLN:HB3	2.00	0.44
75:A3:144:ARG:HH21	75:A3:147:VAL:HG11	1.83	0.44
76:A4:320:LEU:HA	76:A4:323:MET:HG3	1.99	0.44
11:A:2093:U:H2'	11:A:2094:G:C8	2.53	0.44
11:A:2457:A:H3'	22:O:10:SER:HB3	1.99	0.44
11:A:2495:U:O4	11:A:2509:A:H2	2.01	0.44
11:A:2750:U:H2'	11:A:2751:G:H8	1.82	0.44
14:F:249:ASN:ND2	14:F:252:SER:H	2.15	0.44
16:I:62:PRO:HA	16:I:65:LEU:HD12	1.99	0.44
18:k:131:GLU:HA	18:k:131:GLU:OE1	2.16	0.44
35:e:139:GLU:HA	35:e:142:GLU:HG2	2.00	0.44
45:r:189:ARG:HD3	45:r:189:ARG:HA	1.79	0.44
46:AA:1129:U:H2'	46:AA:1130:G:H8	1.83	0.44
46:AA:1279:C:H2'	46:AA:1280:C:C6	2.53	0.44
47:AB:231:LEU:HD23	47:AB:231:LEU:HA	1.88	0.44
48:AC:44:VAL:HA	48:AC:167:LEU:HG	2.00	0.44
80:B:43:G:H2'	80:B:44:A:C8	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:101:ARG:HG3	8:7:101:ARG:NH1	2.32	0.44
8:7:236:LYS:HA	8:7:236:LYS:HD3	1.73	0.44
11:A:2404:U:C6	92:A:3472:NMY:N9	2.85	0.44
12:D:218:ARG:NH2	12:D:220:VAL:HG21	2.33	0.44
20:M:142:GLU:HB2	20:M:162:LEU:HD12	1.99	0.44
24:Q:59:LYS:HG3	67:AV:90:TYR:CE2	2.53	0.44
42:m:89:ARG:O	42:m:93:LEU:HG	2.17	0.44
46:AA:1144:U:H2'	46:AA:1145:A:H8	1.82	0.44
46:AA:1485:G:H2'	46:AA:1486:B8T:O4'	2.17	0.44
49:AD:148:LEU:HD22	76:A4:109:ALA:HB2	2.00	0.44
49:AD:259:GLY:HA3	49:AD:271:ALA:HB2	2.00	0.44
59:AN:24:LYS:HB3	59:AN:24:LYS:HE2	1.81	0.44
66:AU:59:ARG:H	66:AU:59:ARG:HG2	1.60	0.44
70:AY:298:PHE:O	70:AY:302:ILE:HG12	2.18	0.44
70:AY:364:LEU:HB3	70:AY:368:GLN:HB2	2.00	0.44
75:A3:138:MET:HE3	75:A3:142:LYS:HG3	1.98	0.44
80:B:5:G:H2'	80:B:6:U:O4'	2.18	0.44
80:B:27:C:H2'	80:B:28:C:H6	1.82	0.44
82:c:175:VAL:O	82:c:179:THR:HG23	2.18	0.44
6:5:117:VAL:O	6:5:121:LEU:HG	2.18	0.43
7:6:240:ILE:HD12	7:6:240:ILE:O	2.17	0.43
11:A:2042:U:H2'	11:A:2043:C:C6	2.52	0.43
11:A:2753:A:C4	11:A:2754:A:C8	3.06	0.43
29:W:45:LYS:HE3	29:W:45:LYS:HB3	1.86	0.43
46:AA:715:G:H2'	46:AA:716:U:C6	2.53	0.43
46:AA:839:A:H2'	46:AA:840:A:C8	2.52	0.43
46:AA:853:C:H2'	46:AA:854:U:C6	2.53	0.43
46:AA:1395:C:H2'	46:AA:1396:C:H6	1.83	0.43
47:AB:101:PHE:CZ	64:AS:47:GLN:HG2	2.53	0.43
51:AF:205:LEU:HD23	51:AF:205:LEU:HA	1.85	0.43
61:AP:75:LYS:HE3	61:AP:75:LYS:HB2	1.60	0.43
76:A4:580:ALA:HA	76:A4:583:PHE:CD2	2.53	0.43
82:c:148:MET:HG3	82:c:149:PRO:HD2	1.99	0.43
86:s:332:LEU:HD13	86:s:372:TYR:HB2	2.00	0.43
6:5:333:ALA:HB1	6:5:363:ASP:HA	1.98	0.43
11:A:2807:U:H2'	11:A:2808:U:C6	2.53	0.43
11:A:2815:OMG:HM23	11:A:2815:OMG:H1'	1.53	0.43
13:E:218:VAL:HB	13:E:224:PHE:CD2	2.52	0.43
15:H:184:LEU:HB2	15:H:213:ILE:HB	1.99	0.43
16:I:101:ASN:HB2	16:I:150:HIS:HB3	1.99	0.43
40:n:39:SER:O	40:n:43:ARG:HG3	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:m:90:ARG:HH22	46:AA:1396:C:H3'	1.54	0.43
46:AA:1209:C:H2'	46:AA:1210:U:C6	2.53	0.43
53:AH:149:THR:OG1	53:AH:152:THR:HG22	2.18	0.43
61:AP:117:MET:HE3	61:AP:117:MET:HB3	1.75	0.43
78:Aw:36:C:C2	78:Aw:37:A:C8	3.06	0.43
78:Aw:68:U:C2	78:Aw:69:A:C8	3.06	0.43
84:f:170:PHE:CD1	84:f:170:PHE:C	2.96	0.43
10:9:69:LYS:HG3	33:V:181:ASP:CG	2.43	0.43
11:A:2550:A:C2	11:A:2551:G:C8	3.06	0.43
11:A:2745:A:H4'	30:X:102:LYS:O	2.19	0.43
11:A:2894:U:H5''	11:A:2895:U:O4'	2.19	0.43
13:E:210:THR:HG22	13:E:290:PRO:HB3	1.99	0.43
15:H:195:LYS:HB3	15:H:195:LYS:HE2	1.77	0.43
21:N:138:HIS:HE1	79:Ax:1:U:H4'	1.82	0.43
22:O:30:ARG:HD2	22:O:78:PHE:O	2.19	0.43
23:P:86:THR:HG23	23:P:89:HIS:H	1.83	0.43
40:n:67:LEU:HD12	40:n:67:LEU:HA	1.80	0.43
46:AA:900:C:H41	55:AJ:74:ASN:HD21	1.66	0.43
46:AA:1220:A:N6	46:AA:1484:C:H42	2.17	0.43
46:AA:1269:U:H4'	46:AA:1270:U:H3'	2.00	0.43
48:AC:156:GLN:HE21	73:A1:101:GLY:H	1.65	0.43
63:AR:241:GLU:H	63:AR:241:GLU:CD	2.26	0.43
76:A4:126:LYS:HE2	76:A4:126:LYS:HB2	1.94	0.43
83:d:90:PRO:HB2	83:d:269:TRP:HE1	1.83	0.43
4:3:126:LYS:HE3	4:3:126:LYS:HB3	1.89	0.43
11:A:2187:C:H2'	11:A:2188:A:H8	1.83	0.43
11:A:3151:A:H4'	24:Q:146:GLY:O	2.18	0.43
12:D:192:LEU:HD23	12:D:215:VAL:HG12	2.00	0.43
17:J:73:LYS:HB2	17:J:77:THR:HG22	2.00	0.43
46:AA:705:C:H2'	72:A0:136:TYR:CZ	2.53	0.43
46:AA:896:A:H2'	46:AA:897:C:C6	2.53	0.43
46:AA:983:C:H2'	46:AA:984:C:H6	1.83	0.43
46:AA:1207:U:H2'	46:AA:1208:U:H6	1.83	0.43
47:AB:151:PHE:CE2	47:AB:246:VAL:HG21	2.53	0.43
52:AG:382:PRO:HD3	53:AH:133:GLN:HE22	1.82	0.43
62:C:66:MET:HE2	74:G:4:PRO:HD3	1.99	0.43
74:G:48:GLU:HA	74:G:51:VAL:HG12	2.01	0.43
76:A4:397:MET:C	76:A4:397:MET:HE2	2.44	0.43
79:Ax:43:A:H3'	79:Ax:44:A:C8	2.51	0.43
8:7:78:VAL:HG22	83:d:282:ILE:HB	2.01	0.43
8:7:309:HIS:CE1	13:E:155:PHE:HA	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:1710:A:H5''	11:A:1711:C:H5	1.83	0.43
11:A:1805:A:H5'	33:V:96:ARG:HD3	2.00	0.43
11:A:1993:A:H8	11:A:2498:U:O2'	2.01	0.43
11:A:2746:U:H2'	11:A:2747:U:H6	1.83	0.43
14:F:216:VAL:HG22	14:F:258:THR:HB	2.00	0.43
16:I:95:MET:HE1	16:I:164:MET:HG3	2.01	0.43
19:L:47:GLY:HA2	19:L:77:ILE:HD11	2.00	0.43
29:W:35:SER:O	79:Ax:2:A:H5'	2.17	0.43
42:m:107:GLU:HA	71:AZ:13:ARG:HH12	1.82	0.43
44:q:113:LYS:HD2	44:q:113:LYS:HA	1.56	0.43
46:AA:664:G:H2'	46:AA:665:C:C6	2.53	0.43
48:AC:112:ARG:HB3	73:A1:159:SER:HB2	1.99	0.43
52:AG:165:VAL:HG11	52:AG:224:LEU:HB3	2.01	0.43
65:AT:24:LYS:HA	65:AT:108:LYS:HZ3	1.84	0.43
69:AX:212:LYS:HE2	69:AX:212:LYS:HB2	1.86	0.43
73:A1:253:TRP:CZ3	73:A1:259:GLU:HG3	2.53	0.43
76:A4:302:VAL:HG21	76:A4:341:CYS:HB3	2.00	0.43
76:A4:403:LYS:HB3	76:A4:405:PHE:CE1	2.53	0.43
9:8:131:MET:O	9:8:135:THR:HG23	2.17	0.43
9:8:157:LEU:HD22	35:e:184:LEU:HD21	2.00	0.43
11:A:1759:U:H2'	11:A:1760:G:O4'	2.19	0.43
11:A:1944:C:C2	11:A:1945:A:C8	3.07	0.43
15:H:65:ALA:HB2	15:H:71:PRO:HA	2.00	0.43
18:k:73:GLU:N	18:k:73:GLU:OE2	2.52	0.43
42:m:69:ARG:HG2	42:m:69:ARG:NH1	2.33	0.43
46:AA:672:A:H2'	46:AA:673:U:C6	2.53	0.43
47:AB:102:MET:HE3	47:AB:102:MET:HB3	1.78	0.43
48:AC:94:LYS:NZ	49:AD:92:LYS:HB2	2.32	0.43
69:AX:86:ARG:HD2	69:AX:392:GLU:OE1	2.19	0.43
76:A4:497:LEU:HA	76:A4:500:LEU:HD12	1.99	0.43
78:Aw:25:C:H2'	78:Aw:26:U:O4'	2.19	0.43
86:s:332:LEU:HD21	86:s:359:ALA:HB2	2.00	0.43
10:9:88:ALA:HA	31:Y:152:ALA:HB1	2.00	0.43
11:A:2017:U:H2'	11:A:2018:G:H8	1.82	0.43
11:A:2805:A:H2'	11:A:2806:U:C6	2.53	0.43
15:H:99:THR:HG22	15:H:140:PHE:CZ	2.54	0.43
30:X:131:THR:HA	30:X:134:LEU:HB2	2.01	0.43
32:Z:125:PRO:HD3	32:Z:144:GLU:HB2	2.01	0.43
33:V:102:MET:C	33:V:102:MET:HE2	2.44	0.43
45:r:136:PRO:HG2	45:r:139:VAL:HG21	2.00	0.43
48:AC:156:GLN:NE2	73:A1:101:GLY:H	2.17	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:AP:63:LYS:HD2	61:AP:63:LYS:C	2.43	0.43
64:AS:41:LEU:HD12	64:AS:41:LEU:H	1.82	0.43
66:AU:92:GLU:H	66:AU:92:GLU:HG2	1.68	0.43
72:A0:40:THR:HG23	72:A0:42:THR:HG23	2.01	0.43
74:G:81:GLN:O	74:G:85:LYS:HG2	2.19	0.43
76:A4:251:MET:O	76:A4:251:MET:HG3	2.18	0.43
76:A4:360:MET:HB3	76:A4:365:ILE:O	2.18	0.43
86:s:117:GLY:O	86:s:394:TRP:HB3	2.19	0.43
11:A:1718:A:H2'	11:A:1719:G:O4'	2.18	0.43
11:A:2006:C:H2'	11:A:2007:U:H6	1.83	0.43
11:A:2405:C:H5'	12:D:78:LYS:HZ2	1.82	0.43
11:A:2661:U:H2'	11:A:2662:A:H8	1.83	0.43
11:A:2994:U:H4'	78:Aw:75:C:O2'	2.18	0.43
15:H:122:ARG:O	15:H:126:GLN:HG3	2.19	0.43
19:L:63:LYS:HE3	19:L:63:LYS:HB3	1.85	0.43
20:M:99:ASN:OD1	20:M:144:GLY:HA3	2.18	0.43
20:M:277:MET:HE2	20:M:277:MET:HB3	1.83	0.43
21:N:116:LYS:CD	21:N:116:LYS:H	2.32	0.43
26:S:101:PHE:HE1	39:j:49:TRP:HB3	1.84	0.43
34:b:78:ALA:HB2	34:b:105:LEU:HD13	2.00	0.43
37:h:95:ARG:HG2	37:h:95:ARG:HH11	1.84	0.43
46:AA:671:U:H2'	46:AA:672:A:C8	2.54	0.43
46:AA:1033:U:H2'	46:AA:1034:U:C6	2.54	0.43
46:AA:1464:G:H21	46:AA:1467:C:N4	2.17	0.43
46:AA:1488:5MC:H2'	46:AA:1489:G:H8	1.83	0.43
49:AD:260:LYS:HB3	49:AD:260:LYS:HE2	1.78	0.43
68:AW:134:TYR:CZ	68:AW:172:ILE:HD11	2.54	0.43
68:AW:171:GLY:C	68:AW:172:ILE:HD12	2.44	0.43
72:A0:95:TRP:CD2	72:A0:131:ILE:HG12	2.54	0.43
76:A4:376:ILE:HD12	76:A4:376:ILE:H	1.84	0.43
78:Aw:50:A:C2	78:Aw:65:A:C4	3.07	0.43
78:Aw:69:A:H3'	78:Aw:70:C:H6	1.83	0.43
8:7:107:LEU:HD12	8:7:107:LEU:HA	1.76	0.43
8:7:276:PHE:CD2	8:7:277:GLN:HG3	2.54	0.43
9:8:135:THR:O	9:8:139:MET:HG2	2.18	0.43
11:A:1707:C:C4	31:Y:185:VAL:HG21	2.53	0.43
11:A:1751:A:C5	11:A:1752:U:H1'	2.54	0.43
11:A:1989:C:H2'	11:A:1990:G:C8	2.54	0.43
11:A:2983:G:OP1	21:N:140:MET:HG2	2.19	0.43
12:D:172:MET:HE1	50:AE:86:ILE:CG2	2.27	0.43
13:E:256:LYS:H	13:E:256:LYS:HG2	1.60	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Q:64:ASP:HA	67:AV:51:ALA:HB2	1.87	0.43
24:Q:265:LEU:HD23	24:Q:265:LEU:HA	1.80	0.43
33:V:86:VAL:HG21	33:V:120:VAL:HG21	2.01	0.43
34:b:43:GLY:HA3	34:b:93:LYS:O	2.18	0.43
35:e:123:MET:HE3	35:e:123:MET:N	2.28	0.43
46:AA:696:U:H2'	46:AA:697:G:C8	2.54	0.43
53:AH:96:VAL:O	53:AH:100:LYS:HG2	2.19	0.43
60:AO:237:LYS:HE2	60:AO:237:LYS:HB2	1.68	0.43
78:Aw:3:G:C2	78:Aw:71:C:C2	3.07	0.43
78:Aw:71:C:H6	78:Aw:71:C:H5''	1.83	0.43
82:c:72:ILE:HD13	82:c:72:ILE:HA	1.90	0.43
7:6:59:ARG:HB2	7:6:59:ARG:CZ	2.49	0.43
11:A:1895:C:H2'	11:A:1896:U:C6	2.54	0.43
11:A:2688:C:H2'	11:A:2689:C:C6	2.54	0.43
14:F:160:SER:HB3	38:i:80:LEU:HD22	2.01	0.43
20:M:161:GLU:HG3	20:M:236:LEU:HD11	2.01	0.43
24:Q:58:PRO:O	67:AV:90:TYR:CD1	2.72	0.43
37:h:56:ARG:H	37:h:56:ARG:HG2	1.67	0.43
46:AA:735:A:H61	72:A0:195:ARG:HH21	1.66	0.43
46:AA:757:A:H4'	46:AA:758:U:H5''	2.00	0.43
46:AA:911:U:H2'	46:AA:912:U:H6	1.83	0.43
46:AA:916:C:H2'	46:AA:917:C:H6	1.82	0.43
46:AA:990:U:H3	46:AA:997:A:H61	1.66	0.43
46:AA:1069:A:H5''	46:AA:1070:C:C5	2.53	0.43
46:AA:1261:C:H2'	46:AA:1262:C:H6	1.83	0.43
46:AA:1553:A:H2'	46:AA:1554:G:H8	1.82	0.43
92:AA:1784:NMY:O11	92:AA:1784:NMY:H1	2.19	0.43
49:AD:223:LEU:HD23	49:AD:223:LEU:HA	1.86	0.43
51:AF:53:LYS:NZ	51:AF:58:LEU:HG	2.34	0.43
52:AG:55:VAL:O	77:Az:15:U:N3	2.42	0.43
52:AG:148:HIS:HE1	52:AG:160:SER:HB3	1.83	0.43
60:AO:55:PRO:HD2	60:AO:56:TRP:CZ3	2.53	0.43
66:AU:55:VAL:O	66:AU:59:ARG:HG2	2.19	0.43
72:A0:19:ARG:O	72:A0:23:GLU:HG2	2.18	0.43
72:A0:103:ASP:C	72:A0:103:ASP:OD1	2.62	0.43
76:A4:462:PHE:HE2	76:A4:496:LEU:HD23	1.84	0.43
79:Ax:11:U:H2'	79:Ax:12:U:H6	1.78	0.43
79:Ax:67:U:H2'	79:Ax:68:C:H6	1.81	0.43
6:5:55:LEU:HD23	6:5:55:LEU:HA	1.82	0.42
8:7:247:ASN:HD22	8:7:251:ILE:H	1.67	0.42
10:9:44:LEU:HD23	10:9:44:LEU:HA	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:1851:G:H2'	11:A:2693:A:N7	2.34	0.42
11:A:2134:A:H62	11:A:2135:A:H62	1.67	0.42
11:A:3024:U:H2'	11:A:3025:A:C8	2.51	0.42
17:J:28:LEU:HD13	41:l:56:LEU:HD22	2.00	0.42
33:V:54:TRP:CD1	33:V:81:ARG:HD3	2.54	0.42
46:AA:1359:U:H2'	46:AA:1360:G:H8	1.83	0.42
46:AA:1471:A:OP2	92:AA:1783:NMY:C7	2.67	0.42
57:AL:84:LYS:HA	57:AL:84:LYS:HD2	1.72	0.42
69:AX:106:LEU:HD23	69:AX:106:LEU:HA	1.88	0.42
72:A0:64:LEU:HD12	72:A0:139:TRP:CZ2	2.54	0.42
78:Aw:69:A:N3	78:Aw:69:A:H2'	2.34	0.42
11:A:1839:C:OP1	18:k:115:ASN:HB2	2.19	0.42
11:A:2005:C:H2'	11:A:2006:C:H6	1.84	0.42
11:A:2184:A:C5	11:A:2185:G:C8	3.07	0.42
11:A:2558:A:C2	46:AA:1001:C:C4	3.07	0.42
11:A:2847:C:H2'	11:A:2848:A:O4'	2.18	0.42
33:V:81:ARG:HA	33:V:81:ARG:HD2	1.86	0.42
46:AA:874:G:H2'	46:AA:875:U:C6	2.55	0.42
46:AA:1044:U:H2'	46:AA:1045:G:O4'	2.19	0.42
46:AA:1265:C:H4'	53:AH:122:GLN:HG3	2.01	0.42
56:AK:53:ARG:H	56:AK:53:ARG:HG2	1.64	0.42
65:AT:146:GLN:HE21	65:AT:146:GLN:HB3	1.71	0.42
69:AX:361:LEU:HD11	69:AX:372:PRO:HG3	2.01	0.42
78:Aw:53:A:H2'	78:Aw:53:A:N3	2.33	0.42
78:Aw:61:U:H2'	78:Aw:62:C:H6	1.79	0.42
79:Ax:9:A:C5'	79:Ax:46:A:H1'	2.49	0.42
9:8:65:LYS:HE2	9:8:65:LYS:HB3	1.70	0.42
11:A:2187:C:C2	11:A:2188:A:C8	3.08	0.42
11:A:2332:C:OP2	92:A:3471:NMY:O18	2.36	0.42
11:A:2764:A:H4'	15:H:248:TYR:HD2	1.84	0.42
11:A:3041:U:H2'	11:A:3042:U:C6	2.55	0.42
26:S:94:ARG:HG3	82:c:313:PRO:HG3	2.02	0.42
30:X:49:LYS:HA	30:X:49:LYS:HD2	1.74	0.42
35:e:200:MET:HE1	35:e:243:PHE:CE1	2.54	0.42
37:h:86:TRP:CD1	37:h:87:GLN:N	2.87	0.42
39:j:67:LYS:HE3	39:j:67:LYS:HB3	1.62	0.42
45:r:35:PHE:N	45:r:56:THR:HG1	2.17	0.42
46:AA:944:U:H2'	46:AA:945:G:C8	2.54	0.42
46:AA:1236:C:H4'	46:AA:1237:A:O4'	2.19	0.42
54:AI:140:LYS:HE3	54:AI:140:LYS:HB3	1.72	0.42
59:AN:14:VAL:HG22	59:AN:65:LEU:HD23	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:AX:203:LYS:HG2	69:AX:221:PRO:HA	2.00	0.42
70:AY:362:PRO:HG2	70:AY:363:TYR:CE1	2.54	0.42
9:8:52:LYS:HG2	78:Aw:40:C:OP2	2.19	0.42
10:9:27:PRO:O	10:9:31:ARG:HG3	2.19	0.42
92:A:3474:NMY:H18	92:A:3474:NMY:H16	1.16	0.42
17:J:169:LYS:HE3	17:J:169:LYS:HB3	1.73	0.42
21:N:191:SER:H	21:N:194:THR:HB	1.84	0.42
22:O:33:LEU:HD21	22:O:59:LEU:HD22	2.00	0.42
46:AA:740:G:H2'	46:AA:741:A:C8	2.51	0.42
46:AA:1498:C:H2'	46:AA:1499:U:H6	1.85	0.42
67:AV:352:LEU:HD12	67:AV:353:LEU:N	2.34	0.42
73:A1:314:GLU:O	73:A1:318:ARG:HG2	2.18	0.42
75:A3:187:GLU:OE1	75:A3:187:GLU:N	2.51	0.42
76:A4:372:TYR:HE2	76:A4:400:LEU:HD21	1.85	0.42
76:A4:493:MET:HE3	76:A4:493:MET:HB3	1.81	0.42
76:A4:528:ARG:O	76:A4:531:ILE:HG13	2.20	0.42
78:Aw:53:A:H5''	78:Aw:55:A:C2	2.54	0.42
8:7:43:MET:O	8:7:47:LEU:HD13	2.18	0.42
11:A:2533:A:H2'	11:A:2534:G:H8	1.85	0.42
24:Q:59:LYS:N	67:AV:90:TYR:CE1	2.87	0.42
40:n:80:HIS:O	45:r:36:ARG:HD2	2.20	0.42
46:AA:983:C:H2'	46:AA:984:C:C6	2.55	0.42
46:AA:1414:C:H3'	46:AA:1415:G:N2	2.34	0.42
47:AB:167:HIS:CD2	52:AG:153:THR:HA	2.55	0.42
49:AD:218:PHE:HE2	49:AD:279:LEU:HD11	1.84	0.42
50:AE:15:ARG:HE	50:AE:15:ARG:HB3	1.50	0.42
59:AN:29:ARG:HD3	59:AN:46:ARG:HE	1.85	0.42
61:AP:105:LYS:HA	61:AP:105:LYS:HD3	1.89	0.42
69:AX:79:PHE:HZ	69:AX:143:HIS:HB2	1.84	0.42
76:A4:405:PHE:CE2	76:A4:438:LEU:HD11	2.54	0.42
76:A4:415:PHE:CD1	76:A4:415:PHE:C	2.98	0.42
78:Aw:4:U:C2	78:Aw:5:A:C8	3.07	0.42
78:Aw:23:A:H3'	78:Aw:24:A:C8	2.53	0.42
78:Aw:52:G:C2	78:Aw:63:A:N3	2.88	0.42
79:Ax:50:G:C2	79:Ax:51:A:C4	3.08	0.42
79:Ax:57:A:C2	79:Ax:58:A:C4	3.08	0.42
1:0:95:ARG:HG3	27:T:82:TRP:CH2	2.54	0.42
10:9:24:LYS:HE3	28:U:74:HIS:HB2	2.02	0.42
10:9:123:GLN:HE22	10:9:130:LEU:H	1.68	0.42
11:A:1812:C:H41	38:i:36:LEU:HD13	1.85	0.42
17:J:101:ALA:HB2	17:J:109:ALA:HB2	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Q:59:LYS:HG3	67:AV:90:TYR:CZ	2.54	0.42
46:AA:1497:C:H2'	46:AA:1498:C:H6	1.85	0.42
46:AA:1557:A:H5''	55:AJ:72:LYS:HG3	2.01	0.42
63:AR:216:ARG:CZ	63:AR:216:ARG:HB2	2.48	0.42
70:AY:349:HIS:CG	71:AZ:24:ARG:HD2	2.54	0.42
72:A0:23:GLU:O	72:A0:27:ARG:HB3	2.20	0.42
76:A4:117:ALA:O	76:A4:121:ILE:HG12	2.19	0.42
76:A4:461:PHE:HE1	76:A4:465:ILE:HD11	1.81	0.42
78:Aw:52:G:H22	78:Aw:63:A:H1'	1.84	0.42
78:Aw:53:A:H61	78:Aw:61:U:H3	1.67	0.42
79:Ax:55:U:C2	79:Ax:57:A:H3'	2.54	0.42
11:A:2080:U:O2'	43:o:60:ARG:HA	2.20	0.42
11:A:2098:G:OP1	92:A:3474:NMY:C6	2.67	0.42
11:A:2112:A:N6	21:N:140:MET:HE2	2.25	0.42
11:A:3041:U:O2	78:Aw:74:C:C5	2.73	0.42
12:D:172:MET:SD	50:AE:86:ILE:CB	3.08	0.42
16:I:47:LEU:O	16:I:51:THR:HG23	2.20	0.42
20:M:280:LYS:HG3	36:g:45:TYR:CE2	2.55	0.42
26:S:109:THR:O	26:S:112:ASP:HB2	2.19	0.42
35:e:114:ILE:HA	69:AX:234:ARG:HD2	1.16	0.42
46:AA:1162:A:H2'	46:AA:1163:C:C6	2.55	0.42
46:AA:1279:C:H2'	46:AA:1280:C:H6	1.84	0.42
47:AB:156:GLU:HB3	52:AG:163:HIS:CE1	2.54	0.42
49:AD:362:LEU:HD21	63:AR:105:LEU:HD21	2.02	0.42
53:AH:115:ILE:HG12	53:AH:137:ARG:HG2	2.02	0.42
53:AH:166:GLU:OE1	53:AH:166:GLU:N	2.53	0.42
67:AV:277:ARG:HA	67:AV:280:LEU:HD23	2.02	0.42
69:AX:225:VAL:HG21	69:AX:242:ILE:HB	2.02	0.42
71:AZ:18:LEU:HD23	73:A1:228:VAL:HG13	2.02	0.42
76:A4:483:PRO:HB3	76:A4:519:TYR:CE1	2.54	0.42
78:Aw:52:G:C6	78:Aw:53:A:C6	3.07	0.42
83:d:288:LYS:HB2	83:d:288:LYS:HE2	1.78	0.42
84:f:63:ILE:C	84:f:63:ILE:HD12	2.45	0.42
1:0:176:GLU:OE1	1:0:176:GLU:N	2.53	0.42
7:6:240:ILE:HG22	7:6:248:GLY:HA3	2.02	0.42
9:8:93:LYS:H	9:8:93:LYS:CE	2.32	0.42
11:A:1979:U:H2'	11:A:1980:A:H8	1.84	0.42
11:A:2700:G:H2'	11:A:2701:G:C8	2.55	0.42
11:A:3109:U:H1'	18:k:83:TYR:CD2	2.54	0.42
12:D:193:ILE:HD11	12:D:226:ILE:HD12	2.02	0.42
13:E:144:THR:HB	13:E:178:ILE:HG23	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:V:44:VAL:HG11	33:V:83:ARG:NH2	2.35	0.42
36:g:164:LYS:HE3	36:g:164:LYS:HB3	1.64	0.42
47:AB:176:LEU:HD12	47:AB:211:ASP:HB3	2.01	0.42
55:AJ:109:LEU:HD23	55:AJ:126:VAL:HG11	2.01	0.42
67:AV:148:MET:C	67:AV:148:MET:HE2	2.45	0.42
69:AX:253:LEU:HB2	69:AX:255:MET:SD	2.59	0.42
72:A0:63:ARG:HB2	72:A0:66:GLN:HG3	2.02	0.42
76:A4:360:MET:HB3	76:A4:367:PRO:HD3	2.02	0.42
76:A4:564:ILE:HD13	76:A4:564:ILE:HA	1.88	0.42
78:Aw:6:U:H3	78:Aw:7:A:N6	2.18	0.42
79:Ax:4:G:H1	79:Ax:69:C:N4	2.16	0.42
80:B:69:U:H2'	80:B:70:C:H6	1.83	0.42
2:1:43:LEU:HA	44:q:135:TRP:CZ2	2.55	0.42
6:5:299:LEU:HD11	11:A:2405:C:C6	2.55	0.42
7:6:187:VAL:HG13	7:6:319:PHE:HB3	2.02	0.42
8:7:52:LYS:HE2	8:7:52:LYS:HB2	1.86	0.42
11:A:2226:U:O2'	11:A:2227:A:H5'	2.19	0.42
11:A:2761:C:H4'	11:A:2762:C:C4	2.55	0.42
11:A:2812:U:H2'	11:A:2813:U:O4'	2.20	0.42
11:A:3065:U:H4'	13:E:239:ARG:NH2	2.34	0.42
14:F:131:LYS:HB3	14:F:131:LYS:HE3	1.76	0.42
30:X:24:LEU:HB2	30:X:29:LEU:HD21	2.02	0.42
30:X:125:VAL:HG23	30:X:127:VAL:HG13	2.01	0.42
36:g:160:TRP:O	36:g:164:LYS:HG3	2.20	0.42
46:AA:656:U:OP2	92:AA:1785:NMY:N9	2.53	0.42
46:AA:1016:U:O4	61:AP:112:LYS:HE3	2.20	0.42
46:AA:1057:G:H4'	46:AA:1578:A:H4'	2.01	0.42
46:AA:1068:A:H5''	54:AI:190:LYS:HD3	2.02	0.42
47:AB:248:LEU:O	47:AB:252:LEU:HG	2.20	0.42
57:AL:218:GLN:OE1	57:AL:218:GLN:HA	2.20	0.42
63:AR:271:MET:HE2	63:AR:271:MET:HB3	1.90	0.42
69:AX:197:ARG:HH21	69:AX:198:PHE:HZ	1.68	0.42
76:A4:166:VAL:O	76:A4:170:VAL:HG13	2.20	0.42
78:Aw:28:A:H3'	78:Aw:29:U:H6	1.85	0.42
79:Ax:42:G:C2	79:Ax:43:A:H1'	2.55	0.42
79:Ax:54:U:H3'	79:Ax:55:U:C5	2.54	0.42
86:s:165:ARG:CZ	86:s:165:ARG:HB3	2.50	0.42
11:A:1748:G:O5'	11:A:1749:C:H5''	2.20	0.42
11:A:1982:G:H2'	11:A:1983:U:C6	2.55	0.42
11:A:2104:A:H2'	11:A:2105:G:O4'	2.20	0.42
11:A:2610:U:H2'	11:A:2611:C:C6	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:2667:U:C2	11:A:2668:A:C8	3.08	0.42
17:J:53:PHE:C	17:J:53:PHE:HD1	2.27	0.42
17:J:85:PRO:HG2	17:J:90:PHE:HE1	1.84	0.42
22:O:50:ASP:HB2	22:O:107:MET:HE1	2.02	0.42
23:P:39:VAL:HG12	23:P:41:ASN:H	1.85	0.42
23:P:63:ARG:HD3	29:W:93:GLU:HG2	2.01	0.42
25:R:90:LEU:HD12	25:R:90:LEU:HA	1.80	0.42
27:T:123:VAL:HA	27:T:128:VAL:HB	2.01	0.42
41:l:110:LEU:HB3	41:l:117:TYR:HB2	2.02	0.42
42:m:46:GLN:OE1	42:m:46:GLN:HA	2.18	0.42
44:q:28:ARG:HE	44:q:28:ARG:HB3	1.57	0.42
44:q:61:PHE:CD2	44:q:75:LEU:HD11	2.54	0.42
46:AA:1542:U:H2'	46:AA:1543:U:C6	2.55	0.42
51:AF:44:PRO:HD3	51:AF:75:LYS:HB2	2.00	0.42
52:AG:86:ARG:HH11	73:A1:62:VAL:HG11	1.85	0.42
52:AG:95:ASP:OD1	52:AG:95:ASP:C	2.63	0.42
52:AG:168:MET:HE3	52:AG:237:GLU:OE2	2.20	0.42
52:AG:396:ARG:NH1	79:Ax:33:U:OP2	2.50	0.42
60:AO:211:ARG:HA	67:AV:319:ILE:HD13	2.02	0.42
64:AS:28:LYS:HD3	64:AS:29:PRO:HD2	2.01	0.42
64:AS:89:ASN:OD1	64:AS:92:PHE:HB2	2.20	0.42
76:A4:357:LEU:HA	76:A4:360:MET:SD	2.60	0.42
76:A4:556:LYS:HD2	76:A4:556:LYS:C	2.45	0.42
79:Ax:59:U:H3'	79:Ax:60:U:H6	1.85	0.42
79:Ax:61:C:H6	79:Ax:61:C:H5'	1.85	0.42
82:c:79:LEU:HD13	82:c:214:PHE:HE1	1.84	0.42
86:s:63:ILE:HA	86:s:66:TRP:CD1	2.55	0.42
11:A:3117:C:H2'	11:A:3118:U:H6	1.85	0.41
21:N:214:THR:O	21:N:218:ILE:HG13	2.19	0.41
24:Q:165:GLU:HB2	24:Q:168:ASN:HB2	2.01	0.41
35:e:164:LYS:HD2	35:e:167:ASP:HA	2.02	0.41
36:g:155:GLN:OE1	36:g:155:GLN:HA	2.19	0.41
42:m:58:LYS:HB2	42:m:60:ASP:OD1	2.20	0.41
46:AA:990:U:H2'	46:AA:991:G:O4'	2.20	0.41
46:AA:1020:C:H4'	61:AP:94:ARG:NH1	2.35	0.41
46:AA:1240:A:H2'	46:AA:1241:C:C6	2.54	0.41
46:AA:1577:U:H2'	46:AA:1578:A:C8	2.55	0.41
51:AF:176:ASP:OD1	51:AF:176:ASP:C	2.63	0.41
57:AL:85:VAL:HG23	57:AL:90:LYS:HG3	2.01	0.41
57:AL:176:ASP:OD1	57:AL:176:ASP:N	2.52	0.41
58:AM:114:ARG:HG3	58:AM:114:ARG:NH1	2.34	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:AP:139:ARG:HB3	61:AP:139:ARG:CZ	2.50	0.41
63:AR:194:GLN:NE2	63:AR:199:LYS:H	2.18	0.41
68:AW:135:GLN:O	68:AW:138:THR:HG22	2.19	0.41
72:A0:170:LEU:HD23	72:A0:173:MET:HG3	2.02	0.41
82:c:72:ILE:HD13	82:c:178:LEU:HD13	2.01	0.41
86:s:139:LEU:HD13	86:s:419:LEU:HD21	2.01	0.41
11:A:2410:U:H2'	11:A:2411:U:C6	2.54	0.41
15:H:99:THR:HA	15:H:108:ARG:HG3	2.01	0.41
17:J:118:TYR:HD2	41:l:96:LEU:HD22	1.85	0.41
20:M:129:ILE:HD11	20:M:138:VAL:HG13	2.01	0.41
20:M:168:GLU:OE1	20:M:233:ARG:HG2	2.20	0.41
26:S:111:GLU:HG2	34:b:20:LEU:HD11	2.03	0.41
36:g:143:VAL:HG13	36:g:144:THR:HG23	2.02	0.41
46:AA:944:U:H2'	46:AA:945:G:H8	1.86	0.41
46:AA:1461:A:H4'	46:AA:1462:G:C8	2.55	0.41
46:AA:1464:G:H2'	46:AA:1465:C:C6	2.54	0.41
72:A0:91:GLU:CD	72:A0:91:GLU:H	2.28	0.41
73:A1:149:ILE:HD13	73:A1:175:VAL:HB	2.01	0.41
79:Ax:66:U:H2'	79:Ax:67:U:H6	1.81	0.41
86:s:119:PRO:HG3	86:s:394:TRP:CD2	2.55	0.41
6:5:135:LYS:NZ	6:5:135:LYS:HB3	2.35	0.41
8:7:192:TRP:O	8:7:193:MET:HE2	2.21	0.41
9:8:99:ARG:HD2	35:e:89:LEU:HD11	2.02	0.41
10:9:120:GLU:OE1	10:9:121:PRO:HD2	2.20	0.41
11:A:3112:A:C5	11:A:3200:U:O2	2.72	0.41
25:R:111:LYS:HG2	81:a:45:CYS:HB3	2.02	0.41
29:W:101:LYS:HD2	84:f:56:ILE:HG21	2.01	0.41
46:AA:862:A:H2'	46:AA:863:C:C6	2.56	0.41
46:AA:1489:G:H2'	46:AA:1490:U:H6	1.86	0.41
49:AD:198:TRP:HA	49:AD:201:ILE:HD12	2.02	0.41
58:AM:95:GLY:O	72:A0:167:PRO:HB2	2.20	0.41
67:AV:97:HIS:C	72:A0:104:TYR:HB2	2.45	0.41
67:AV:219:VAL:HG21	67:AV:359:LEU:HD22	2.02	0.41
72:A0:41:LEU:HD11	72:A0:59:ARG:NH2	2.34	0.41
72:A0:138:ASP:OD1	72:A0:138:ASP:C	2.64	0.41
76:A4:420:MET:HE3	76:A4:420:MET:HB3	1.79	0.41
76:A4:451:ASP:HA	76:A4:454:ARG:NE	2.36	0.41
77:Az:9:U:O2	78:Aw:34:A:N1	2.53	0.41
79:Ax:59:U:H3'	79:Ax:60:U:C6	2.55	0.41
84:f:84:THR:H	84:f:87:GLU:HB2	1.85	0.41
1:0:128:GLU:HG2	83:d:289:PRO:HG2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:1879:G:H2'	11:A:1880:C:C6	2.54	0.41
11:A:1912:A:H2'	11:A:1913:G:C8	2.55	0.41
11:A:2181:A:C4	11:A:2207:A:H4'	2.54	0.41
11:A:2215:C:C2	11:A:2216:A:C8	3.08	0.41
11:A:2296:U:H5''	11:A:2297:A:OP1	2.21	0.41
11:A:2382:A:H2'	11:A:2383:U:C6	2.55	0.41
12:D:196:VAL:HG22	12:D:206:TYR:HB2	2.02	0.41
16:I:96:ILE:HG23	16:I:155:VAL:HG12	2.02	0.41
18:k:169:LEU:HD22	45:r:75:TRP:CD1	2.55	0.41
21:N:61:LYS:HD3	21:N:130:PRO:HD3	2.02	0.41
26:S:74:ARG:O	26:S:78:GLU:HG3	2.20	0.41
35:e:171:TRP:CG	35:e:263:TYR:HB3	2.56	0.41
46:AA:1007:G:H2'	46:AA:1008:A:H8	1.84	0.41
46:AA:1227:G:OP1	53:AH:128:LYS:HE3	2.19	0.41
54:AI:110:ALA:HB3	54:AI:135:ALA:HB2	2.01	0.41
61:AP:112:LYS:HD2	61:AP:112:LYS:HA	1.78	0.41
63:AR:200:GLU:OE1	63:AR:200:GLU:N	2.49	0.41
66:AU:94:LYS:HB2	66:AU:94:LYS:HE3	1.79	0.41
67:AV:102:TRP:HD1	72:A0:74:PHE:HD1	1.67	0.41
67:AV:175:VAL:HG12	67:AV:178:THR:H	1.84	0.41
67:AV:263:MET:HE3	67:AV:263:MET:HB3	1.88	0.41
72:A0:73:LEU:O	72:A0:76:LEU:HG	2.20	0.41
73:A1:248:MET:H	73:A1:248:MET:HG2	1.70	0.41
74:G:67:ARG:O	74:G:70:ILE:HG22	2.20	0.41
80:B:39:PSU:H2'	80:B:40:U:C6	2.56	0.41
86:s:239:ASN:HB2	86:s:299:PHE:HB2	2.01	0.41
6:5:327:LEU:HD23	6:5:328:LEU:HD23	2.02	0.41
9:8:123:LEU:O	9:8:126:GLN:HB3	2.20	0.41
11:A:2277:U:H2'	11:A:2278:A:C8	2.54	0.41
11:A:2362:A:O2'	11:A:2363:A:H2'	2.20	0.41
11:A:2439:U:H2'	11:A:2440:G:H8	1.86	0.41
12:D:292:MET:HE2	12:D:292:MET:HB3	1.73	0.41
18:k:171:THR:HG23	45:r:59:GLU:H	1.85	0.41
24:Q:195:PRO:O	24:Q:199:THR:HG23	2.21	0.41
33:V:168:GLU:HG2	33:V:169:THR:N	2.36	0.41
46:AA:798:C:H2'	46:AA:799:A:H8	1.84	0.41
46:AA:1462:G:H2'	46:AA:1463:G:H8	1.84	0.41
52:AG:317:PHE:CE2	52:AG:348:MET:HE3	2.52	0.41
56:AK:31:ASP:C	56:AK:31:ASP:OD1	2.64	0.41
57:AL:83:GLU:OE2	57:AL:83:GLU:N	2.54	0.41
63:AR:142:LEU:HD21	72:A0:172:ALA:HB2	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:AR:331:PHE:C	63:AR:331:PHE:CD1	2.99	0.41
67:AV:30:LEU:HD22	67:AV:34:TYR:CD1	2.55	0.41
74:G:66:CYS:O	74:G:70:ILE:HB	2.20	0.41
78:Aw:4:U:O2'	78:Aw:5:A:O4'	2.37	0.41
83:d:118:SER:O	83:d:122:ILE:HG13	2.21	0.41
6:5:48:ARG:NH1	30:X:125:VAL:HG12	2.36	0.41
6:5:157:VAL:HG22	6:5:183:ASN:HB3	2.03	0.41
6:5:395:ARG:HH22	6:5:397:VAL:HG23	1.84	0.41
7:6:214:TRP:CZ3	7:6:274:LYS:HG3	2.55	0.41
8:7:204:LYS:HB3	8:7:204:LYS:HE2	1.75	0.41
11:A:2109:A:C6	11:A:2946:A:C8	3.08	0.41
11:A:2332:C:H3'	11:A:2333:G:H8	1.85	0.41
11:A:2810:G:H2'	11:A:2811:G:H8	1.85	0.41
11:A:2951:A:H2'	11:A:2952:U:C6	2.56	0.41
14:F:222:THR:OG1	14:F:225:GLU:HB2	2.21	0.41
16:I:101:ASN:OD1	16:I:152:MET:HE2	2.20	0.41
16:I:146:LEU:HD11	16:I:177:LEU:HB3	2.01	0.41
16:I:160:LYS:O	16:I:164:MET:HB2	2.20	0.41
16:I:187:SER:O	16:I:191:PHE:HD1	2.03	0.41
21:N:223:MET:HE2	21:N:223:MET:HB3	1.91	0.41
46:AA:1007:G:H2'	46:AA:1008:A:C8	2.55	0.41
57:AL:75:ASP:HB3	66:AU:153:LYS:HD2	2.02	0.41
58:AM:21:LEU:HD21	58:AM:87:MET:HE3	2.03	0.41
58:AM:70:LEU:HD23	58:AM:70:LEU:HA	1.88	0.41
60:AO:74:TRP:CD2	60:AO:140:THR:HG22	2.56	0.41
64:AS:102:LYS:O	64:AS:106:LEU:HD13	2.21	0.41
65:AT:121:LYS:N	65:AT:121:LYS:HD3	2.36	0.41
73:A1:190:LEU:HD11	73:A1:229:LEU:HD13	2.01	0.41
73:A1:194:VAL:HB	73:A1:197:ARG:HB2	2.03	0.41
76:A4:436:HIS:HB2	76:A4:461:PHE:HE2	1.86	0.41
77:Az:1:U:H3'	77:Az:2:A:H8	1.85	0.41
1:0:132:LYS:HD3	1:0:132:LYS:HA	1.75	0.41
10:9:77:LEU:HD21	33:V:167:PRO:O	2.21	0.41
11:A:1719:G:H2'	11:A:1720:C:C6	2.55	0.41
11:A:2171:U:C2	11:A:2173:G:H5'	2.56	0.41
11:A:2765:A:H4'	15:H:244:LYS:HG2	2.02	0.41
11:A:3213:A:H2'	11:A:3214:C:H6	1.85	0.41
12:D:172:MET:HE3	50:AE:84:ARG:C	2.45	0.41
12:D:215:VAL:HG22	12:D:227:GLN:HB3	2.02	0.41
15:H:247:ARG:HG2	15:H:251:TRP:HE3	1.86	0.41
16:I:163:GLU:O	16:I:167:ILE:HG12	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:J:25:ARG:HB2	41:l:56:LEU:HD13	2.01	0.41
17:J:149:ARG:NH2	41:l:103:PRO:HA	2.33	0.41
32:Z:132:GLU:OE1	32:Z:132:GLU:N	2.51	0.41
41:l:76:ASN:HB2	41:l:83:ASP:HA	2.02	0.41
42:m:122:PHE:CE1	53:AH:183:HIS:CD2	2.68	0.41
44:q:128:MET:HE2	44:q:128:MET:HB2	1.86	0.41
46:AA:715:G:H2'	46:AA:716:U:H6	1.85	0.41
46:AA:1020:C:C5	46:AA:1021:U:C4	3.09	0.41
67:AV:241:ARG:HA	67:AV:244:TYR:CE2	2.56	0.41
73:A1:137:LEU:HD22	73:A1:143:CYS:HA	2.02	0.41
74:G:24:ASN:OD1	74:G:25:LYS:HG3	2.20	0.41
76:A4:476:LYS:HD3	76:A4:476:LYS:HA	1.96	0.41
78:Aw:22:A:H2'	78:Aw:23:A:H8	1.86	0.41
79:Ax:62:C:H2'	79:Ax:63:U:H6	1.79	0.41
83:d:165:THR:CG2	83:d:262:HIS:HA	2.50	0.41
83:d:181:VAL:HG22	83:d:224:ILE:HG12	2.02	0.41
6:5:165:GLN:NE2	6:5:179:VAL:HG21	2.35	0.41
8:7:67:VAL:HG23	8:7:79:PHE:HD2	1.86	0.41
8:7:166:LEU:H	8:7:166:LEU:HD22	1.85	0.41
9:8:51:ARG:HD2	9:8:51:ARG:N	2.36	0.41
11:A:1950:U:H2'	11:A:1951:C:C6	2.56	0.41
11:A:2235:C:H2'	11:A:2236:C:O4'	2.21	0.41
11:A:2442:U:H5''	86:s:81:ARG:HH22	1.85	0.41
11:A:2700:G:H2'	11:A:2701:G:H8	1.86	0.41
11:A:2993:U:O2'	78:Aw:76:A:H4'	2.21	0.41
36:g:47:PHE:HA	36:g:50:ARG:NH1	2.36	0.41
46:AA:786:G:H2'	46:AA:787:C:C6	2.54	0.41
46:AA:799:A:H2'	46:AA:800:C:H6	1.86	0.41
46:AA:1395:C:H2'	46:AA:1396:C:C6	2.56	0.41
51:AF:48:LYS:O	51:AF:52:ARG:HG2	2.21	0.41
53:AH:178:GLU:O	73:A1:149:ILE:HB	2.21	0.41
60:AO:217:ARG:HA	60:AO:224:LEU:HD21	2.03	0.41
63:AR:218:MET:HE2	63:AR:223:ARG:CZ	2.51	0.41
70:AY:386:ILE:HD12	70:AY:387:LEU:N	2.35	0.41
73:A1:56:ARG:NH1	76:A4:84:ALA:HB2	2.36	0.41
77:Az:8:U:O2'	77:Az:9:U:H5'	2.20	0.41
78:Aw:53:A:N6	78:Aw:61:U:H3	2.18	0.41
6:5:380:GLN:HB3	6:5:410:THR:HG23	2.03	0.41
9:8:67:ARG:NH1	79:Ax:46:A:O3'	2.54	0.41
10:9:130:LEU:HB3	31:Y:154:ARG:HG3	2.02	0.41
11:A:1677:C:OP1	82:c:31:VAL:HA	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:1860:A:H2'	11:A:1861:U:C6	2.55	0.41
11:A:1897:A:H2'	11:A:1898:A:H8	1.85	0.41
11:A:1917:A:N1	11:A:1997:C:H1'	2.36	0.41
11:A:2005:C:H2'	11:A:2006:C:C6	2.55	0.41
11:A:2298:A:H61	14:F:145:LEU:HD22	1.86	0.41
11:A:2338:A:C4	11:A:2339:G:C8	3.09	0.41
11:A:2583:C:OP1	46:AA:1582:G:C5	2.74	0.41
11:A:2776:G:H2'	11:A:2777:G:H8	1.86	0.41
11:A:2804:A:H2'	11:A:2805:A:C8	2.56	0.41
11:A:2810:G:H2'	11:A:2811:G:C8	2.56	0.41
11:A:3117:C:H2'	11:A:3118:U:C6	2.56	0.41
11:A:3213:A:H2'	11:A:3214:C:C6	2.56	0.41
15:H:99:THR:HG22	15:H:140:PHE:HZ	1.86	0.41
15:H:168:LYS:HD3	15:H:231:VAL:HG13	2.02	0.41
16:I:57:LYS:HE2	16:I:57:LYS:HB2	1.73	0.41
16:I:90:PHE:CE1	16:I:96:ILE:HG21	2.55	0.41
16:I:98:VAL:HG11	16:I:146:LEU:HG	2.01	0.41
17:J:161:SER:HB2	41:I:69:THR:HG21	2.02	0.41
26:S:185:ILE:HD13	26:S:185:ILE:HA	1.89	0.41
27:T:68:TYR:CZ	27:T:171:LYS:HD2	2.55	0.41
28:U:81:ASP:HB3	28:U:87:ILE:HD11	2.03	0.41
32:Z:46:PHE:CZ	32:Z:111:LYS:HG2	2.56	0.41
33:V:51:ASP:HA	33:V:81:ARG:HH22	1.86	0.41
37:h:62:PRO:HB3	37:h:130:TYR:O	2.21	0.41
40:n:15:GLN:HE21	40:n:52:ILE:HD13	1.84	0.41
42:m:96:ARG:HH12	42:m:97:GLU:HG3	1.85	0.41
46:AA:914:A:H2'	46:AA:915:C:C6	2.56	0.41
46:AA:1012:A:H2'	46:AA:1013:A:C8	2.56	0.41
46:AA:1155:G:H2'	46:AA:1156:C:C6	2.56	0.41
46:AA:1156:C:H2'	46:AA:1157:U:H6	1.86	0.41
46:AA:1317:A:H3'	46:AA:1318:A:H8	1.85	0.41
46:AA:1412:G:C5	46:AA:1413:U:C5	3.09	0.41
51:AF:163:LYS:HD2	51:AF:163:LYS:HA	1.90	0.41
52:AG:224:LEU:HD23	52:AG:224:LEU:HA	1.86	0.41
52:AG:268:ALA:HB3	52:AG:287:LYS:HD2	2.03	0.41
53:AH:159:TYR:CE1	76:A4:74:LEU:HD21	2.56	0.41
57:AL:76:TYR:HE1	66:AU:153:LYS:HD3	1.85	0.41
57:AL:89:VAL:HG22	66:AU:164:VAL:HG21	2.03	0.41
63:AR:191:ARG:HG2	63:AR:192:MET:HE2	2.03	0.41
66:AU:176:ARG:HD2	66:AU:176:ARG:HA	1.84	0.41
67:AV:216:LYS:HB2	67:AV:216:LYS:HE2	1.71	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:AV:246:ASN:HB3	72:A0:70:ARG:NH2	2.34	0.41
73:A1:46:ARG:HB2	73:A1:47:PRO:HD3	2.03	0.41
73:A1:66:TRP:HZ2	73:A1:112:LEU:HB3	1.86	0.41
73:A1:133:TRP:CD2	73:A1:134:PRO:HD2	2.56	0.41
76:A4:115:ASN:HA	76:A4:118:LYS:HB2	2.02	0.41
76:A4:356:VAL:O	76:A4:359:GLU:HG3	2.21	0.41
77:Az:1:U:P	77:Az:1:U:C6	3.13	0.41
78:Aw:14:A:N1	78:Aw:21:A:O2'	2.48	0.41
79:Ax:21:A:H2'	79:Ax:46:A:H61	1.85	0.41
84:f:155:ARG:HA	84:f:155:ARG:HD3	1.66	0.41
85:p:45:LEU:HD13	85:p:45:LEU:HA	1.93	0.41
1:0:144:GLN:C	1:0:144:GLN:OE1	2.64	0.41
5:4:103:MET:HE3	5:4:103:MET:HB3	1.83	0.41
6:5:354:PHE:HB3	6:5:417:LEU:HD11	2.03	0.41
7:6:331:PHE:CD1	7:6:337:MET:HE3	2.56	0.41
9:8:171:PHE:CD1	9:8:171:PHE:C	2.98	0.41
10:9:43:PHE:CE2	10:9:53:ILE:HD11	2.56	0.41
10:9:43:PHE:HE2	10:9:53:ILE:HD11	1.85	0.41
11:A:2343:G:H3'	11:A:2343:G:N3	2.35	0.41
11:A:2506:A:H1'	11:A:2601:A:N6	2.36	0.41
12:D:123:GLU:OE2	12:D:164:LEU:HD12	2.21	0.41
12:D:172:MET:SD	50:AE:86:ILE:HG12	2.60	0.41
12:D:262:ARG:O	12:D:266:LEU:HD22	2.21	0.41
14:F:51:VAL:HG13	14:F:81:ASP:OD1	2.21	0.41
21:N:170:GLU:OE1	41:l:132:LEU:HB3	2.21	0.41
40:n:85:GLU:CD	40:n:85:GLU:H	2.29	0.41
41:l:71:TYR:HB3	41:l:83:ASP:OD2	2.20	0.41
46:AA:1119:U:C5	64:AS:48:ARG:HD2	2.56	0.41
46:AA:1309:A:H2'	46:AA:1310:C:C6	2.56	0.41
46:AA:1520:U:H4'	46:AA:1521:U:O5'	2.21	0.41
48:AC:154:HIS:HD1	73:A1:75:PRO:HG3	1.86	0.41
49:AD:265:MET:HE2	52:AG:56:ILE:HG23	2.02	0.41
49:AD:411:VAL:O	49:AD:415:GLN:HG3	2.21	0.41
63:AR:173:VAL:HG11	72:A0:169:LEU:HD23	2.03	0.41
63:AR:266:ARG:H	63:AR:266:ARG:HG3	1.67	0.41
66:AU:189:TRP:CE3	66:AU:197:VAL:HG13	2.56	0.41
69:AX:237:THR:O	69:AX:240:VAL:HG22	2.21	0.41
71:AZ:81:GLU:OE1	71:AZ:81:GLU:HA	2.21	0.41
73:A1:115:THR:O	73:A1:119:ILE:HG13	2.21	0.41
73:A1:266:LEU:O	73:A1:270:LYS:HG2	2.20	0.41
76:A4:62:LYS:HE2	76:A4:62:LYS:HB3	1.90	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
76:A4:401:MET:HG3	76:A4:434:GLN:HE22	1.86	0.41
77:Az:7:G:O6	78:Aw:36:C:C4	2.71	0.41
78:Aw:54:U:H5	78:Aw:55:A:N3	2.19	0.41
79:Ax:27:U:H3	79:Ax:43:A:H61	1.69	0.41
84:f:51:LYS:HD3	84:f:51:LYS:HA	1.74	0.41
84:f:82:LEU:HD13	84:f:83:GLY:N	2.36	0.41
6:5:301:PRO:HB3	11:A:2389:C:P	2.61	0.40
11:A:1897:A:H2'	11:A:1898:A:C8	2.57	0.40
11:A:2386:C:H1'	11:A:2407:U:O2	2.22	0.40
11:A:2682:A:H4'	25:R:41:LEU:HD13	2.02	0.40
11:A:2769:A:H2'	11:A:2770:C:O4'	2.21	0.40
14:F:271:ASP:C	14:F:271:ASP:OD1	2.64	0.40
17:J:138:SER:O	17:J:141:VAL:HG12	2.21	0.40
33:V:175:LYS:HE3	33:V:175:LYS:HB2	1.87	0.40
36:g:66:TYR:CD2	36:g:74:PRO:HD3	2.56	0.40
40:n:76:MET:HE3	40:n:76:MET:HB2	2.00	0.40
40:n:84:LEU:HD12	40:n:84:LEU:HA	1.88	0.40
46:AA:1504:U:H2'	46:AA:1505:A:C8	2.56	0.40
49:AD:412:LYS:HE3	49:AD:418:LYS:HD3	2.03	0.40
52:AG:279:ALA:HB2	52:AG:335:GLY:HA3	2.01	0.40
57:AL:221:LYS:HD2	57:AL:221:LYS:HA	1.82	0.40
60:AO:49:SER:O	60:AO:52:LYS:HG3	2.21	0.40
67:AV:274:LYS:HB2	67:AV:348:GLU:OE2	2.21	0.40
67:AV:328:PRO:O	67:AV:332:GLU:HG2	2.22	0.40
76:A4:80:ARG:NH1	76:A4:484:SER:HB3	2.36	0.40
78:Aw:21:A:C6	78:Aw:46:A:C4	3.08	0.40
78:Aw:71:C:H2'	78:Aw:72:A:C8	2.56	0.40
6:5:257:TYR:CG	6:5:258:PRO:HA	2.57	0.40
8:7:79:PHE:HD1	83:d:281:MET:HG2	1.86	0.40
8:7:97:GLU:O	8:7:101:ARG:HG2	2.22	0.40
9:8:157:LEU:H	9:8:157:LEU:HG	1.74	0.40
11:A:2007:U:H2'	11:A:2008:G:H8	1.85	0.40
11:A:2056:G:H2'	11:A:2057:C:C6	2.55	0.40
11:A:2132:A:H62	43:o:16:GLN:NE2	2.19	0.40
11:A:2398:A:H2'	11:A:2399:A:O4'	2.21	0.40
11:A:2538:C:H2'	11:A:2539:A:O4'	2.21	0.40
12:D:207:ILE:HG12	12:D:229:PRO:HD3	2.03	0.40
14:F:46:PRO:HB3	37:h:98:PHE:CD2	2.57	0.40
16:I:130:VAL:C	16:I:133:PRO:HD2	2.46	0.40
16:I:188:ARG:HD3	40:n:55:VAL:HB	2.04	0.40
24:Q:74:ARG:HG3	24:Q:283:TRP:CZ2	2.56	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:U:11:ARG:HH21	33:V:211:LYS:NZ	2.19	0.40
30:X:32:LEU:HD23	30:X:32:LEU:HA	1.78	0.40
40:n:22:PRO:HD3	40:n:55:VAL:HG13	2.02	0.40
41:l:87:LYS:HB3	41:l:91:GLU:HB2	2.02	0.40
45:r:99:MET:HB3	45:r:99:MET:HE3	1.77	0.40
46:AA:1065:C:H2'	46:AA:1066:C:O4'	2.21	0.40
46:AA:1587:U:H2'	46:AA:1588:G:H8	1.86	0.40
51:AF:200:LEU:HB3	51:AF:202:PRO:HD2	2.03	0.40
53:AH:151:SER:HB2	73:A1:131:THR:HG23	2.03	0.40
56:AK:62:ILE:HD12	56:AK:63:LEU:N	2.36	0.40
63:AR:351:GLU:H	63:AR:351:GLU:HG2	1.73	0.40
73:A1:69:VAL:HG12	73:A1:70:TYR:HD1	1.86	0.40
76:A4:427:ARG:CA	76:A4:468:MET:HE1	2.52	0.40
76:A4:583:PHE:HD1	76:A4:588:ARG:NH2	2.19	0.40
77:Az:2:A:C3'	77:Az:3:A:H8	2.34	0.40
77:Az:11:U:H1'	77:Az:12:U:H5	1.86	0.40
78:Aw:14:A:C6	78:Aw:15:A:C4	3.09	0.40
78:Aw:65:A:H2'	78:Aw:66:U:C6	2.56	0.40
78:Aw:65:A:H2'	78:Aw:66:U:H6	1.87	0.40
79:Ax:49:G:N2	79:Ax:66:U:H1'	2.36	0.40
82:c:79:LEU:HD13	82:c:214:PHE:CE1	2.56	0.40
9:8:47:SER:HA	77:Az:7:G:OP2	2.21	0.40
10:9:111:PRO:HA	10:9:114:LEU:HD23	2.04	0.40
11:A:1928:A:OP2	92:A:3472:NMY:H81	2.22	0.40
11:A:2545:U:H1'	11:A:2635:G:N2	2.36	0.40
14:F:114:THR:HG21	14:F:154:GLY:HA3	2.04	0.40
35:e:221:MET:HE2	35:e:221:MET:C	2.47	0.40
46:AA:661:C:H2'	46:AA:662:U:H6	1.87	0.40
46:AA:686:A:H2'	46:AA:687:G:H8	1.87	0.40
46:AA:1109:A:H2'	46:AA:1110:A:H8	1.86	0.40
46:AA:1190:C:H2'	46:AA:1191:C:H6	1.87	0.40
46:AA:1322:C:OP2	48:AC:36:LYS:HE3	2.20	0.40
51:AF:133:GLU:O	51:AF:137:ILE:HG12	2.21	0.40
52:AG:313:LEU:O	52:AG:316:PRO:HD2	2.22	0.40
56:AK:29:TYR:HB3	56:AK:34:MET:HE3	2.03	0.40
60:AO:122:LEU:O	60:AO:125:GLN:HB3	2.21	0.40
61:AP:141:ARG:HG3	61:AP:141:ARG:NH1	2.36	0.40
67:AV:149:ASP:HA	67:AV:152:ILE:HG22	2.03	0.40
69:AX:125:LEU:HD11	69:AX:310:LEU:HG	2.03	0.40
72:A0:4:LYS:HB3	72:A0:5:LYS:HE2	2.04	0.40
74:G:58:GLN:OE1	74:G:58:GLN:HA	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
76:A4:299:GLU:HG3	76:A4:341:CYS:SG	2.60	0.40
76:A4:317:LEU:HB3	76:A4:321:ARG:NH2	2.36	0.40
78:Aw:22:A:H2'	78:Aw:23:A:C8	2.56	0.40
79:Ax:72:A:H2'	79:Ax:73:A:H8	1.85	0.40
80:B:49:U:H2'	80:B:50:U:C6	2.56	0.40
82:c:42:GLN:O	82:c:46:GLU:HG3	2.21	0.40
86:s:91:TYR:HE2	86:s:229:LEU:HD22	1.87	0.40
2:1:19:ARG:HB2	2:1:62:ILE:HD11	2.03	0.40
11:A:2186:C:H2'	11:A:2187:C:H6	1.85	0.40
12:D:171:ARG:CZ	50:AE:86:ILE:HD11	2.52	0.40
12:D:199:GLU:HG2	12:D:202:ARG:HB2	2.04	0.40
14:F:282:PRO:HB3	14:F:286:PHE:CZ	2.56	0.40
15:H:78:ARG:HG3	30:X:88:GLY:HA2	2.04	0.40
22:O:20:LEU:H	22:O:24:SER:CB	2.35	0.40
30:X:166:LEU:HD23	30:X:166:LEU:HA	1.93	0.40
33:V:72:LYS:HE3	83:d:256:TYR:CD1	2.57	0.40
45:r:87:LEU:HD23	45:r:87:LEU:HA	1.88	0.40
50:AE:36:VAL:HG12	66:AU:168:ILE:HB	2.04	0.40
51:AF:155:MET:H	51:AF:155:MET:HG2	1.69	0.40
69:AX:56:PRO:HA	69:AX:59:HIS:CE1	2.57	0.40
76:A4:264:ARG:HH22	76:A4:292:TYR:HD2	1.70	0.40
83:d:177:LYS:HE2	83:d:177:LYS:HB2	1.84	0.40
2:1:55:LEU:HD23	2:1:55:LEU:HA	1.83	0.40
6:5:193:LEU:HD13	6:5:193:LEU:HA	1.92	0.40
6:5:310:ARG:NH1	6:5:378:SER:HB3	2.36	0.40
7:6:221:LEU:HD12	7:6:221:LEU:H	1.86	0.40
8:7:79:PHE:CD1	83:d:281:MET:HG2	2.56	0.40
8:7:233:SER:HB2	8:7:236:LYS:HB2	2.03	0.40
10:9:45:THR:HG22	10:9:49:ARG:O	2.20	0.40
11:A:2313:A:H2'	11:A:2314:C:C6	2.56	0.40
11:A:2603:C:H2'	11:A:2604:A:H8	1.87	0.40
11:A:2950:U:H2'	11:A:2951:A:H8	1.87	0.40
11:A:3057:C:H2'	11:A:3058:U:O4'	2.21	0.40
14:F:279:ARG:NH1	14:F:282:PRO:HD3	2.33	0.40
16:I:90:PHE:HD1	16:I:96:ILE:HD13	1.85	0.40
16:I:103:ALA:HB3	40:n:39:SER:HA	2.02	0.40
18:k:20:LEU:HB2	18:k:141:LEU:HD13	2.02	0.40
21:N:116:LYS:H	21:N:116:LYS:HD3	1.86	0.40
23:P:72:PHE:HB2	29:W:107:HIS:HA	2.04	0.40
34:b:10:ARG:HB3	34:b:114:ILE:HD11	2.04	0.40
40:n:64:VAL:O	40:n:75:ILE:HA	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:l:119:ARG:HG2	41:l:119:ARG:NH1	2.36	0.40
44:q:33:ARG:NH2	44:q:34:ARG:HB2	2.36	0.40
46:AA:877:G:H2'	46:AA:878:G:C8	2.57	0.40
46:AA:1067:A:H2'	46:AA:1068:A:O4'	2.21	0.40
46:AA:1499:U:H2'	46:AA:1500:C:C6	2.56	0.40
48:AC:48:ASP:OD1	48:AC:48:ASP:N	2.54	0.40
49:AD:221:ARG:HD2	49:AD:322:THR:HG23	2.03	0.40
49:AD:241:ILE:HG21	49:AD:264:ARG:HG3	2.03	0.40
53:AH:113:ARG:HB3	53:AH:139:LEU:HD13	2.04	0.40
60:AO:150:LEU:HD23	60:AO:150:LEU:HA	1.87	0.40
67:AV:85:ILE:HG23	67:AV:112:TRP:CH2	2.56	0.40
69:AX:136:LEU:HD23	69:AX:136:LEU:HA	1.90	0.40
69:AX:349:ASN:CG	69:AX:352:GLU:HG3	2.46	0.40
76:A4:429:LEU:HB2	76:A4:468:MET:HB3	2.04	0.40
76:A4:571:TRP:HE3	76:A4:576:LEU:HD21	1.85	0.40
79:Ax:12:U:H2'	79:Ax:13:U:O4'	2.22	0.40
84:f:109:TYR:CD1	84:f:109:TYR:C	2.98	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	
1	0	108/188 (57%)	107 (99%)	1 (1%)	0	100	100
2	1	54/65 (83%)	52 (96%)	2 (4%)	0	100	100
3	2	44/92 (48%)	44 (100%)	0	0	100	100
4	3	93/188 (50%)	92 (99%)	1 (1%)	0	100	100
5	4	36/103 (35%)	36 (100%)	0	0	100	100
6	5	392/423 (93%)	385 (98%)	7 (2%)	0	100	100
7	6	352/380 (93%)	343 (97%)	9 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	7	292/338 (86%)	283 (97%)	9 (3%)	0	100	100
9	8	155/206 (75%)	152 (98%)	3 (2%)	0	100	100
10	9	122/137 (89%)	119 (98%)	3 (2%)	0	100	100
12	D	236/305 (77%)	231 (98%)	5 (2%)	0	100	100
13	E	303/348 (87%)	296 (98%)	7 (2%)	0	100	100
14	F	250/311 (80%)	249 (100%)	1 (0%)	0	100	100
15	H	200/267 (75%)	198 (99%)	2 (1%)	0	100	100
16	I	166/261 (64%)	163 (98%)	3 (2%)	0	100	100
17	J	173/192 (90%)	170 (98%)	3 (2%)	0	100	100
18	k	176/178 (99%)	172 (98%)	4 (2%)	0	100	100
19	L	113/145 (78%)	111 (98%)	2 (2%)	0	100	100
20	M	287/296 (97%)	284 (99%)	3 (1%)	0	100	100
21	N	220/251 (88%)	218 (99%)	2 (1%)	0	100	100
22	O	152/175 (87%)	149 (98%)	3 (2%)	0	100	100
23	P	142/180 (79%)	142 (100%)	0	0	100	100
24	Q	237/292 (81%)	234 (99%)	2 (1%)	1 (0%)	30	59
25	R	138/149 (93%)	138 (100%)	0	0	100	100
26	S	159/205 (78%)	158 (99%)	1 (1%)	0	100	100
27	T	164/206 (80%)	159 (97%)	5 (3%)	0	100	100
28	U	151/153 (99%)	150 (99%)	1 (1%)	0	100	100
29	W	114/148 (77%)	113 (99%)	1 (1%)	0	100	100
30	X	242/256 (94%)	239 (99%)	3 (1%)	0	100	100
31	Y	179/250 (72%)	177 (99%)	2 (1%)	0	100	100
32	Z	120/161 (74%)	119 (99%)	1 (1%)	0	100	100
33	V	203/216 (94%)	199 (98%)	4 (2%)	0	100	100
34	b	149/215 (69%)	144 (97%)	5 (3%)	0	100	100
35	e	236/279 (85%)	225 (95%)	11 (5%)	0	100	100
36	g	132/166 (80%)	132 (100%)	0	0	100	100
37	h	108/158 (68%)	105 (97%)	3 (3%)	0	100	100
38	i	95/128 (74%)	95 (100%)	0	0	100	100
39	j	92/123 (75%)	91 (99%)	1 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	n	100/112 (89%)	98 (98%)	2 (2%)	0	100	100
41	l	80/138 (58%)	80 (100%)	0	0	100	100
42	m	90/128 (70%)	85 (94%)	5 (6%)	0	100	100
43	o	92/102 (90%)	91 (99%)	1 (1%)	0	100	100
44	q	126/222 (57%)	125 (99%)	1 (1%)	0	100	100
45	r	160/196 (82%)	158 (99%)	2 (1%)	0	100	100
47	AB	220/296 (74%)	217 (99%)	3 (1%)	0	100	100
48	AC	130/167 (78%)	128 (98%)	2 (2%)	0	100	100
49	AD	341/430 (79%)	335 (98%)	6 (2%)	0	100	100
50	AE	120/125 (96%)	119 (99%)	1 (1%)	0	100	100
51	AF	206/242 (85%)	205 (100%)	1 (0%)	0	100	100
52	AG	323/396 (82%)	316 (98%)	7 (2%)	0	100	100
53	AH	138/201 (69%)	136 (99%)	1 (1%)	1 (1%)	18	48
54	AI	134/194 (69%)	132 (98%)	2 (2%)	0	100	100
55	AJ	106/138 (77%)	103 (97%)	3 (3%)	0	100	100
56	AK	99/128 (77%)	99 (100%)	0	0	100	100
57	AL	172/257 (67%)	170 (99%)	2 (1%)	0	100	100
58	AM	117/137 (85%)	116 (99%)	1 (1%)	0	100	100
59	AN	108/130 (83%)	105 (97%)	3 (3%)	0	100	100
60	AO	191/258 (74%)	188 (98%)	3 (2%)	0	100	100
61	AP	95/142 (67%)	94 (99%)	1 (1%)	0	100	100
62	C	85/87 (98%)	83 (98%)	2 (2%)	0	100	100
63	AR	293/360 (81%)	288 (98%)	5 (2%)	0	100	100
64	AS	133/190 (70%)	132 (99%)	1 (1%)	0	100	100
65	AT	166/173 (96%)	164 (99%)	2 (1%)	0	100	100
66	AU	174/205 (85%)	173 (99%)	1 (1%)	0	100	100
67	AV	358/414 (86%)	352 (98%)	6 (2%)	0	100	100
68	AW	98/187 (52%)	98 (100%)	0	0	100	100
69	AX	350/398 (88%)	346 (99%)	4 (1%)	0	100	100
70	AY	147/395 (37%)	145 (99%)	2 (1%)	0	100	100
71	AZ	98/106 (92%)	97 (99%)	1 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
72	A0	213/217 (98%)	207 (97%)	6 (3%)	0	100	100
73	A1	277/323 (86%)	271 (98%)	6 (2%)	0	100	100
74	G	116/118 (98%)	114 (98%)	2 (2%)	0	100	100
75	A3	68/199 (34%)	67 (98%)	1 (2%)	0	100	100
76	A4	584/689 (85%)	575 (98%)	9 (2%)	0	100	100
81	a	96/142 (68%)	95 (99%)	1 (1%)	0	100	100
82	c	282/332 (85%)	279 (99%)	3 (1%)	0	100	100
83	d	235/306 (77%)	228 (97%)	7 (3%)	0	100	100
84	f	153/212 (72%)	149 (97%)	4 (3%)	0	100	100
85	p	141/206 (68%)	138 (98%)	3 (2%)	0	100	100
86	s	382/439 (87%)	375 (98%)	7 (2%)	0	100	100
All	All	14182/17971 (79%)	13950 (98%)	230 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
53	AH	126	ILE
24	Q	62	ILE

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	
1	0	99/164 (60%)	98 (99%)	1 (1%)	68	89
2	1	53/60 (88%)	51 (96%)	2 (4%)	29	64
3	2	40/72 (56%)	38 (95%)	2 (5%)	22	53
4	3	88/166 (53%)	87 (99%)	1 (1%)	65	88
5	4	37/89 (42%)	37 (100%)	0	100	100
6	5	353/368 (96%)	346 (98%)	7 (2%)	48	78
7	6	313/332 (94%)	310 (99%)	3 (1%)	68	89

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	7	270/303 (89%)	264 (98%)	6 (2%)	45	77
9	8	146/190 (77%)	140 (96%)	6 (4%)	27	61
10	9	104/112 (93%)	100 (96%)	4 (4%)	29	64
12	D	192/245 (78%)	191 (100%)	1 (0%)	81	93
13	E	260/290 (90%)	257 (99%)	3 (1%)	63	86
14	F	219/262 (84%)	215 (98%)	4 (2%)	51	80
15	H	182/228 (80%)	179 (98%)	3 (2%)	55	83
16	I	153/232 (66%)	151 (99%)	2 (1%)	61	86
17	J	138/150 (92%)	132 (96%)	6 (4%)	26	60
18	k	155/155 (100%)	152 (98%)	3 (2%)	50	79
19	L	98/124 (79%)	96 (98%)	2 (2%)	48	78
20	M	245/249 (98%)	244 (100%)	1 (0%)	84	94
21	N	189/211 (90%)	188 (100%)	1 (0%)	81	93
22	O	134/150 (89%)	132 (98%)	2 (2%)	57	84
23	P	126/155 (81%)	126 (100%)	0	100	100
24	Q	221/256 (86%)	220 (100%)	1 (0%)	81	93
25	R	118/126 (94%)	115 (98%)	3 (2%)	42	74
26	S	146/180 (81%)	146 (100%)	0	100	100
27	T	146/176 (83%)	141 (97%)	5 (3%)	32	66
28	U	134/134 (100%)	128 (96%)	6 (4%)	24	58
29	W	94/119 (79%)	93 (99%)	1 (1%)	65	88
30	X	220/229 (96%)	219 (100%)	1 (0%)	81	93
31	Y	163/223 (73%)	161 (99%)	2 (1%)	63	86
32	Z	113/147 (77%)	112 (99%)	1 (1%)	70	90
33	V	183/191 (96%)	176 (96%)	7 (4%)	29	64
34	b	132/185 (71%)	127 (96%)	5 (4%)	29	64
35	e	207/236 (88%)	201 (97%)	6 (3%)	37	71
36	g	124/148 (84%)	121 (98%)	3 (2%)	43	75
37	h	104/148 (70%)	99 (95%)	5 (5%)	23	55
38	i	86/110 (78%)	85 (99%)	1 (1%)	63	86
39	j	74/97 (76%)	72 (97%)	2 (3%)	39	73

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	n	83/89 (93%)	82 (99%)	1 (1%)	63	86
41	l	76/116 (66%)	76 (100%)	0	100	100
42	m	85/113 (75%)	82 (96%)	3 (4%)	32	66
43	o	80/87 (92%)	78 (98%)	2 (2%)	42	74
44	q	110/178 (62%)	110 (100%)	0	100	100
45	r	147/169 (87%)	143 (97%)	4 (3%)	39	73
47	AB	197/249 (79%)	193 (98%)	4 (2%)	48	78
48	AC	115/143 (80%)	110 (96%)	5 (4%)	26	60
49	AD	286/357 (80%)	283 (99%)	3 (1%)	68	89
50	AE	104/107 (97%)	103 (99%)	1 (1%)	68	89
51	AF	185/209 (88%)	182 (98%)	3 (2%)	55	83
52	AG	285/342 (83%)	283 (99%)	2 (1%)	76	92
53	AH	130/180 (72%)	126 (97%)	4 (3%)	35	69
54	AI	104/146 (71%)	102 (98%)	2 (2%)	50	79
55	AJ	93/118 (79%)	92 (99%)	1 (1%)	65	88
56	AK	91/113 (80%)	90 (99%)	1 (1%)	65	88
57	AL	158/226 (70%)	157 (99%)	1 (1%)	78	93
58	AM	97/113 (86%)	96 (99%)	1 (1%)	68	89
59	AN	96/115 (84%)	94 (98%)	2 (2%)	47	77
60	AO	174/230 (76%)	173 (99%)	1 (1%)	78	93
61	AP	88/123 (72%)	87 (99%)	1 (1%)	65	88
62	C	78/78 (100%)	78 (100%)	0	100	100
63	AR	264/318 (83%)	258 (98%)	6 (2%)	44	76
64	AS	116/164 (71%)	114 (98%)	2 (2%)	53	82
65	AT	153/157 (98%)	150 (98%)	3 (2%)	48	78
66	AU	152/174 (87%)	148 (97%)	4 (3%)	40	73
67	AV	325/364 (89%)	318 (98%)	7 (2%)	45	77
68	AW	87/158 (55%)	81 (93%)	6 (7%)	14	41
69	AX	311/351 (89%)	308 (99%)	3 (1%)	68	89
70	AY	137/357 (38%)	137 (100%)	0	100	100
71	AZ	90/95 (95%)	89 (99%)	1 (1%)	65	88

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
72	A0	188/189 (100%)	185 (98%)	3 (2%)	55	83
73	A1	257/291 (88%)	253 (98%)	4 (2%)	55	83
74	G	100/100 (100%)	99 (99%)	1 (1%)	68	89
75	A3	65/166 (39%)	61 (94%)	4 (6%)	16	46
76	A4	526/609 (86%)	515 (98%)	11 (2%)	47	77
81	a	96/133 (72%)	94 (98%)	2 (2%)	47	77
82	c	251/288 (87%)	249 (99%)	2 (1%)	73	90
83	d	223/274 (81%)	219 (98%)	4 (2%)	51	80
84	f	139/188 (74%)	135 (97%)	4 (3%)	37	71
85	p	135/181 (75%)	134 (99%)	1 (1%)	76	92
86	s	340/381 (89%)	334 (98%)	6 (2%)	51	80
All	All	12676/15551 (82%)	12451 (98%)	225 (2%)	51	80

All (225) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	108	ASP
2	1	37	LEU
2	1	54	VAL
3	2	56	SER
3	2	72	THR
4	3	164	SER
6	5	41	SER
6	5	89	ARG
6	5	140	VAL
6	5	155	LEU
6	5	252	VAL
6	5	370	VAL
6	5	391	VAL
7	6	100	THR
7	6	219	THR
7	6	338	ARG
8	7	55	GLN
8	7	59	THR
8	7	143	TRP
8	7	184	VAL
8	7	187	SER
8	7	257	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	8	90	THR
9	8	154	SER
9	8	157	LEU
9	8	164	ARG
9	8	195	ILE
9	8	198	VAL
10	9	29	SER
10	9	94	GLU
10	9	96	VAL
10	9	122	THR
12	D	71	LYS
13	E	45	SER
13	E	111	THR
13	E	256	LYS
14	F	228	GLN
14	F	236	ARG
14	F	242	LEU
14	F	258	THR
15	H	102	VAL
15	H	148	GLN
15	H	193	PHE
16	I	169	ARG
16	I	174	LEU
17	J	21	ARG
17	J	44	VAL
17	J	46	ILE
17	J	127	ASP
17	J	135	VAL
17	J	141	VAL
18	k	67	PHE
18	k	78	SER
18	k	171	THR
19	L	83	LYS
19	L	135	SER
20	M	155	GLU
21	N	87	PHE
22	O	109	GLN
22	O	115	LEU
24	Q	141	SER
25	R	15	THR
25	R	23	GLU
25	R	121	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
27	T	52	VAL
27	T	66	GLU
27	T	84	LEU
27	T	151	ARG
27	T	164	VAL
28	U	28	LEU
28	U	46	MET
28	U	48	MET
28	U	70	THR
28	U	110	LEU
28	U	131	GLU
29	W	93	GLU
30	X	151	GLU
31	Y	86	THR
31	Y	128	SER
32	Z	39	SER
33	V	23	MET
33	V	47	GLU
33	V	56	LEU
33	V	108	MET
33	V	146	VAL
33	V	166	VAL
33	V	193	THR
34	b	63	VAL
34	b	95	VAL
34	b	108	GLN
34	b	112	ASP
34	b	149	VAL
35	e	53	LEU
35	e	60	SER
35	e	77	ILE
35	e	172	ILE
35	e	240	THR
35	e	255	VAL
36	g	143	VAL
36	g	147	LEU
36	g	149	ILE
37	h	61	THR
37	h	70	LEU
37	h	87	GLN
37	h	96	LEU
37	h	157	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
38	i	43	VAL
39	j	89	GLN
39	j	115	SER
40	n	57	HIS
42	m	41	THR
42	m	73	ARG
42	m	114	LEU
43	o	11	ARG
43	o	69	GLU
45	r	39	VAL
45	r	73	CYS
45	r	140	VAL
45	r	146	GLN
47	AB	150	GLN
47	AB	152	SER
47	AB	236	VAL
47	AB	254	GLN
48	AC	52	THR
48	AC	76	LEU
48	AC	115	ASN
48	AC	142	LEU
48	AC	162	VAL
49	AD	276	VAL
49	AD	332	MET
49	AD	382	ILE
50	AE	29	LEU
51	AF	45	LEU
51	AF	67	GLU
51	AF	226	LEU
52	AG	129	GLU
52	AG	247	SER
53	AH	64	THR
53	AH	80	VAL
53	AH	172	VAL
53	AH	179	GLN
54	AI	104	ASN
54	AI	179	THR
55	AJ	127	ARG
56	AK	30	VAL
57	AL	116	VAL
58	AM	93	LEU
59	AN	6	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
59	AN	65	LEU
60	AO	164	ILE
61	AP	50	LEU
63	AR	111	LEU
63	AR	125	ARG
63	AR	159	THR
63	AR	192	MET
63	AR	205	LEU
63	AR	307	LEU
64	AS	63	ILE
64	AS	116	LYS
65	AT	94	SER
65	AT	136	LEU
65	AT	158	GLU
66	AU	56	LEU
66	AU	89	VAL
66	AU	127	GLU
66	AU	165	LYS
67	AV	116	CYS
67	AV	208	LEU
67	AV	247	MET
67	AV	352	LEU
67	AV	366	THR
67	AV	367	CYS
67	AV	404	TYR
68	AW	147	LEU
68	AW	148	GLU
68	AW	150	THR
68	AW	159	ASP
68	AW	161	THR
68	AW	173	GLN
69	AX	107	GLU
69	AX	125	LEU
69	AX	259	LEU
71	AZ	74	GLU
72	A0	61	GLU
72	A0	91	GLU
72	A0	119	THR
73	A1	95	VAL
73	A1	206	THR
73	A1	275	ASN
73	A1	278	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
74	G	70	ILE
75	A3	158	GLN
75	A3	170	GLU
75	A3	178	LEU
75	A3	196	LEU
76	A4	70	VAL
76	A4	90	GLN
76	A4	114	GLU
76	A4	183	VAL
76	A4	259	TYR
76	A4	308	LYS
76	A4	316	ILE
76	A4	329	LYS
76	A4	396	ILE
76	A4	409	ASP
76	A4	486	TYR
81	a	37	SER
81	a	91	VAL
82	c	31	VAL
82	c	106	GLN
83	d	75	SER
83	d	150	LEU
83	d	155	SER
83	d	247	VAL
84	f	53	THR
84	f	132	ILE
84	f	135	LEU
84	f	149	VAL
85	p	191	LYS
86	s	161	ARG
86	s	185	VAL
86	s	312	LEU
86	s	362	THR
86	s	392	ILE
86	s	396	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (117) such sidechains are listed below:

Mol	Chain	Res	Type
2	1	31	ASN
6	5	160	HIS
6	5	214	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	5	269	ASN
6	5	384	GLN
7	6	354	GLN
8	7	247	ASN
9	8	62	GLN
9	8	158	HIS
10	9	52	GLN
10	9	123	GLN
12	D	94	HIS
12	D	194	ASN
12	D	195	ASN
12	D	235	GLN
13	E	88	HIS
13	E	137	ASN
13	E	174	GLN
13	E	202	GLN
14	F	63	GLN
14	F	103	GLN
14	F	105	ASN
14	F	228	GLN
14	F	241	ASN
15	H	156	GLN
15	H	204	HIS
15	H	226	ASN
16	I	43	GLN
17	J	133	GLN
18	k	89	GLN
19	L	33	GLN
19	L	48	ASN
19	L	103	ASN
21	N	178	GLN
21	N	210	GLN
23	P	115	HIS
24	Q	132	GLN
24	Q	172	GLN
24	Q	258	GLN
24	Q	261	ASN
24	Q	262	GLN
25	R	89	ASN
25	R	149	HIS
26	S	140	ASN
28	U	27	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
28	U	77	ASN
30	X	93	ASN
32	Z	62	ASN
34	b	26	GLN
34	b	28	GLN
38	i	120	HIS
38	i	124	HIS
39	j	26	GLN
40	n	15	GLN
44	q	134	ASN
45	r	76	ASN
45	r	79	HIS
45	r	109	GLN
45	r	131	HIS
49	AD	341	ASN
49	AD	369	HIS
51	AF	214	HIS
52	AG	288	HIS
52	AG	318	HIS
52	AG	340	GLN
52	AG	384	GLN
53	AH	83	HIS
53	AH	176	GLN
53	AH	183	HIS
54	AI	87	HIS
54	AI	96	GLN
54	AI	163	HIS
55	AJ	77	ASN
55	AJ	134	HIS
56	AK	28	HIS
57	AL	162	GLN
58	AM	69	ASN
59	AN	44	ASN
60	AO	103	ASN
60	AO	147	HIS
61	AP	47	ASN
61	AP	71	HIS
61	AP	115	GLN
61	AP	137	ASN
63	AR	139	ASN
63	AR	305	HIS
63	AR	347	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
63	AR	356	HIS
65	AT	35	ASN
65	AT	85	GLN
66	AU	62	HIS
66	AU	186	ASN
67	AV	170	GLN
67	AV	224	GLN
67	AV	324	GLN
67	AV	396	GLN
67	AV	399	GLN
69	AX	66	GLN
69	AX	363	ASN
70	AY	285	GLN
73	A1	231	HIS
75	A3	141	HIS
75	A3	158	GLN
76	A4	189	ASN
76	A4	288	HIS
76	A4	436	HIS
81	a	90	GLN
81	a	126	HIS
82	c	128	GLN
82	c	168	HIS
82	c	204	GLN
83	d	217	HIS
84	f	94	HIS
86	s	71	HIS
86	s	107	GLN
86	s	375	ASN
86	s	423	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	A	1556/1561 (99%)	246 (15%)	3 (0%)
46	AA	953/954 (99%)	146 (15%)	1 (0%)
77	Az	15/32 (46%)	4 (26%)	0
78	Aw	67/68 (98%)	39 (58%)	0
79	Ax	68/70 (97%)	34 (50%)	0
80	B	71/72 (98%)	16 (22%)	0
All	All	2730/2757 (99%)	485 (17%)	4 (0%)

All (485) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	A	1681	G
11	A	1689	C
11	A	1692	A
11	A	1699	C
11	A	1700	U
11	A	1704	U
11	A	1708	A
11	A	1713	A
11	A	1724	A
11	A	1727	A
11	A	1736	A
11	A	1748	G
11	A	1765	C
11	A	1805	A
11	A	1807	U
11	A	1821	A
11	A	1827	C
11	A	1828	A
11	A	1832	A
11	A	1836	A
11	A	1844	A
11	A	1854	U
11	A	1856	A
11	A	1869	A
11	A	1878	U
11	A	1882	A
11	A	1887	A
11	A	1888	G
11	A	1893	A
11	A	1902	C
11	A	1903	C
11	A	1909	A
11	A	1918	G
11	A	1937	A
11	A	1940	A
11	A	1985	G
11	A	1992	C
11	A	1993	A
11	A	1994	A
11	A	2002	G
11	A	2003	A
11	A	2015	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	A	2022	G
11	A	2030	U
11	A	2031	A
11	A	2036	C
11	A	2037	U
11	A	2039	A
11	A	2054	U
11	A	2055	U
11	A	2060	A
11	A	2069	U
11	A	2070	C
11	A	2071	U
11	A	2079	C
11	A	2098	G
11	A	2099	U
11	A	2105	G
11	A	2111	C
11	A	2113	G
11	A	2125	C
11	A	2126	U
11	A	2131	A
11	A	2147	G
11	A	2159	U
11	A	2163	A
11	A	2168	U
11	A	2181	A
11	A	2182	G
11	A	2198	A
11	A	2200	A
11	A	2214	A
11	A	2219	C
11	A	2221	C
11	A	2225	C
11	A	2226	U
11	A	2227	A
11	A	2228	A
11	A	2230	A
11	A	2233	U
11	A	2237	A
11	A	2241	A
11	A	2243	A
11	A	2245	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	A	2246	A
11	A	2262	C
11	A	2263	C
11	A	2283	C
11	A	2284	C
11	A	2285	U
11	A	2297	A
11	A	2300	G
11	A	2322	C
11	A	2331	C
11	A	2332	C
11	A	2333	G
11	A	2345	G
11	A	2349	G
11	A	2350	A
11	A	2353	A
11	A	2354	A
11	A	2363	A
11	A	2372	U
11	A	2374	A
11	A	2399	A
11	A	2401	A
11	A	2404	U
11	A	2405	C
11	A	2406	A
11	A	2407	U
11	A	2414	C
11	A	2415	C
11	A	2451	A
11	A	2452	A
11	A	2458	A
11	A	2471	G
11	A	2478	G
11	A	2484	C
11	A	2485	U
11	A	2493	C
11	A	2502	C
11	A	2506	A
11	A	2520	C
11	A	2521	A
11	A	2527	A
11	A	2540	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	A	2557	C
11	A	2558	A
11	A	2570	C
11	A	2571	G
11	A	2592	G
11	A	2593	G
11	A	2599	U
11	A	2600	A
11	A	2601	A
11	A	2618	U
11	A	2627	G
11	A	2630	U
11	A	2633	A
11	A	2635	G
11	A	2654	U
11	A	2655	G
11	A	2656	U
11	A	2683	C
11	A	2686	G
11	A	2694	A
11	A	2696	A
11	A	2706	A
11	A	2708	C
11	A	2718	C
11	A	2719	G
11	A	2723	A
11	A	2724	G
11	A	2732	G
11	A	2745	A
11	A	2757	A
11	A	2758	G
11	A	2761	C
11	A	2762	C
11	A	2764	A
11	A	2765	A
11	A	2766	C
11	A	2767	A
11	A	2768	A
11	A	2773	A
11	A	2774	C
11	A	2776	G
11	A	2778	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	A	2780	C
11	A	2782	A
11	A	2783	A
11	A	2786	U
11	A	2791	A
11	A	2801	A
11	A	2804	A
11	A	2810	G
11	A	2832	A
11	A	2833	A
11	A	2847	C
11	A	2864	U
11	A	2865	C
11	A	2882	U
11	A	2883	A
11	A	2884	C
11	A	2887	U
11	A	2888	A
11	A	2889	C
11	A	2893	A
11	A	2911	C
11	A	2913	A
11	A	2915	C
11	A	2916	G
11	A	2917	G
11	A	2918	A
11	A	2919	A
11	A	2922	A
11	A	2928	C
11	A	2935	A
11	A	2956	A
11	A	2962	C
11	A	2965	A
11	A	2971	A
11	A	2985	C
11	A	2989	G
11	A	2990	A
11	A	2992	G
11	A	3000	A
11	A	3005	A
11	A	3007	C
11	A	3016	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	A	3022	G
11	A	3041	U
11	A	3053	A
11	A	3054	G
11	A	3066	C
11	A	3070	G
11	A	3090	G
11	A	3096	U
11	A	3100	U
11	A	3102	U
11	A	3110	C
11	A	3111	A
11	A	3112	A
11	A	3113	A
11	A	3150	U
11	A	3157	C
11	A	3158	A
11	A	3162	C
11	A	3172	C
11	A	3176	A
11	A	3180	A
11	A	3183	U
11	A	3190	A
11	A	3199	U
11	A	3200	U
11	A	3207	A
11	A	3209	A
11	A	3210	C
11	A	3212	C
11	A	3217	A
11	A	3218	A
11	A	3220	A
11	A	3228	U
11	A	3229	U
11	A	3230	G
11	A	3231	U
46	AA	651	A
46	AA	672	A
46	AA	673	U
46	AA	680	U
46	AA	688	A
46	AA	704	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
46	AA	721	U
46	AA	737	C
46	AA	738	A
46	AA	753	A
46	AA	761	A
46	AA	766	G
46	AA	773	U
46	AA	777	G
46	AA	783	A
46	AA	791	G
46	AA	794	U
46	AA	796	G
46	AA	808	C
46	AA	815	C
46	AA	817	G
46	AA	829	C
46	AA	830	U
46	AA	832	U
46	AA	835	C
46	AA	836	A
46	AA	851	A
46	AA	860	A
46	AA	861	U
46	AA	866	A
46	AA	868	C
46	AA	871	A
46	AA	881	A
46	AA	890	C
46	AA	893	G
46	AA	903	U
46	AA	904	C
46	AA	907	A
46	AA	919	A
46	AA	923	A
46	AA	929	A
46	AA	930	G
46	AA	932	C
46	AA	938	A
46	AA	939	A
46	AA	941	G
46	AA	942	A
46	AA	943	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
46	AA	946	U
46	AA	947	U
46	AA	954	C
46	AA	958	C
46	AA	960	C
46	AA	962	C
46	AA	963	C
46	AA	967	A
46	AA	992	U
46	AA	1001	C
46	AA	1002	C
46	AA	1015	A
46	AA	1031	G
46	AA	1042	U
46	AA	1080	A
46	AA	1081	U
46	AA	1082	A
46	AA	1103	A
46	AA	1105	C
46	AA	1106	C
46	AA	1107	U
46	AA	1109	A
46	AA	1116	A
46	AA	1118	A
46	AA	1119	U
46	AA	1120	C
46	AA	1121	A
46	AA	1126	A
46	AA	1137	A
46	AA	1151	C
46	AA	1152	A
46	AA	1153	C
46	AA	1155	G
46	AA	1160	A
46	AA	1167	A
46	AA	1187	U
46	AA	1189	U
46	AA	1190	C
46	AA	1193	U
46	AA	1209	C
46	AA	1215	U
46	AA	1220	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
46	AA	1223	C
46	AA	1225	C
46	AA	1230	C
46	AA	1235	U
46	AA	1247	G
46	AA	1248	C
46	AA	1251	A
46	AA	1271	C
46	AA	1273	G
46	AA	1275	A
46	AA	1283	A
46	AA	1284	U
46	AA	1285	G
46	AA	1290	C
46	AA	1291	U
46	AA	1326	A
46	AA	1327	G
46	AA	1330	C
46	AA	1343	A
46	AA	1354	A
46	AA	1356	A
46	AA	1376	C
46	AA	1378	C
46	AA	1387	A
46	AA	1390	A
46	AA	1391	U
46	AA	1405	C
46	AA	1407	U
46	AA	1420	U
46	AA	1430	A
46	AA	1469	G
46	AA	1470	A
46	AA	1481	C
46	AA	1482	A
46	AA	1503	G
46	AA	1512	A
46	AA	1519	A
46	AA	1521	U
46	AA	1522	U
46	AA	1525	C
46	AA	1526	U
46	AA	1527	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
46	AA	1533	C
46	AA	1536	A
46	AA	1537	C
46	AA	1540	A
46	AA	1541	U
46	AA	1544	A
46	AA	1557	A
46	AA	1568	U
46	AA	1571	U
46	AA	1582	G
46	AA	1584	MA6
46	AA	1594	G
46	AA	1595	G
46	AA	1599	A
77	Az	4	A
77	Az	11	U
77	Az	12	U
77	Az	13	U
78	Aw	5	A
78	Aw	6	U
78	Aw	7	A
78	Aw	8	U
78	Aw	9	A
78	Aw	12	U
78	Aw	14	A
78	Aw	15	A
78	Aw	16	A
78	Aw	20	C
78	Aw	21	A
78	Aw	22	A
78	Aw	24	A
78	Aw	26	U
78	Aw	27	A
78	Aw	28	A
78	Aw	29	U
78	Aw	30	G
78	Aw	34	A
78	Aw	35	A
78	Aw	36	C
78	Aw	42	U
78	Aw	45	A
78	Aw	46	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
78	Aw	48	U
78	Aw	49	U
78	Aw	51	U
78	Aw	53	A
78	Aw	55	A
78	Aw	56	A
78	Aw	61	U
78	Aw	63	A
78	Aw	64	U
78	Aw	67	U
78	Aw	69	A
78	Aw	70	C
78	Aw	71	C
78	Aw	74	C
78	Aw	75	C
79	Ax	3	G
79	Ax	5	G
79	Ax	6	A
79	Ax	7	A
79	Ax	8	U
79	Ax	9	A
79	Ax	11	U
79	Ax	12	U
79	Ax	14	A
79	Ax	22	A
79	Ax	24	A
79	Ax	28	C
79	Ax	30	G
79	Ax	34	C
79	Ax	43	A
79	Ax	44	A
79	Ax	45	G
79	Ax	46	A
79	Ax	48	U
79	Ax	49	G
79	Ax	50	G
79	Ax	52	G
79	Ax	53	G
79	Ax	54	U
79	Ax	55	U
79	Ax	58	A
79	Ax	61	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
79	Ax	62	C
79	Ax	63	U
79	Ax	64	C
79	Ax	65	C
79	Ax	69	C
79	Ax	75	C
79	Ax	76	A
80	B	4	A
80	B	8	U
80	B	10	2MG
80	B	16	C
80	B	21	A
80	B	24	G
80	B	45	G
80	B	48	U
80	B	49	U
80	B	54	C
80	B	55	U
80	B	56	U
80	B	58	A
80	B	59	A
80	B	64	A
80	B	76	A

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
11	A	2030	U
11	A	2245	A
11	A	2331	C
46	AA	1539	C

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

14 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
11	OMU	A	3039	11,88	19,22,23	3.03	8 (42%)	26,31,34	1.70	5 (19%)
11	OMG	A	2815	11,79,88	23,26,27	3.05	10 (43%)	33,38,41	2.69	11 (33%)
46	MA6	AA	1583	46	23,26,27	1.54	4 (17%)	34,38,41	3.96	13 (38%)
11	PSU	A	3067	11	18,21,22	1.98	8 (44%)	22,30,33	1.81	4 (18%)
46	MA6	AA	1584	46	23,26,27	1.52	4 (17%)	34,38,41	3.91	13 (38%)
80	1MA	B	9	80	21,25,26	3.18	6 (28%)	31,37,40	2.28	8 (25%)
80	2MG	B	10	80	23,26,27	2.86	9 (39%)	32,38,41	2.21	11 (34%)
46	B8T	AA	1486	46,91	19,22,23	3.30	8 (42%)	26,31,34	0.84	1 (3%)
11	1MA	A	2617	11	21,25,26	3.19	6 (28%)	31,37,40	2.37	8 (25%)
46	5MU	AA	1076	46	19,22,23	7.09	8 (42%)	28,32,35	3.41	10 (35%)
11	OMG	A	3040	11,78	23,26,27	3.06	10 (43%)	33,38,41	2.69	11 (33%)
54	5F0	AI	184	54	8,8,9	1.47	2 (25%)	7,9,11	1.82	2 (28%)
46	5MC	AA	1488	46	18,22,23	3.85	7 (38%)	26,32,35	0.96	1 (3%)
80	PSU	B	39	80	18,21,22	1.92	7 (38%)	22,30,33	1.79	3 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	OMU	A	3039	11,88	-	0/9/27/28	0/2/2/2
11	OMG	A	2815	11,79,88	-	1/9/27/28	0/3/3/3
46	MA6	AA	1583	46	-	0/11/29/30	0/3/3/3
11	PSU	A	3067	11	-	0/7/25/26	0/2/2/2
46	MA6	AA	1584	46	-	1/11/29/30	0/3/3/3
80	1MA	B	9	80	-	2/7/25/26	0/3/3/3
80	2MG	B	10	80	-	0/9/27/28	0/3/3/3
46	B8T	AA	1486	46,91	-	0/7/27/28	0/2/2/2
11	1MA	A	2617	11	-	0/7/25/26	0/3/3/3
46	5MU	AA	1076	46	-	0/7/25/26	0/2/2/2
11	OMG	A	3040	11,78	-	0/9/27/28	0/3/3/3
54	5F0	AI	184	54	-	0/9/9/10	-
46	5MC	AA	1488	46	-	0/7/25/26	0/2/2/2
80	PSU	B	39	80	-	0/7/25/26	0/2/2/2

All (97) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	AA	1076	5MU	C4-C5	20.71	1.79	1.44
46	AA	1076	5MU	C6-N1	14.41	1.62	1.38
46	AA	1076	5MU	C6-C5	-11.51	1.15	1.34
46	AA	1076	5MU	C4-N3	-11.12	1.18	1.38
46	AA	1488	5MC	C6-C5	9.64	1.50	1.34
80	B	9	1MA	C2-N3	8.25	1.45	1.30
11	A	2617	1MA	C2-N3	8.17	1.45	1.30
80	B	9	1MA	C4-N3	7.57	1.51	1.35
11	A	2617	1MA	C4-N3	7.56	1.51	1.35
11	A	3040	OMG	C2-N2	7.49	1.52	1.34
80	B	10	2MG	C2-N3	7.47	1.46	1.31
11	A	2815	OMG	C2-N2	7.46	1.51	1.34
46	AA	1488	5MC	C4-N3	7.37	1.46	1.34
11	A	3040	OMG	C4-N3	7.13	1.51	1.34
11	A	2815	OMG	C4-N3	7.12	1.51	1.34
46	AA	1486	B8T	C4-N3	7.02	1.45	1.32
11	A	3039	OMU	C2-N1	7.00	1.49	1.38
11	A	3039	OMU	C2-N3	6.85	1.50	1.38
11	A	2617	1MA	C2-N1	6.39	1.47	1.35
80	B	10	2MG	C4-N3	6.38	1.49	1.34
80	B	9	1MA	C2-N1	6.33	1.47	1.35
46	AA	1486	B8T	C2-N3	6.24	1.49	1.36
46	AA	1486	B8T	C6-C5	6.23	1.49	1.35
11	A	3040	OMG	C2-N3	6.20	1.48	1.33
46	AA	1488	5MC	C2-N3	6.17	1.48	1.36
11	A	2815	OMG	C2-N3	6.17	1.48	1.33
11	A	3039	OMU	C6-C5	5.67	1.48	1.35
80	B	10	2MG	C2-N2	5.63	1.45	1.33
46	AA	1488	5MC	C6-N1	5.09	1.46	1.38
46	AA	1486	B8T	C4-N4	4.90	1.46	1.35
80	B	10	2MG	C2-N1	4.83	1.44	1.36
46	AA	1488	5MC	C2-N1	4.79	1.50	1.40
80	B	9	1MA	C5-C6	4.78	1.56	1.43
46	AA	1486	B8T	C2-N1	4.74	1.50	1.40
11	A	2617	1MA	C5-C6	4.74	1.56	1.43
46	AA	1076	5MU	O4-C4	-4.71	1.14	1.23
46	AA	1488	5MC	C4-N4	4.39	1.45	1.34
46	AA	1076	5MU	C2-N1	4.19	1.45	1.38
11	A	3039	OMU	C4-N3	4.06	1.45	1.38
11	A	3040	OMG	C6-N1	4.05	1.46	1.38
11	A	2815	OMG	C6-N1	4.00	1.46	1.38
46	AA	1584	MA6	C6-N6	3.99	1.48	1.36
46	AA	1583	MA6	C6-N6	3.99	1.48	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	AA	1486	B8T	C5-C4	3.78	1.48	1.40
46	AA	1076	5MU	C2-N3	3.56	1.44	1.38
11	A	3067	PSU	C4-N3	-3.48	1.32	1.38
80	B	39	PSU	C4-N3	-3.43	1.32	1.38
80	B	39	PSU	C6-C5	3.41	1.39	1.35
11	A	3067	PSU	C2-N1	-3.40	1.32	1.36
11	A	3067	PSU	C6-C5	3.36	1.39	1.35
11	A	2815	OMG	C5-N7	-3.32	1.32	1.39
11	A	2617	1MA	C5-N7	-3.29	1.32	1.39
11	A	3040	OMG	C2-N1	3.26	1.45	1.37
11	A	3040	OMG	C5-N7	-3.23	1.32	1.39
80	B	9	1MA	C5-N7	-3.20	1.32	1.39
80	B	39	PSU	C2-N1	-3.20	1.32	1.36
11	A	2815	OMG	O6-C6	-3.19	1.17	1.23
11	A	2815	OMG	C2-N1	3.18	1.45	1.37
11	A	3067	PSU	C2-N3	-3.16	1.32	1.37
46	AA	1488	5MC	O2-C2	-3.16	1.17	1.23
80	B	39	PSU	C2-N3	-3.14	1.32	1.37
46	AA	1486	B8T	C6-N1	3.13	1.45	1.38
11	A	3040	OMG	O6-C6	-3.11	1.17	1.23
54	AI	184	5F0	OD1-C1	2.90	1.40	1.33
11	A	3039	OMU	O4-C4	-2.89	1.18	1.24
46	AA	1076	5MU	O2-C2	-2.87	1.17	1.23
46	AA	1583	MA6	C5-C4	-2.86	1.33	1.39
11	A	3039	OMU	C6-N1	2.83	1.44	1.38
80	B	10	2MG	C5-N7	-2.80	1.33	1.39
46	AA	1486	B8T	O2-C2	-2.80	1.18	1.23
11	A	3040	OMG	C5-C6	2.79	1.54	1.44
46	AA	1584	MA6	C8-N9	-2.78	1.32	1.37
46	AA	1584	MA6	C5-C4	-2.76	1.33	1.39
46	AA	1583	MA6	C8-N9	-2.74	1.32	1.37
11	A	2815	OMG	C5-C6	2.72	1.54	1.44
80	B	10	2MG	O6-C6	-2.68	1.18	1.23
80	B	10	2MG	C6-N1	2.58	1.43	1.38
46	AA	1584	MA6	C5-N7	-2.52	1.34	1.39
11	A	3067	PSU	C6-N1	-2.49	1.32	1.36
46	AA	1583	MA6	C5-N7	-2.48	1.34	1.39
80	B	10	2MG	C5-C6	2.46	1.53	1.44
11	A	3067	PSU	O4-C4	-2.46	1.18	1.23
11	A	2815	OMG	C4-N9	-2.45	1.31	1.38
11	A	3040	OMG	C4-N9	-2.42	1.31	1.38
80	B	39	PSU	O4-C4	-2.41	1.19	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	2617	1MA	C6-N6	-2.36	1.22	1.28
11	A	3039	OMU	C5-C4	2.36	1.48	1.43
80	B	9	1MA	C6-N6	-2.35	1.22	1.28
11	A	3039	OMU	O2-C2	-2.34	1.18	1.23
80	B	39	PSU	C6-N1	-2.28	1.32	1.36
11	A	3067	PSU	O2-C2	-2.19	1.18	1.23
80	B	39	PSU	O2-C2	-2.15	1.18	1.23
54	AI	184	5F0	OD1-CXT	-2.13	1.40	1.45
11	A	3067	PSU	O4'-C1'	-2.10	1.40	1.43
80	B	10	2MG	C4-N9	-2.08	1.32	1.38
11	A	3040	OMG	O2'-CM2	2.07	1.49	1.42
11	A	2815	OMG	O2'-CM2	2.02	1.49	1.42

All (101) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	AA	1583	MA6	N1-C6-N6	-15.38	100.27	117.08
46	AA	1584	MA6	N1-C6-N6	-15.34	100.31	117.08
46	AA	1076	5MU	C5-C4-N3	10.29	124.09	115.31
11	A	2815	OMG	C1'-N9-C8	-8.79	101.68	126.70
11	A	3040	OMG	C1'-N9-C8	-8.73	101.85	126.70
46	AA	1076	5MU	C5-C6-N1	-8.22	114.88	123.34
46	AA	1583	MA6	C5-C6-N6	8.20	139.58	125.30
46	AA	1584	MA6	C5-C6-N6	8.15	139.50	125.30
11	A	2815	OMG	C1'-N9-C4	7.13	147.67	126.50
11	A	3040	OMG	C1'-N9-C4	7.12	147.66	126.50
46	AA	1076	5MU	C4-N3-C2	-7.09	118.17	127.35
11	A	2617	1MA	C1'-N9-C8	-6.85	107.20	126.70
46	AA	1583	MA6	C4-N9-C1'	-6.52	111.07	126.59
80	B	10	2MG	C2-N3-C4	6.30	119.84	112.04
80	B	9	1MA	C1'-N9-C8	-6.22	109.00	126.70
11	A	2617	1MA	C1'-N9-C4	5.85	143.87	126.50
46	AA	1584	MA6	C4-N9-C1'	-5.70	113.01	126.59
46	AA	1583	MA6	N9-C8-N7	-5.50	106.40	113.91
11	A	3067	PSU	N1-C2-N3	5.41	121.26	115.13
80	B	9	1MA	C1'-N9-C4	5.40	142.53	126.50
80	B	39	PSU	N1-C2-N3	5.33	121.17	115.13
46	AA	1583	MA6	N1-C2-N3	-5.33	120.27	128.60
46	AA	1584	MA6	N1-C2-N3	-5.31	120.30	128.60
11	A	3039	OMU	C4-N3-C2	-5.30	119.59	126.58
46	AA	1584	MA6	N9-C8-N7	-5.20	106.80	113.91
11	A	2617	1MA	N1-C2-N3	-5.18	119.84	126.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	AA	1583	MA6	C1'-N9-C8	5.10	138.65	127.14
46	AA	1584	MA6	C5-C4-N3	-5.07	120.13	126.75
80	B	9	1MA	N1-C2-N3	-5.06	119.98	126.00
46	AA	1076	5MU	C5M-C5-C6	-4.91	116.29	122.85
80	B	9	1MA	C5-C4-N3	-4.77	120.15	127.26
80	B	10	2MG	C5-C4-N3	-4.73	120.78	128.46
11	A	2617	1MA	C5-C4-N3	-4.66	120.31	127.26
46	AA	1583	MA6	C5-C4-N3	-4.64	120.70	126.75
46	AA	1076	5MU	N3-C2-N1	4.53	120.90	114.89
11	A	3040	OMG	C5-C4-N3	-4.50	121.17	128.46
11	A	2815	OMG	C5-C4-N3	-4.46	121.23	128.46
46	AA	1584	MA6	C1'-N9-C8	4.41	137.10	127.14
46	AA	1583	MA6	C4-N9-C8	4.18	110.26	105.73
80	B	10	2MG	C2-N1-C6	-4.13	119.72	124.48
11	A	2815	OMG	C2-N3-C4	4.09	119.59	112.30
11	A	3040	OMG	C2-N3-C4	4.08	119.57	112.30
11	A	2815	OMG	N9-C8-N7	-3.98	105.90	113.39
46	AA	1076	5MU	C5M-C5-C4	3.95	123.11	118.77
11	A	3040	OMG	N9-C8-N7	-3.90	106.04	113.39
11	A	2617	1MA	C2-N3-C4	3.90	120.08	112.41
80	B	9	1MA	C2-N3-C4	3.89	120.06	112.41
11	A	3039	OMU	N3-C2-N1	3.86	120.01	114.89
46	AA	1584	MA6	C4-N9-C8	3.84	109.89	105.73
46	AA	1076	5MU	O4-C4-C5	-3.80	120.50	124.90
46	AA	1584	MA6	N3-C4-N9	3.79	133.32	127.08
80	B	39	PSU	C4-N3-C2	-3.73	120.96	126.34
80	B	10	2MG	N9-C8-N7	-3.62	106.58	113.39
46	AA	1584	MA6	C2-N3-C4	3.51	120.05	111.75
11	A	3067	PSU	C4-N3-C2	-3.48	121.32	126.34
46	AA	1584	MA6	C4-C5-C6	3.48	119.77	115.88
46	AA	1583	MA6	N3-C4-N9	3.42	132.72	127.08
46	AA	1583	MA6	C5-N7-C8	3.40	108.33	103.51
46	AA	1583	MA6	C2-N3-C4	3.38	119.73	111.75
46	AA	1583	MA6	C2-N1-C6	3.37	119.71	111.75
46	AA	1584	MA6	C5-N7-C8	3.36	108.29	103.51
46	AA	1584	MA6	C2-N1-C6	3.30	119.56	111.75
11	A	3039	OMU	C5-C4-N3	3.30	119.77	114.84
54	AI	184	5F0	OD1-C1-CA	3.29	119.94	111.52
80	B	10	2MG	C1'-N9-C8	-3.23	117.49	126.70
11	A	3067	PSU	O2-C2-N1	-3.22	119.25	122.79
11	A	2617	1MA	N9-C8-N7	-3.20	107.36	113.39
46	AA	1583	MA6	C4-C5-C6	3.18	119.44	115.88

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	2815	OMG	N9-C4-N3	3.13	132.22	125.94
11	A	3040	OMG	N9-C4-N3	3.09	132.14	125.94
80	B	10	2MG	N9-C4-N3	3.08	132.13	125.94
80	B	9	1MA	N9-C8-N7	-3.07	107.60	113.39
46	AA	1076	5MU	C6-C5-C4	3.07	120.60	118.03
80	B	39	PSU	O2-C2-N1	-3.04	119.45	122.79
46	AA	1488	5MC	C5-C6-N1	-2.97	120.28	123.34
11	A	3040	OMG	C2-N1-C6	-2.97	119.68	125.10
11	A	2815	OMG	C2-N1-C6	-2.94	119.73	125.10
11	A	3039	OMU	O4-C4-C5	-2.81	120.23	125.16
80	B	10	2MG	C5-C6-N1	2.67	119.97	113.19
11	A	2815	OMG	C5-C6-N1	2.67	119.96	113.19
11	A	3040	OMG	C5-C6-N1	2.64	119.91	113.19
80	B	10	2MG	N1-C2-N3	-2.56	119.99	123.95
11	A	2815	OMG	O6-C6-C5	-2.55	119.83	126.60
80	B	10	2MG	O6-C6-C5	-2.53	119.88	126.60
11	A	3040	OMG	O6-C6-C5	-2.52	119.92	126.60
11	A	3040	OMG	C8-N7-C5	2.49	108.74	104.24
46	AA	1486	B8T	C6-C5-C4	2.46	119.97	116.96
11	A	2815	OMG	C8-N7-C5	2.46	108.70	104.24
46	AA	1076	5MU	O4-C4-N3	-2.45	115.41	120.12
11	A	2815	OMG	C8-N9-C4	2.42	110.65	106.05
11	A	2617	1MA	N9-C4-N3	2.35	132.42	126.94
80	B	10	2MG	C8-N7-C5	2.34	108.48	104.24
11	A	3040	OMG	C8-N9-C4	2.33	110.49	106.05
54	AI	184	5F0	O-C-CB	-2.33	118.63	125.43
46	AA	1076	5MU	O2-C2-N1	-2.27	119.77	122.79
80	B	9	1MA	N9-C4-N3	2.26	132.20	126.94
11	A	3067	PSU	O4'-C1'-C2'	2.24	108.31	105.14
80	B	9	1MA	C8-N7-C5	2.15	108.14	104.24
11	A	2617	1MA	C8-N7-C5	2.14	108.11	104.24
80	B	10	2MG	C1'-N9-C4	2.08	132.67	126.50
11	A	3039	OMU	O2-C2-N1	-2.00	120.12	122.79

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	2815	OMG	C1'-C2'-O2'-CM2
80	B	9	1MA	C3'-C4'-C5'-O5'
46	AA	1584	MA6	C4'-C5'-O5'-P
80	B	9	1MA	O4'-C4'-C5'-O5'

There are no ring outliers.

7 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	2815	OMG	1	0
46	AA	1583	MA6	1	0
46	AA	1486	B8T	1	0
46	AA	1076	5MU	1	0
11	A	3040	OMG	2	0
46	AA	1488	5MC	2	0
80	B	39	PSU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 286 ligands modelled in this entry, 264 are monoatomic - leaving 22 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
96	SPM	AA	1702	-	13,13,13	0.35	0	12,12,12	0.98	0
97	ATP	AX	501	91	29,33,33	2.99	12 (41%)	44,52,52	2.39	14 (31%)
92	NMY	AA	1784	-	45,45,45	0.74	0	63,67,67	1.08	5 (7%)
92	NMY	A	3473	-	45,45,45	0.83	1 (2%)	63,67,67	0.93	2 (3%)
95	NAD	AA	1701	91	45,48,48	0.73	1 (2%)	63,73,73	0.76	2 (3%)
92	NMY	A	3471	-	45,45,45	0.52	0	63,67,67	1.22	7 (11%)
98	GDP	AX	503	-	28,30,30	1.13	3 (10%)	44,47,47	1.83	8 (18%)
89	SPD	A	3301	-	9,9,9	0.27	0	8,8,8	0.28	0
90	PUT	A	3304	-	5,5,5	0.16	0	4,4,4	0.21	0
92	NMY	AA	1786	-	45,45,45	0.66	0	63,67,67	1.03	3 (4%)
93	VAL	e	301	-	4,6,7	0.52	0	6,7,9	0.94	0
92	NMY	AA	1785	-	45,45,45	0.69	0	63,67,67	0.95	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
92	NMY	A	3474	-	45,45,45	0.55	0	63,67,67	1.01	3 (4%)
94	FES	AT	201	58,65	0,4,4	-	-	-		
94	FES	r	201	16,45	0,4,4	-	-	-		
89	SPD	A	3303	91	9,9,9	0.27	0	8,8,8	0.26	0
92	NMY	A	3470	-	45,45,45	0.73	1 (2%)	63,67,67	1.09	4 (6%)
92	NMY	A	3472	11	45,45,45	0.58	0	63,67,67	1.11	5 (7%)
92	NMY	AA	1783	-	45,45,45	0.61	0	63,67,67	0.97	4 (6%)
89	SPD	AA	1703	-	9,9,9	0.26	0	8,8,8	0.31	0
89	SPD	A	3302	-	9,9,9	0.27	0	8,8,8	0.25	0
94	FES	AP	201	50,61	0,4,4	-	-	-		

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
96	SPM	AA	1702	-	-	0/11/11/11	-
97	ATP	AX	501	91	-	7/22/38/38	0/3/3/3
92	NMY	AA	1784	-	-	5/18/94/94	0/4/4/4
92	NMY	A	3473	-	-	8/18/94/94	0/4/4/4
95	NAD	AA	1701	91	-	7/30/62/62	0/5/5/5
92	NMY	A	3471	-	-	10/18/94/94	0/4/4/4
98	GDP	AX	503	-	-	3/16/32/32	0/3/3/3
89	SPD	A	3301	-	-	1/7/7/7	-
90	PUT	A	3304	-	-	0/3/3/3	-
92	NMY	AA	1786	-	-	8/18/94/94	0/4/4/4
93	VAL	e	301	-	-	1/5/6/8	-
92	NMY	AA	1785	-	-	5/18/94/94	1/4/4/4
92	NMY	A	3474	-	-	10/18/94/94	1/4/4/4
94	FES	AT	201	58,65	-	-	0/1/1/1
94	FES	r	201	16,45	-	-	0/1/1/1
89	SPD	A	3303	91	-	0/7/7/7	-
92	NMY	A	3470	-	-	6/18/94/94	0/4/4/4
92	NMY	A	3472	11	-	11/18/94/94	0/4/4/4
92	NMY	AA	1783	-	-	7/18/94/94	1/4/4/4
89	SPD	AA	1703	-	-	2/7/7/7	-
89	SPD	A	3302	-	-	0/7/7/7	-
94	FES	AP	201	50,61	-	-	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
97	AX	501	ATP	C2'-C3'	-10.74	1.23	1.53
97	AX	501	ATP	O4'-C1'	-4.66	1.31	1.42
97	AX	501	ATP	C6-N6	4.54	1.45	1.34
97	AX	501	ATP	C2'-C1'	4.17	1.66	1.53
97	AX	501	ATP	C5'-C4'	-3.95	1.39	1.51
97	AX	501	ATP	O3'-C3'	3.28	1.50	1.43
97	AX	501	ATP	C3'-C4'	3.11	1.60	1.53
98	AX	503	GDP	C5-C4	3.10	1.47	1.38
97	AX	501	ATP	O4'-C4'	2.76	1.51	1.45
97	AX	501	ATP	C5-C4	-2.75	1.33	1.39
97	AX	501	ATP	C5-N7	-2.45	1.34	1.39
98	AX	503	GDP	C6-N1	-2.44	1.34	1.38
92	A	3473	NMY	C13-C14	-2.38	1.49	1.52
92	A	3470	NMY	C13-C14	-2.37	1.49	1.52
95	AA	1701	NAD	O4D-C1D	-2.34	1.37	1.41
97	AX	501	ATP	O2'-C2'	2.28	1.48	1.43
98	AX	503	GDP	C5-N7	-2.12	1.35	1.39
97	AX	501	ATP	C8-N9	-2.10	1.33	1.37

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
98	AX	503	GDP	C5-C4-N3	-6.04	118.67	128.46
97	AX	501	ATP	N3-C2-N1	-5.50	120.00	128.60
97	AX	501	ATP	N6-C6-N1	-5.47	106.37	118.35
97	AX	501	ATP	C5-C4-N3	-5.25	119.90	126.75
98	AX	503	GDP	C2-N3-C4	4.79	120.83	112.30
97	AX	501	ATP	N9-C8-N7	-4.77	107.39	113.91
98	AX	503	GDP	N9-C4-N3	4.52	135.03	125.94
97	AX	501	ATP	C4-N9-C1'	-4.47	115.94	126.59
97	AX	501	ATP	C5-C6-N6	4.37	132.94	123.43
92	A	3470	NMY	C18-O18-C15	-4.26	107.42	117.96
97	AX	501	ATP	C2-N3-C4	3.61	120.28	111.75
92	A	3471	NMY	C1-O1-C10	-3.58	109.10	117.96
97	AX	501	ATP	N3-C4-N9	3.53	132.90	127.08
97	AX	501	ATP	C1'-N9-C8	3.52	135.08	127.14
98	AX	503	GDP	PA-O3A-PB	-3.35	121.34	132.83
92	A	3473	NMY	C13-O11-C11	-3.34	109.70	117.96
97	AX	501	ATP	C5-N7-C8	3.24	108.12	103.51
98	AX	503	GDP	C6-C5-N7	3.09	135.99	130.25
92	A	3472	NMY	C13-O11-C11	-3.04	110.43	117.96
92	AA	1783	NMY	C13-O11-C11	-3.01	110.51	117.96

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
97	AX	501	ATP	C4-N9-C8	2.99	108.97	105.73
92	A	3471	NMY	C13-C14-C15	2.96	105.66	102.10
92	A	3470	NMY	C11-C10-C9	2.81	116.41	111.16
92	A	3471	NMY	C13-O11-C11	-2.78	111.09	117.96
92	AA	1784	NMY	C13-O11-C11	-2.75	111.15	117.96
92	AA	1786	NMY	C13-O11-C11	-2.73	111.21	117.96
97	AX	501	ATP	PB-O3B-PG	-2.72	123.50	132.83
92	AA	1785	NMY	C18-O22-C22	2.72	119.02	113.69
92	A	3471	NMY	O16-C13-C14	2.70	108.46	104.98
92	A	3472	NMY	C1-O1-C10	-2.66	111.39	117.96
92	AA	1786	NMY	C1-O5-C5	-2.57	108.64	113.69
98	AX	503	GDP	C4-C5-N7	-2.55	106.68	110.72
97	AX	501	ATP	C3'-C2'-C1'	2.52	106.22	101.43
92	A	3474	NMY	C13-C14-C15	2.52	105.14	102.10
92	A	3472	NMY	C1-O5-C5	2.52	118.63	113.69
92	AA	1783	NMY	C13-C14-C15	2.49	105.10	102.10
97	AX	501	ATP	PA-O3A-PB	-2.47	124.35	132.83
92	A	3473	NMY	C18-O18-C15	-2.41	112.00	117.96
92	AA	1784	NMY	C11-C12-C7	2.40	115.49	109.63
92	A	3472	NMY	C13-C14-C15	2.38	104.96	102.10
92	A	3471	NMY	C11-C10-C9	-2.36	106.76	111.16
98	AX	503	GDP	C3'-C2'-C1'	2.35	105.89	101.43
92	AA	1786	NMY	O22-C22-C23	2.33	110.34	106.01
92	A	3471	NMY	C8-C7-C12	2.21	113.38	110.04
92	AA	1785	NMY	O11-C13-O16	-2.21	109.04	111.43
92	A	3474	NMY	C18-O18-C15	-2.20	112.52	117.96
92	AA	1784	NMY	C1-O1-C10	-2.20	112.53	117.96
95	AA	1701	NAD	PN-O3-PA	-2.17	125.39	132.83
98	AX	503	GDP	O6-C6-C5	-2.11	121.01	126.60
92	AA	1784	NMY	C12-C11-C10	2.10	116.45	111.66
92	AA	1783	NMY	O22-C22-C23	2.08	109.89	106.01
95	AA	1701	NAD	O2A-PA-O1A	2.07	122.49	112.24
92	AA	1783	NMY	C18-O22-C22	-2.06	109.64	113.69
92	AA	1785	NMY	C13-O11-C11	-2.06	112.87	117.96
92	A	3470	NMY	C1-O1-C10	-2.05	112.90	117.96
92	A	3471	NMY	O1-C1-C2	2.04	111.72	108.22
92	A	3474	NMY	O22-C22-C23	2.03	109.79	106.01
92	AA	1785	NMY	C18-O18-C15	-2.03	112.95	117.96
92	A	3472	NMY	O5-C5-C6	2.02	109.76	106.01
92	A	3470	NMY	O11-C13-O16	-2.01	109.25	111.43
92	AA	1784	NMY	C9-C8-C7	-2.00	107.07	111.18

There are no chirality outliers.

All (91) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
92	A	3470	NMY	C14-C13-O11-C11
92	A	3470	NMY	O16-C13-O11-C11
92	A	3471	NMY	C2-C1-O1-C10
92	A	3471	NMY	C14-C13-O11-C11
92	A	3471	NMY	O22-C22-C23-N19
92	A	3472	NMY	C9-C10-O1-C1
92	A	3473	NMY	O5-C5-C6-N6
92	A	3473	NMY	C14-C13-O11-C11
92	A	3473	NMY	O16-C13-O11-C11
92	A	3473	NMY	C21-C22-C23-N19
92	A	3473	NMY	O22-C22-C23-N19
92	A	3474	NMY	C14-C13-O11-C11
92	A	3474	NMY	O16-C13-O11-C11
92	A	3474	NMY	C16-C15-O18-C18
92	AA	1783	NMY	C4-C5-C6-N6
92	AA	1783	NMY	O5-C5-C6-N6
92	AA	1783	NMY	C19-C18-O18-C15
92	AA	1783	NMY	C21-C22-C23-N19
92	AA	1783	NMY	O22-C22-C23-N19
92	AA	1784	NMY	C21-C22-C23-N19
92	AA	1784	NMY	O22-C22-C23-N19
92	AA	1785	NMY	C4-C5-C6-N6
92	AA	1785	NMY	O5-C5-C6-N6
92	AA	1785	NMY	C14-C13-O11-C11
92	AA	1785	NMY	C14-C15-O18-C18
92	AA	1786	NMY	C2-C1-O1-C10
92	AA	1786	NMY	O22-C18-O18-C15
95	AA	1701	NAD	C5D-O5D-PN-O1N
97	AX	501	ATP	PB-O3B-PG-O2G
97	AX	501	ATP	C5'-O5'-PA-O1A
98	AX	503	GDP	C5'-O5'-PA-O1A
98	AX	503	GDP	C5'-O5'-PA-O2A
92	A	3471	NMY	O22-C18-O18-C15
92	A	3473	NMY	O22-C18-O18-C15
92	AA	1783	NMY	O22-C18-O18-C15
92	A	3471	NMY	C12-C11-O11-C13
92	A	3472	NMY	O22-C18-O18-C15
92	A	3474	NMY	O5-C1-O1-C10
92	AA	1784	NMY	O22-C18-O18-C15
92	AA	1783	NMY	O5-C1-O1-C10
92	AA	1786	NMY	C15-C16-C17-O17
92	A	3471	NMY	O16-C16-C17-O17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
92	A	3471	NMY	C15-C16-C17-O17
92	A	3471	NMY	O5-C1-O1-C10
92	AA	1786	NMY	O16-C16-C17-O17
92	A	3470	NMY	C15-C16-C17-O17
92	A	3471	NMY	O16-C13-O11-C11
92	AA	1785	NMY	O16-C13-O11-C11
97	AX	501	ATP	O4'-C4'-C5'-O5'
92	AA	1784	NMY	C11-C10-O1-C1
92	A	3472	NMY	C15-C16-C17-O17
89	AA	1703	SPD	C3-C4-C5-N6
97	AX	501	ATP	C3'-C4'-C5'-O5'
92	A	3472	NMY	C4-C5-C6-N6
92	A	3473	NMY	C4-C5-C6-N6
92	AA	1786	NMY	C19-C18-O18-C15
92	A	3470	NMY	O16-C16-C17-O17
92	A	3472	NMY	O16-C13-O11-C11
92	AA	1786	NMY	O16-C13-O11-C11
95	AA	1701	NAD	C5D-O5D-PN-O3
92	A	3472	NMY	C14-C13-O11-C11
92	AA	1786	NMY	C14-C13-O11-C11
95	AA	1701	NAD	PA-O3-PN-O1N
95	AA	1701	NAD	C5D-O5D-PN-O2N
92	A	3470	NMY	O5-C5-C6-N6
92	A	3472	NMY	O5-C5-C6-N6
92	A	3474	NMY	O5-C5-C6-N6
92	A	3474	NMY	O22-C22-C23-N19
92	AA	1786	NMY	O5-C5-C6-N6
95	AA	1701	NAD	O4B-C4B-C5B-O5B
97	AX	501	ATP	PA-O3A-PB-O1B
92	A	3474	NMY	C21-C22-C23-N19
89	AA	1703	SPD	N1-C2-C3-C4
95	AA	1701	NAD	C3B-C4B-C5B-O5B
92	A	3472	NMY	C11-C10-O1-C1
93	e	301	VAL	O-C-CA-CB
97	AX	501	ATP	PB-O3B-PG-O1G
97	AX	501	ATP	C5'-O5'-PA-O3A
98	AX	503	GDP	C5'-O5'-PA-O3A
89	A	3301	SPD	N6-C7-C8-C9
95	AA	1701	NAD	PA-O3-PN-O2N
92	A	3470	NMY	C16-C15-O18-C18
92	A	3472	NMY	C16-C15-O18-C18
92	A	3473	NMY	C14-C15-O18-C18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
92	A	3474	NMY	C4-C5-C6-N6
92	A	3474	NMY	C14-C15-O18-C18
92	A	3471	NMY	C19-C18-O18-C15
92	A	3472	NMY	C2-C1-O1-C10
92	A	3474	NMY	C19-C18-O18-C15
92	A	3472	NMY	O16-C16-C17-O17
92	AA	1784	NMY	C12-C11-O11-C13

All (3) ring outliers are listed below:

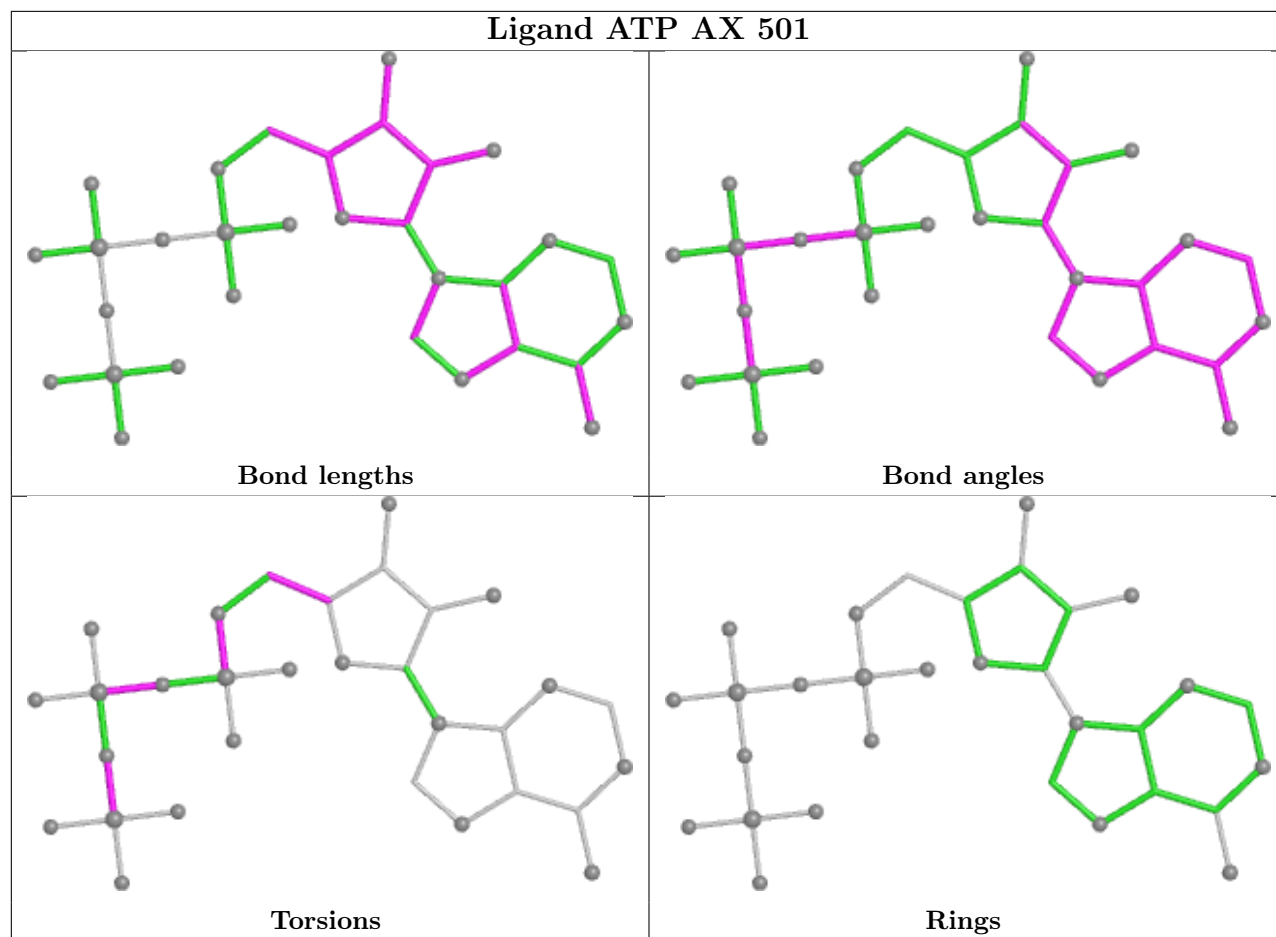
Mol	Chain	Res	Type	Atoms
92	AA	1785	NMY	C18-C19-C20-C21-C22-O22
92	A	3474	NMY	C10-C11-C12-C7-C8-C9
92	AA	1783	NMY	C10-C11-C12-C7-C8-C9

11 monomers are involved in 46 short contacts:

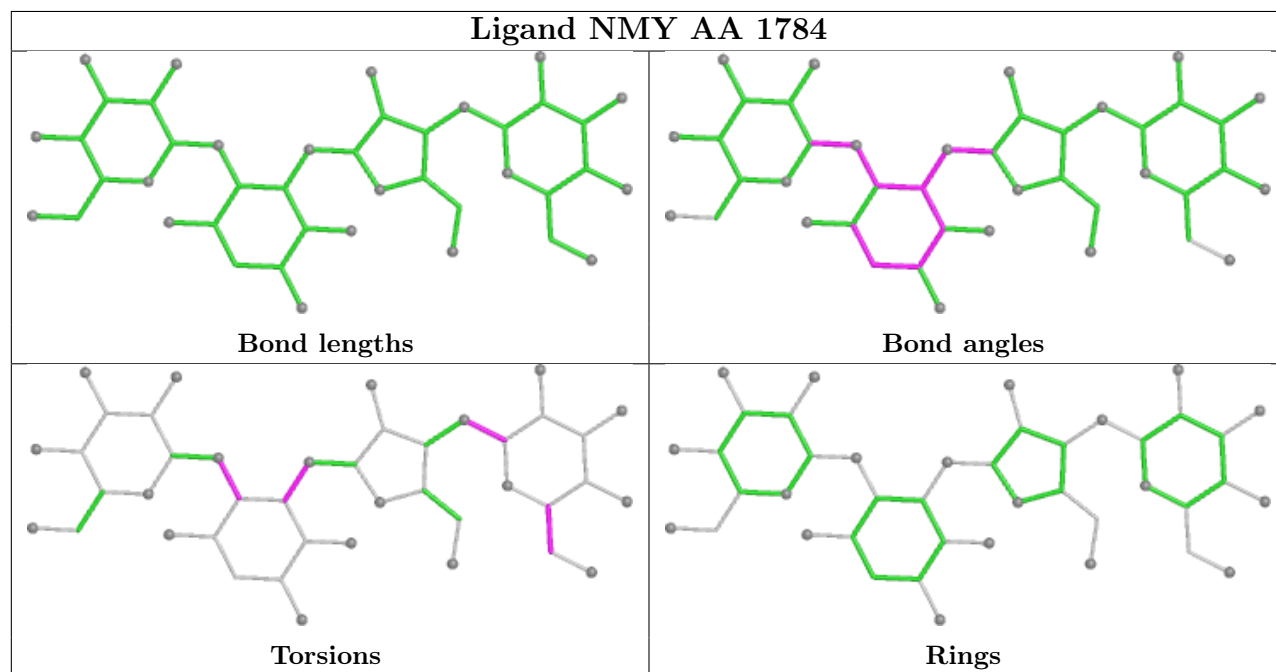
Mol	Chain	Res	Type	Clashes	Symm-Clashes
92	AA	1784	NMY	5	0
92	A	3473	NMY	3	0
92	A	3471	NMY	1	0
98	AX	503	GDP	1	0
92	AA	1786	NMY	3	0
93	e	301	VAL	1	0
92	AA	1785	NMY	5	0
92	A	3474	NMY	6	0
94	r	201	FES	1	0
92	A	3472	NMY	10	0
92	AA	1783	NMY	10	0

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

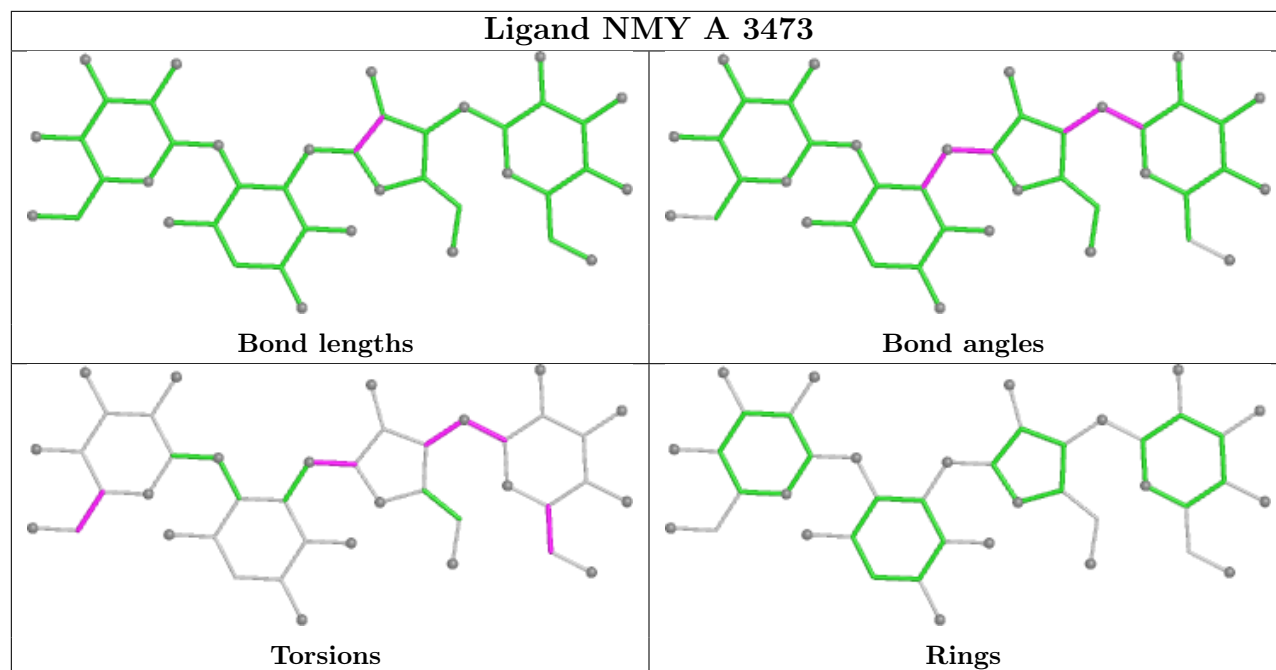
Ligand ATP AX 501



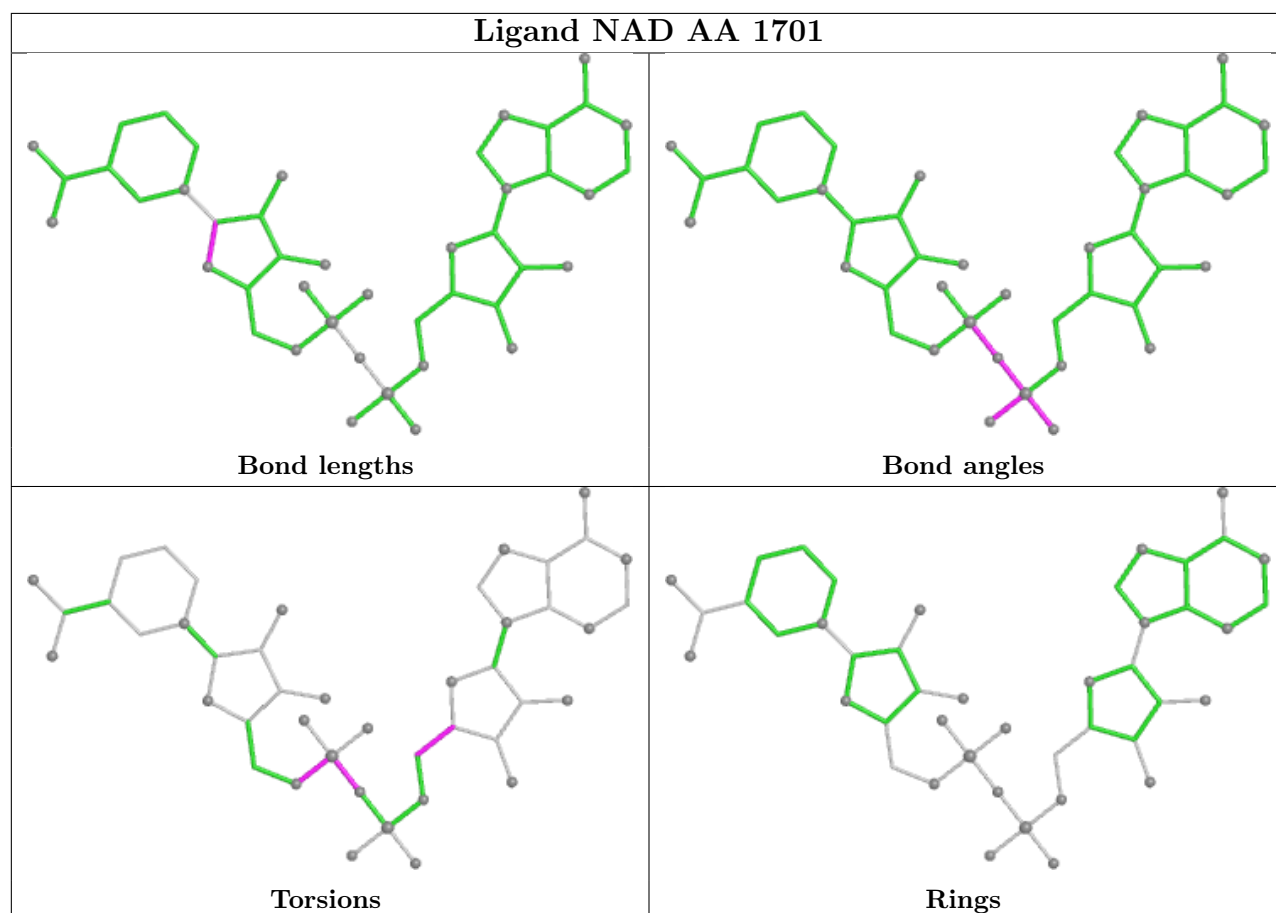
Ligand NMY AA 1784



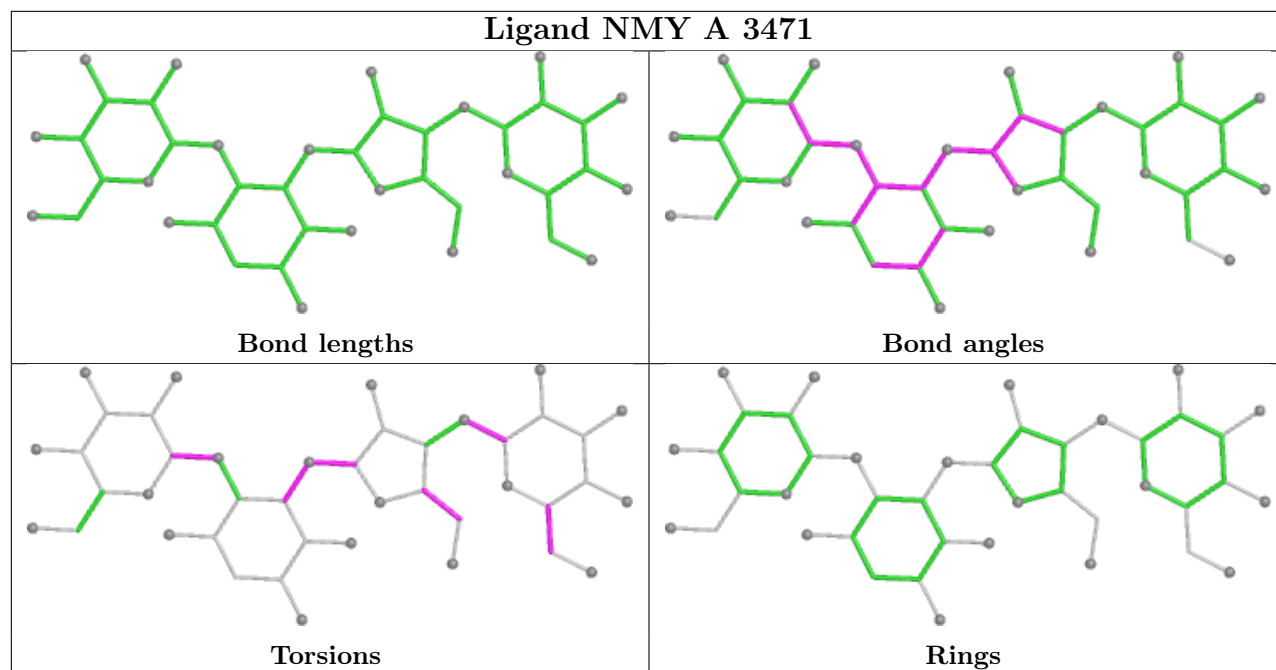
Ligand NMY A 3473



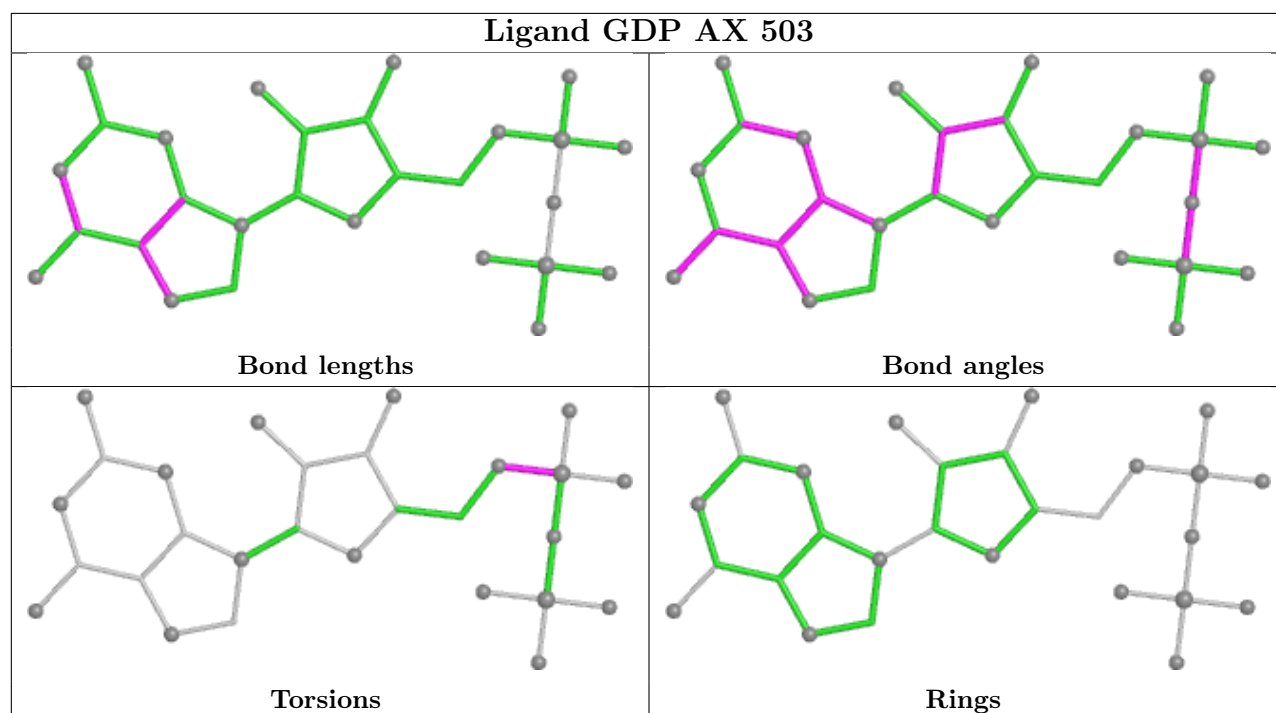
Ligand NAD AA 1701

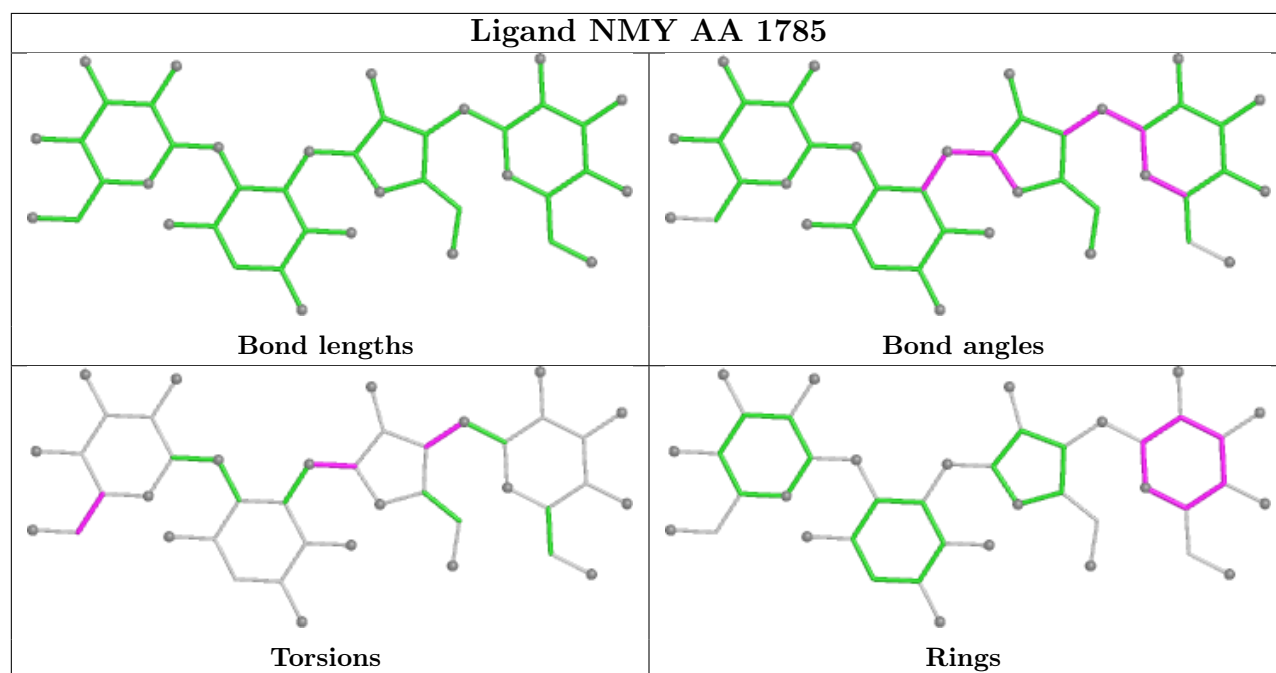
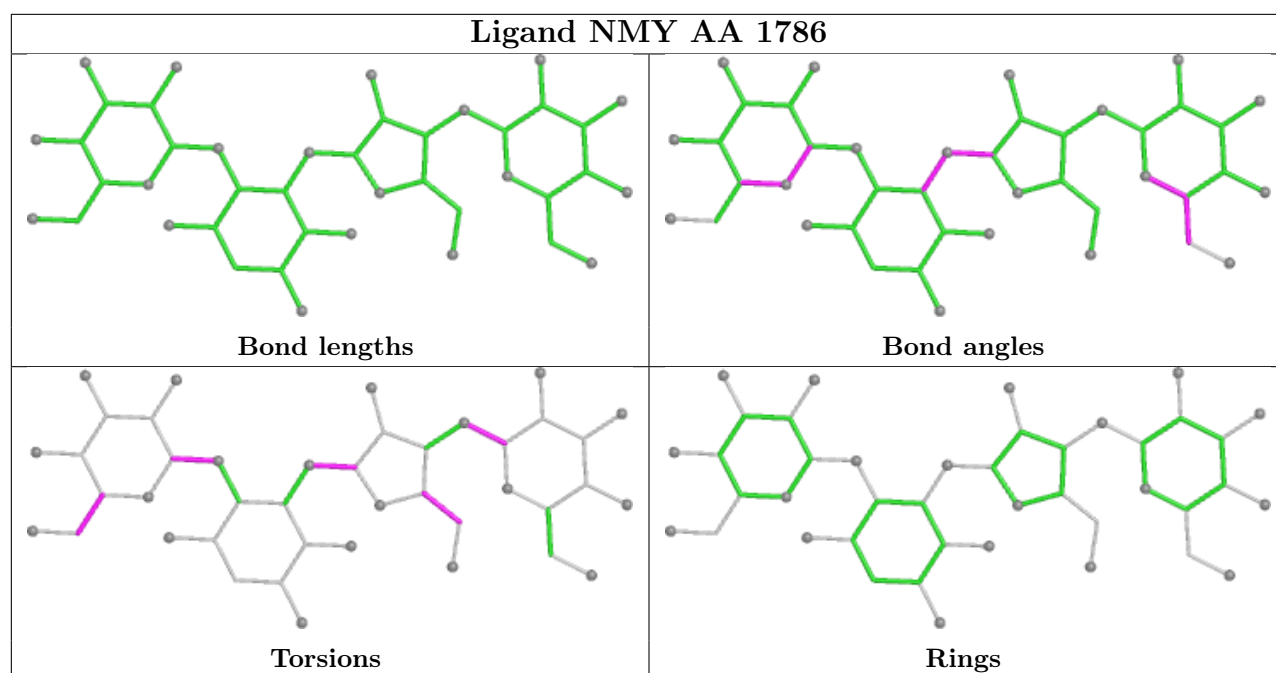


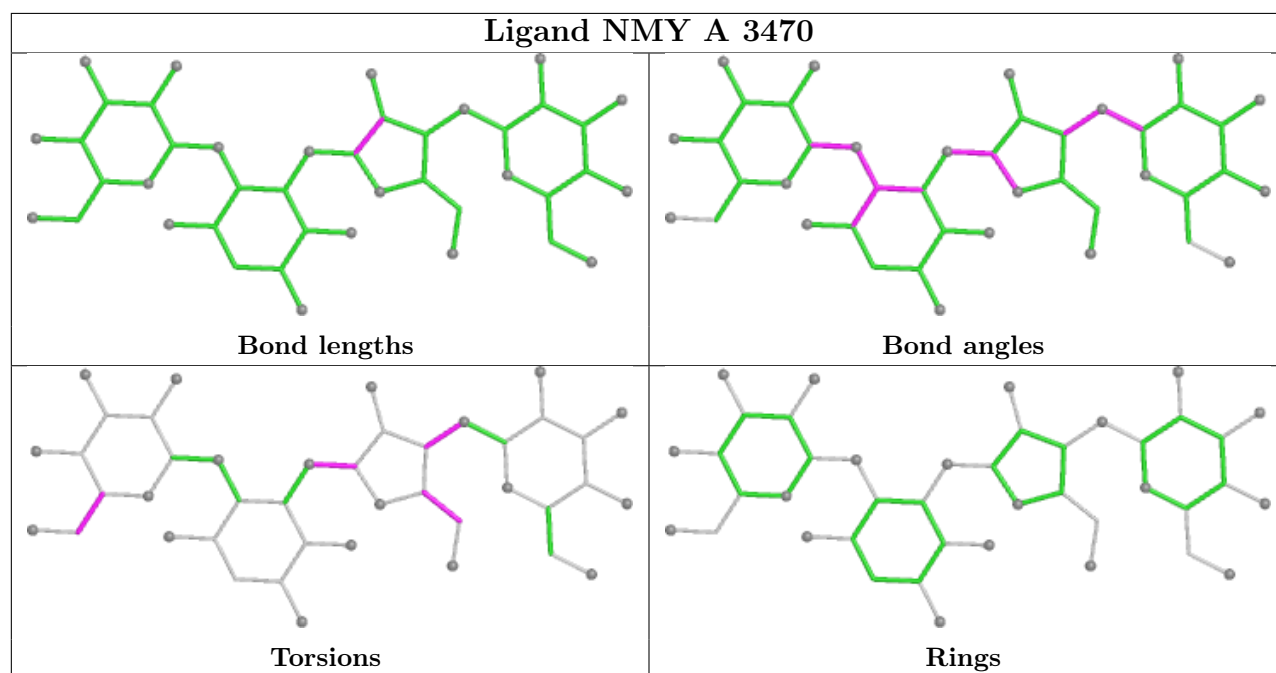
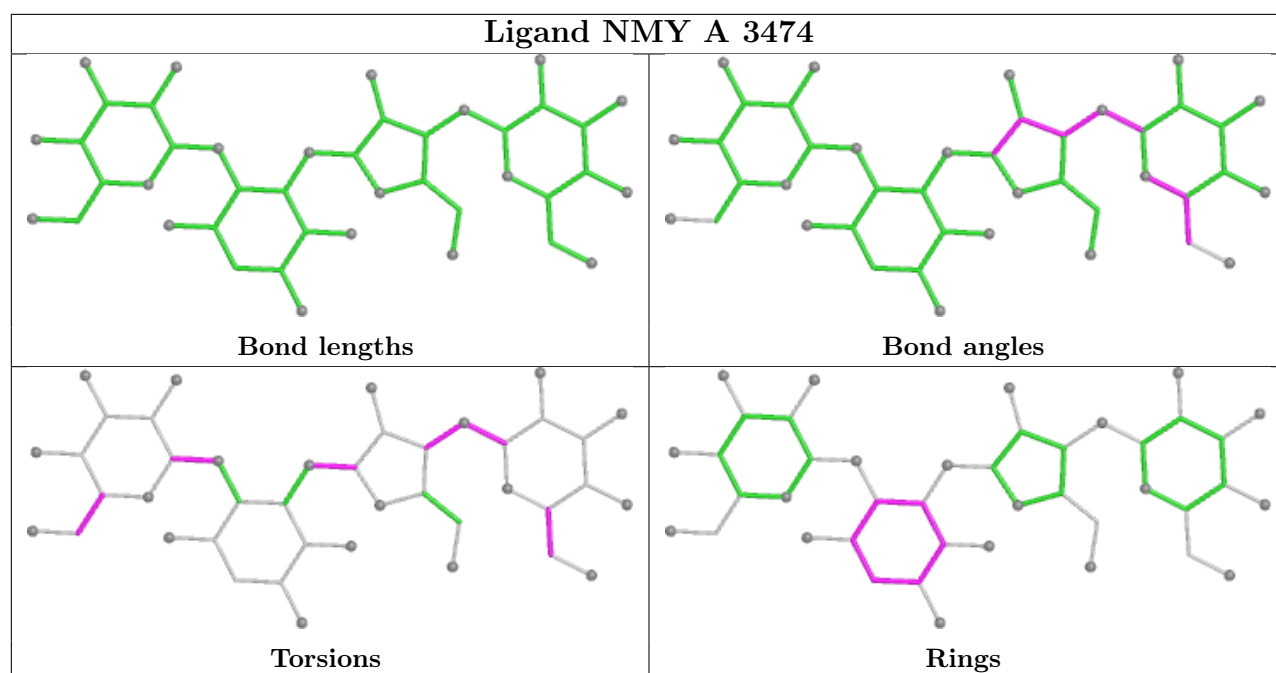
Ligand NMY A 3471

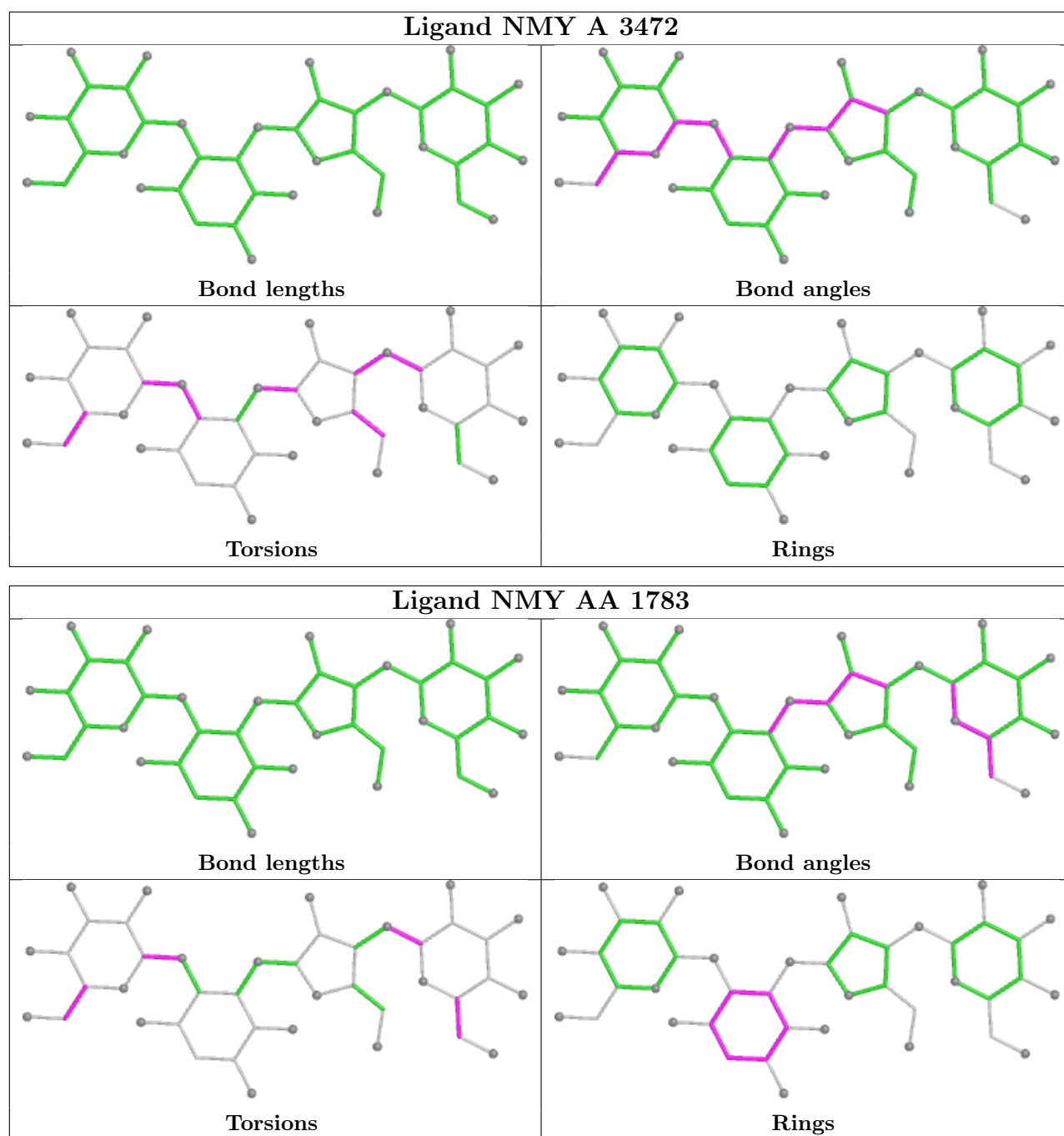


Ligand GDP AX 503









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
79	Ax	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Ax	15:A	O3'	21:A	P	9.38

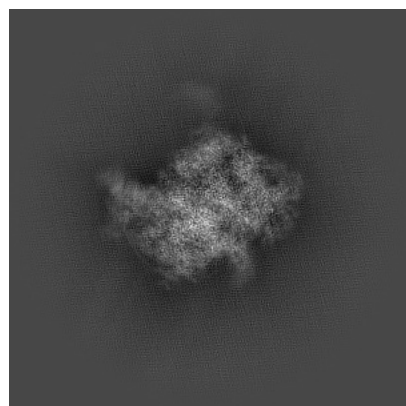
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-65433. These allow visual inspection of the internal detail of the map and identification of artifacts.

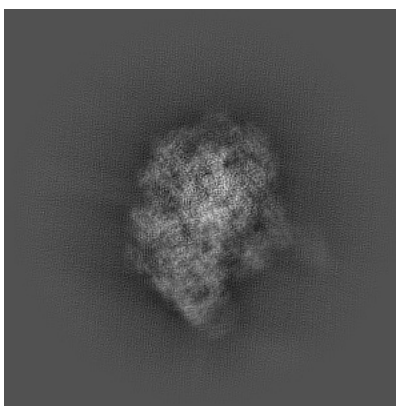
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

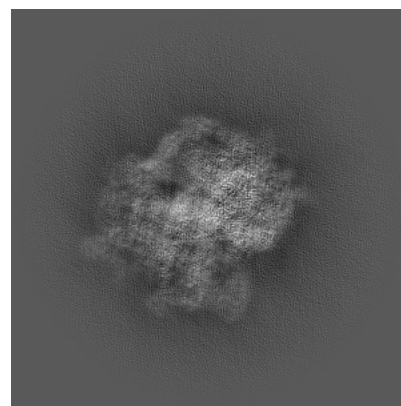
6.1.1 Primary map



X

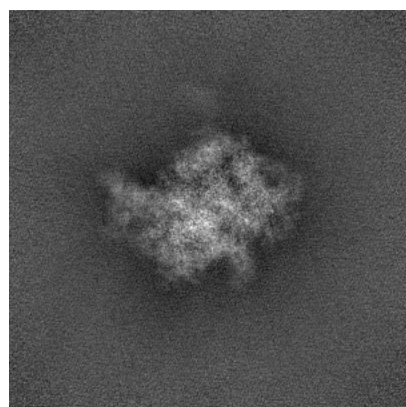


Y

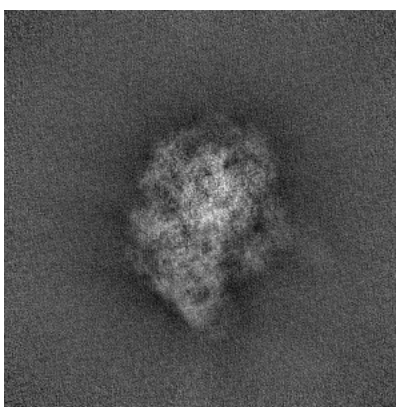


Z

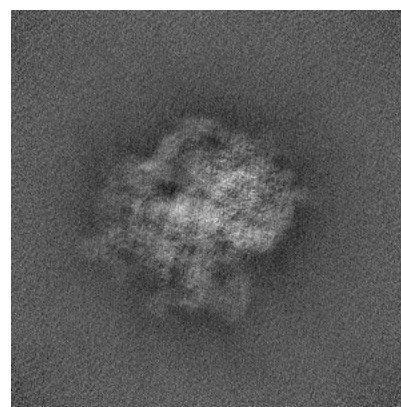
6.1.2 Raw map



X



Y

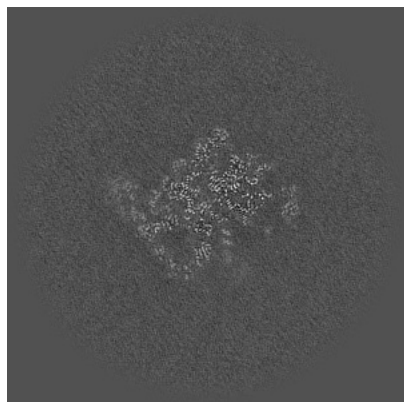


Z

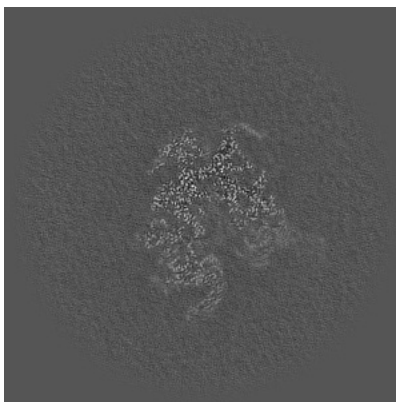
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

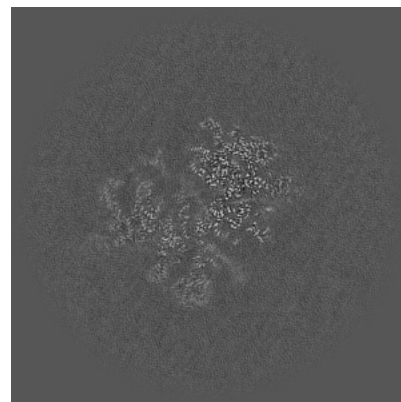
6.2.1 Primary map



X Index: 340

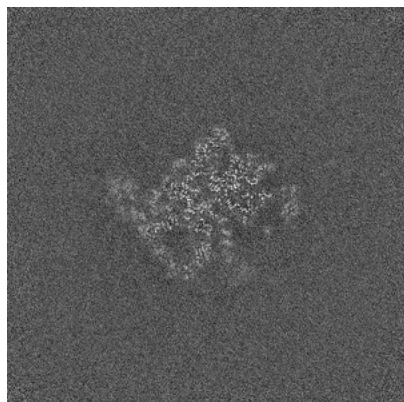


Y Index: 340

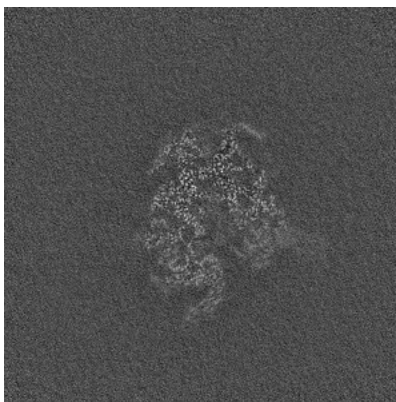


Z Index: 340

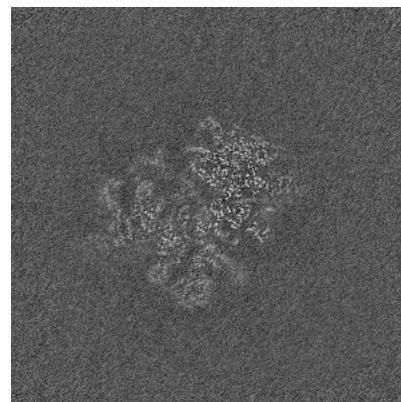
6.2.2 Raw map



X Index: 340



Y Index: 340

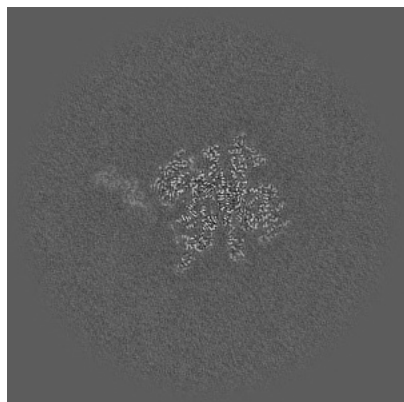


Z Index: 340

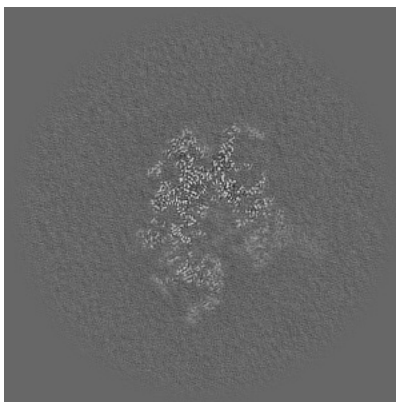
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

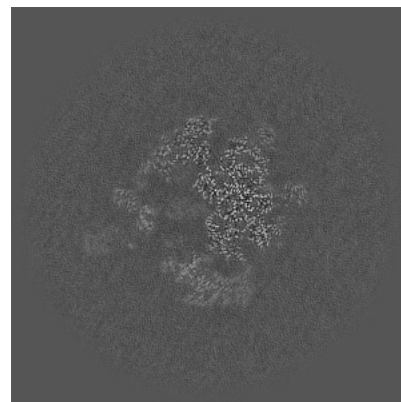
6.3.1 Primary map



X Index: 378

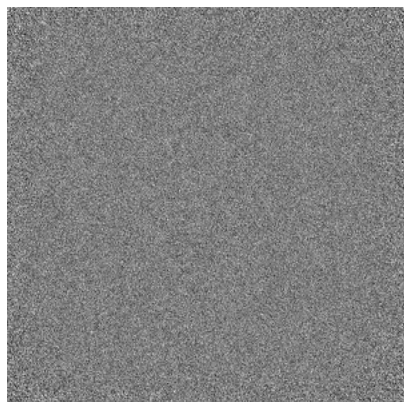


Y Index: 337

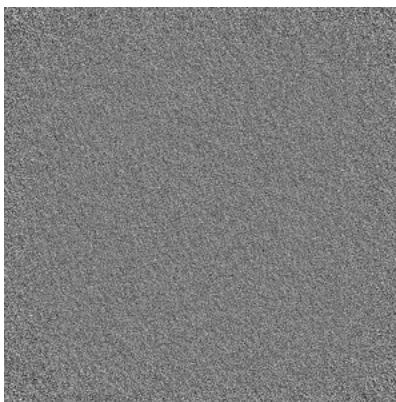


Z Index: 369

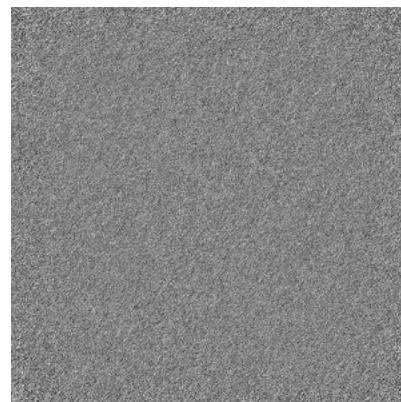
6.3.2 Raw map



X Index: 0



Y Index: 0

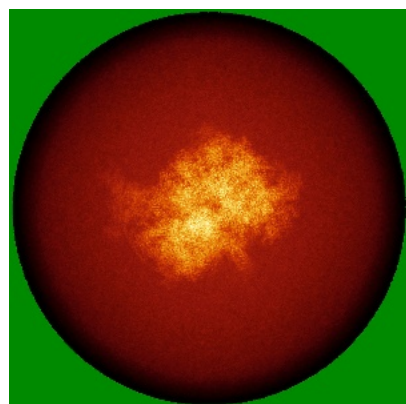


Z Index: 0

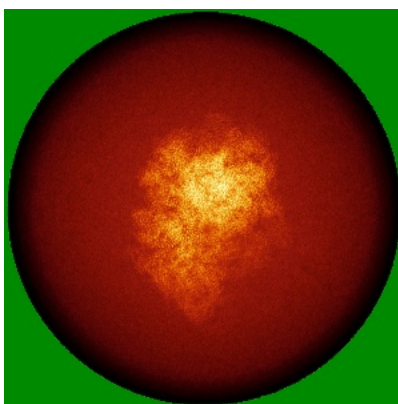
The images above show the largest variance slices of the map in three orthogonal directions.

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

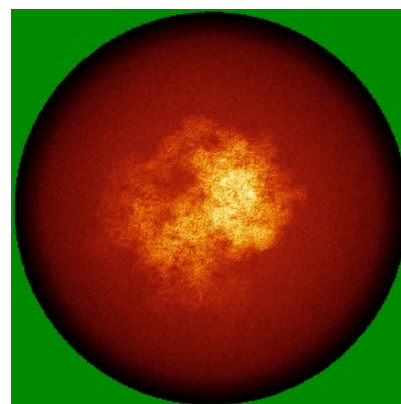
6.4.1 Primary map



X

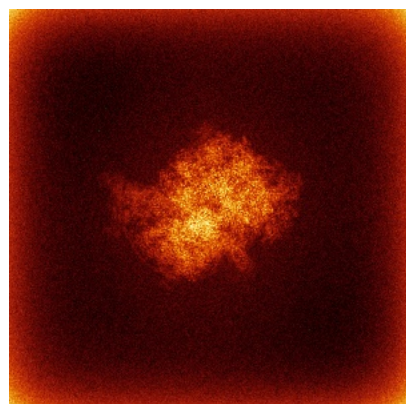


Y

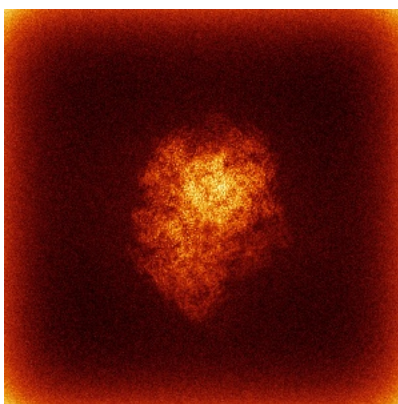


Z

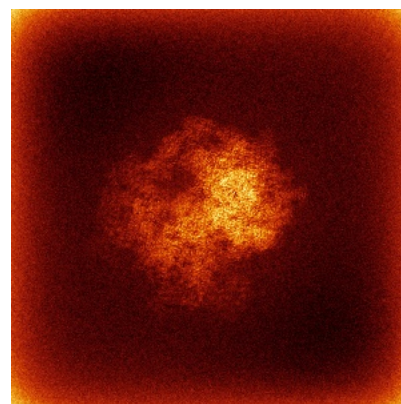
6.4.2 Raw map



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



X



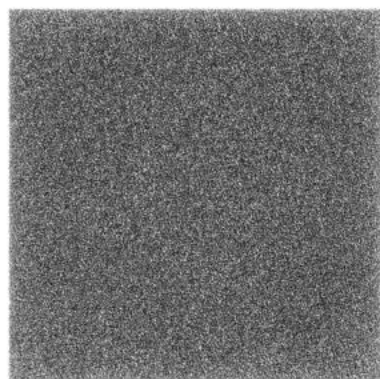
Y



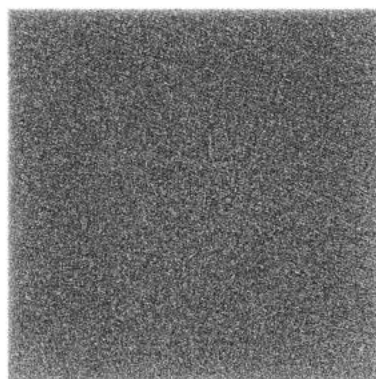
Z

The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

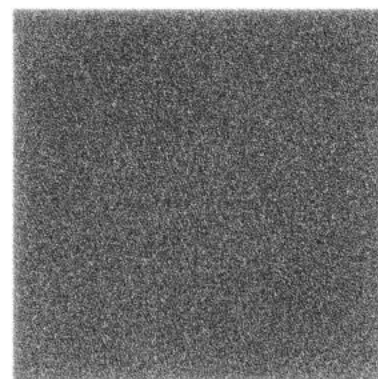
6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

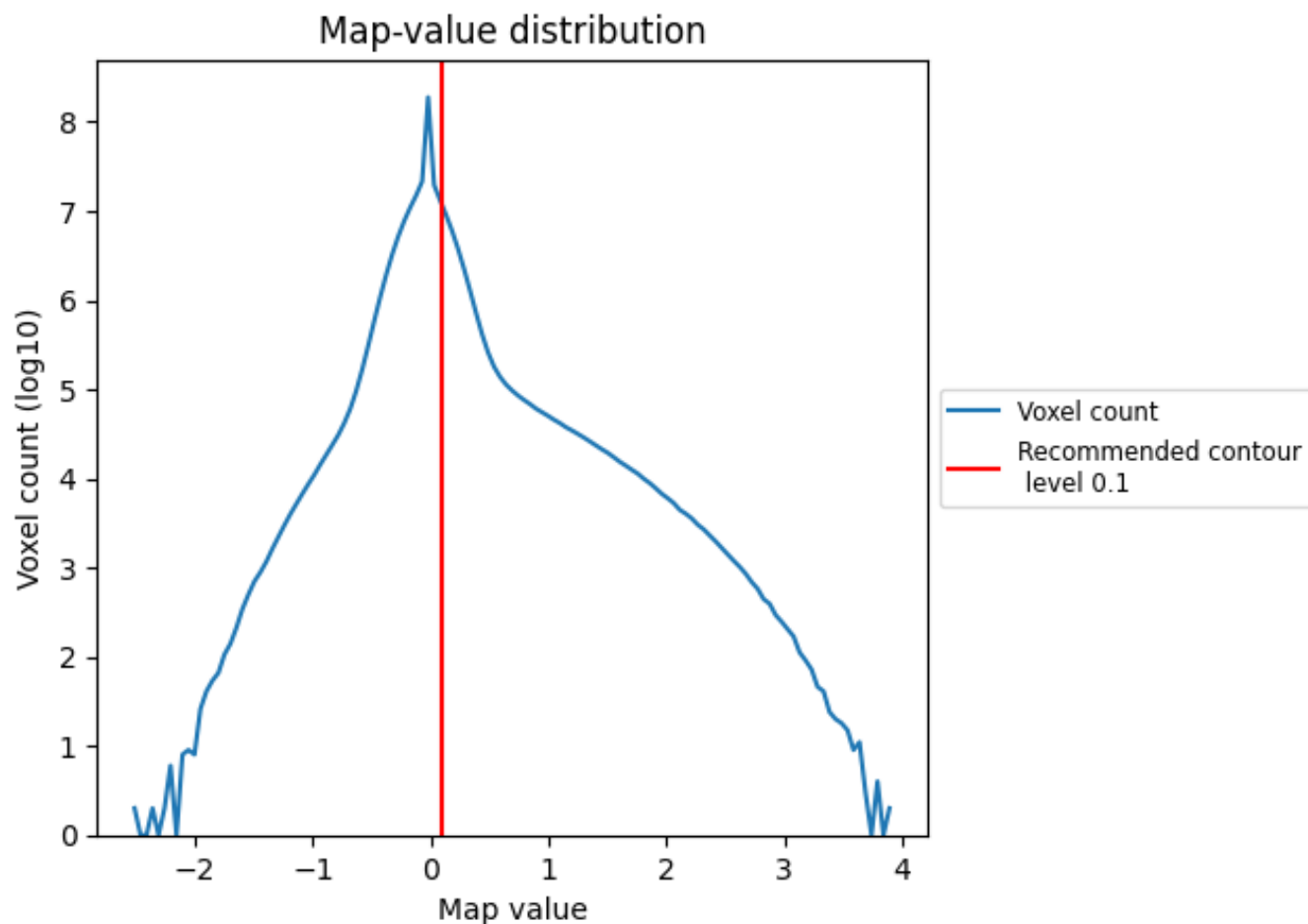
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

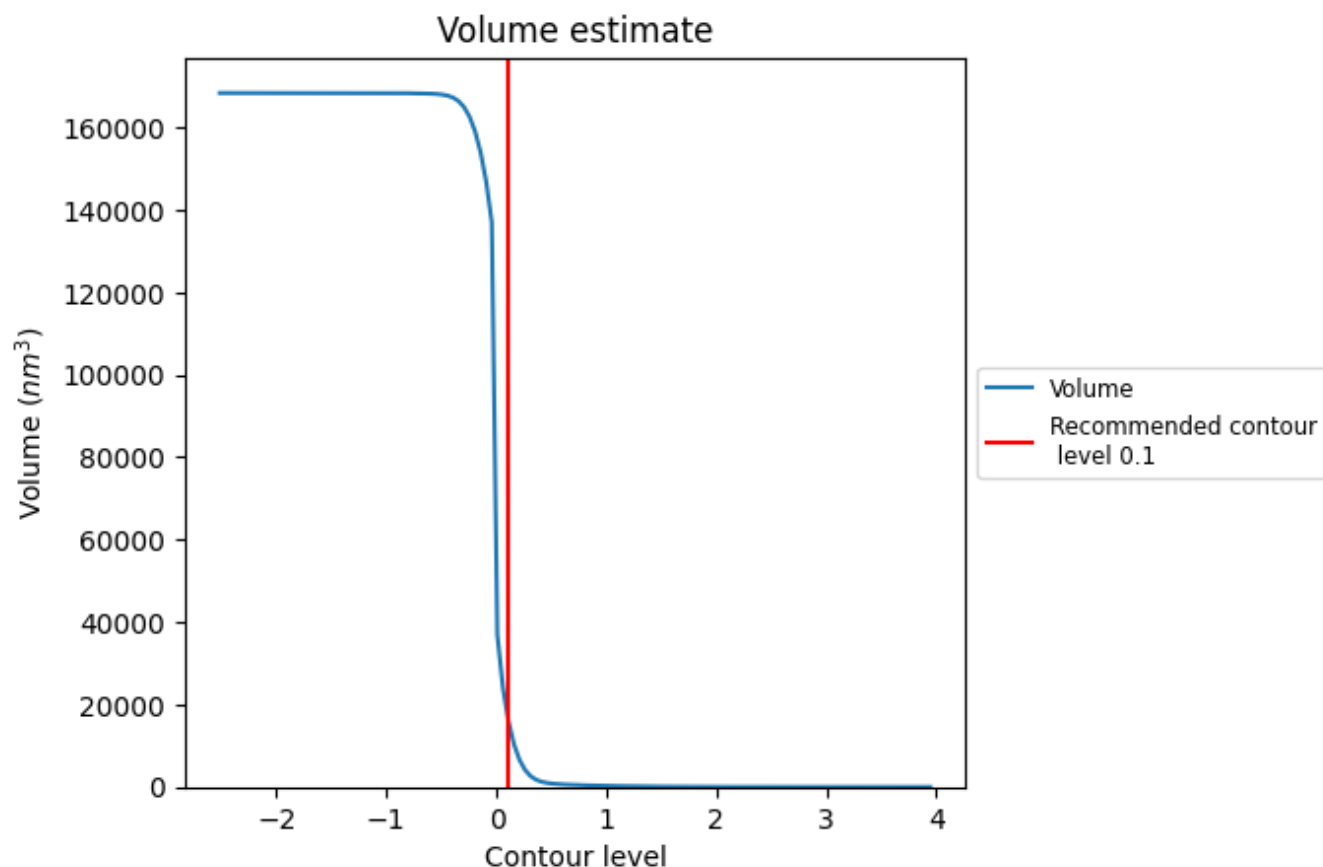
This section contains the results of statistical analysis of the map.

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.

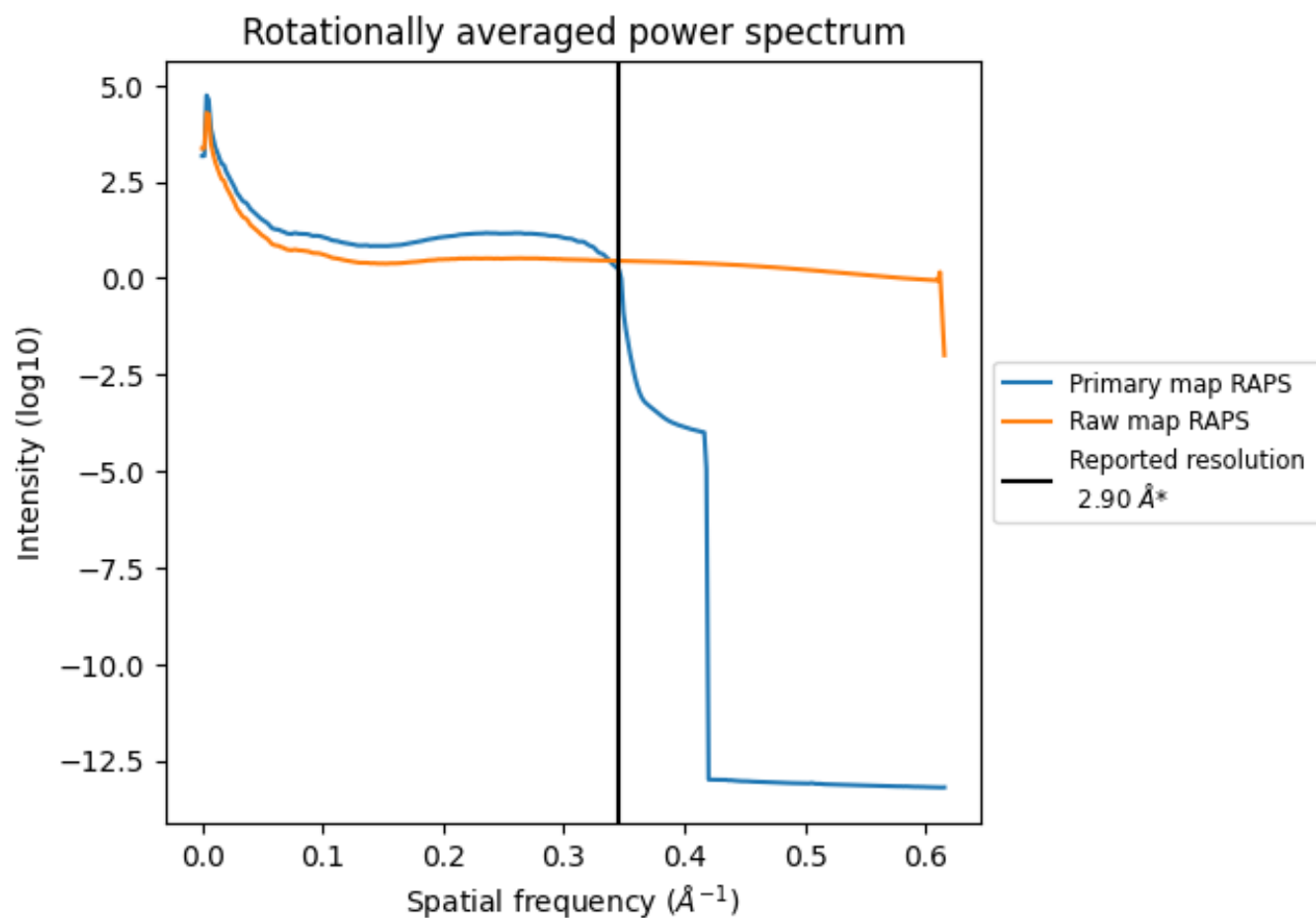
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 17573 nm^3 ; this corresponds to an approximate mass of 15874 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 ⓘ

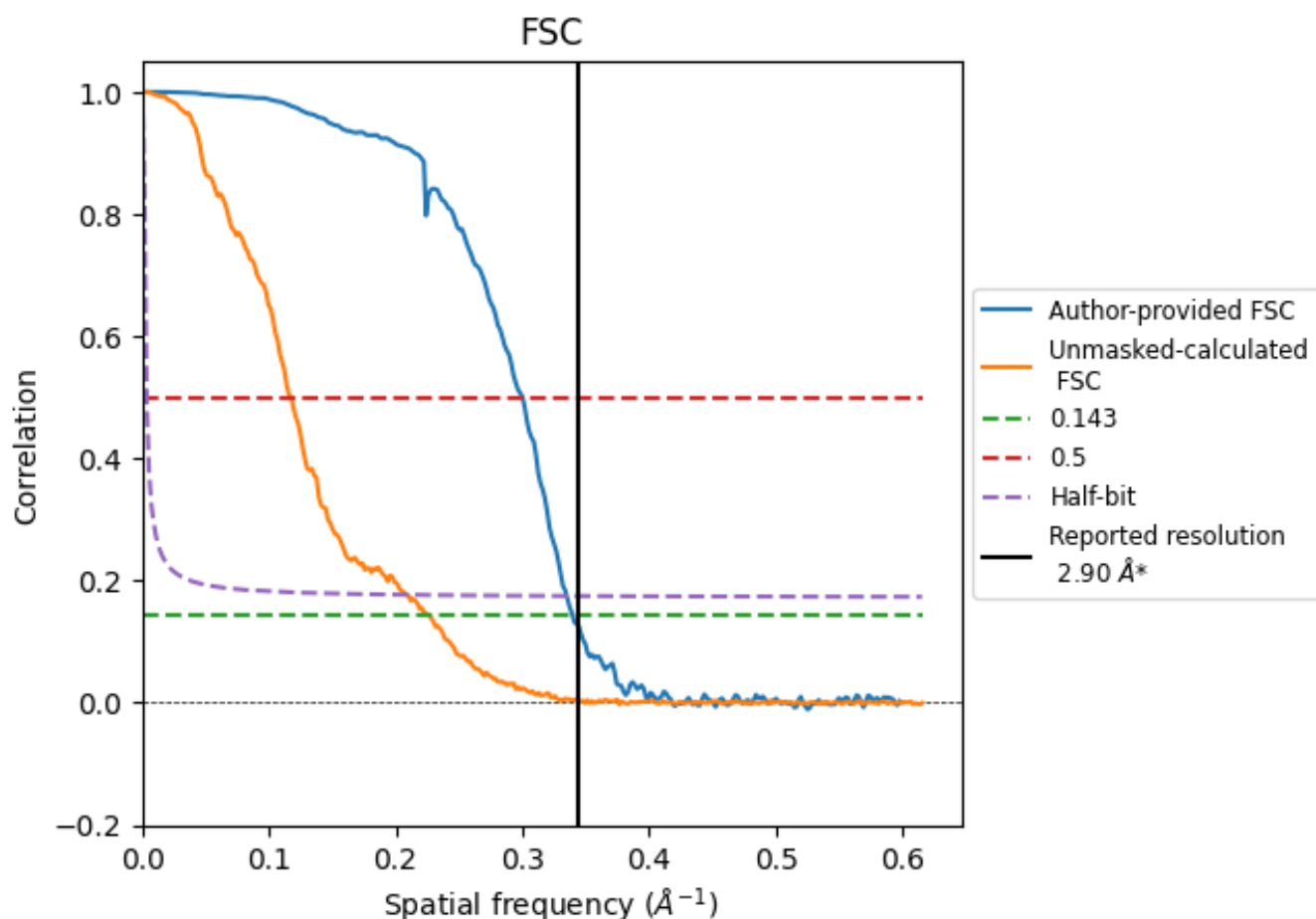


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.345 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

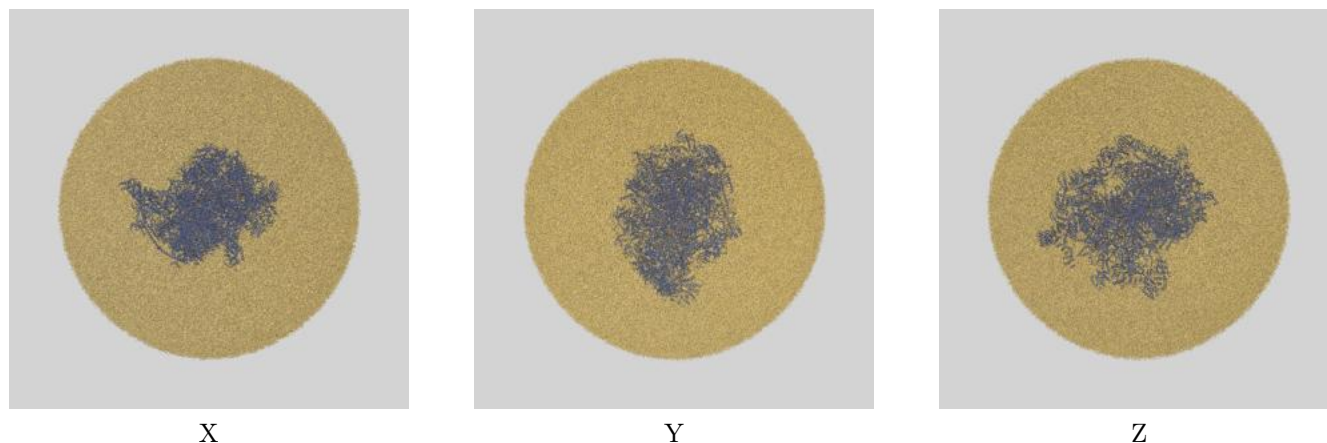
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.94	3.33	2.98
Unmasked-calculated*	4.42	8.49	4.80

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.42 differs from the reported value 2.9 by more than 10 %

9 Map-model fit [i](#)

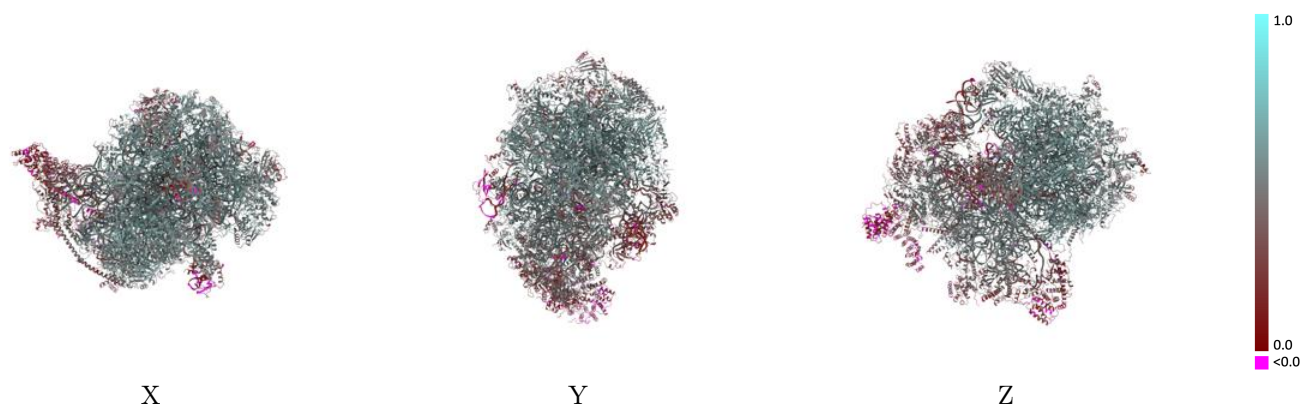
This section contains information regarding the fit between EMDB map EMD-65433 and PDB model 9VXM. Per-residue inclusion information can be found in section [3](#) on page [27](#).

9.1 Map-model overlay [i](#)



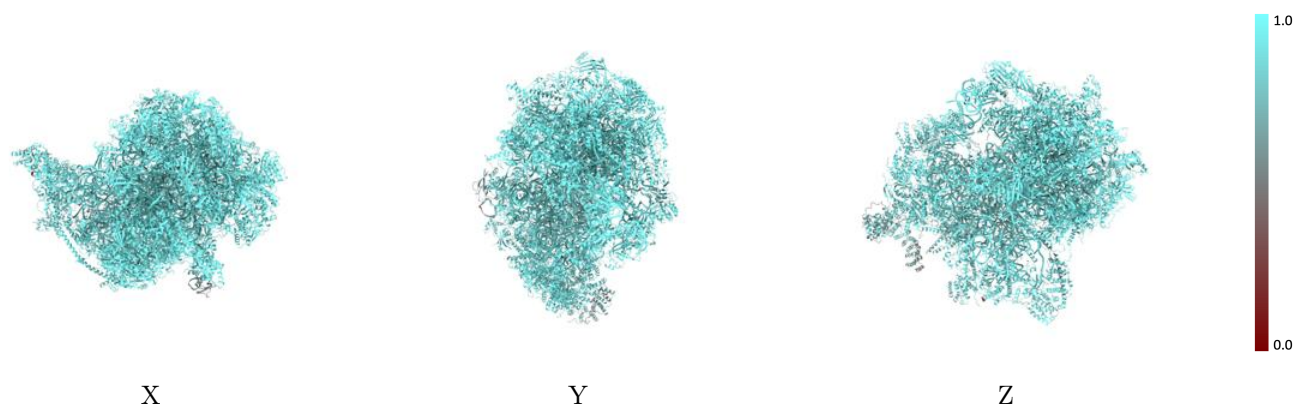
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



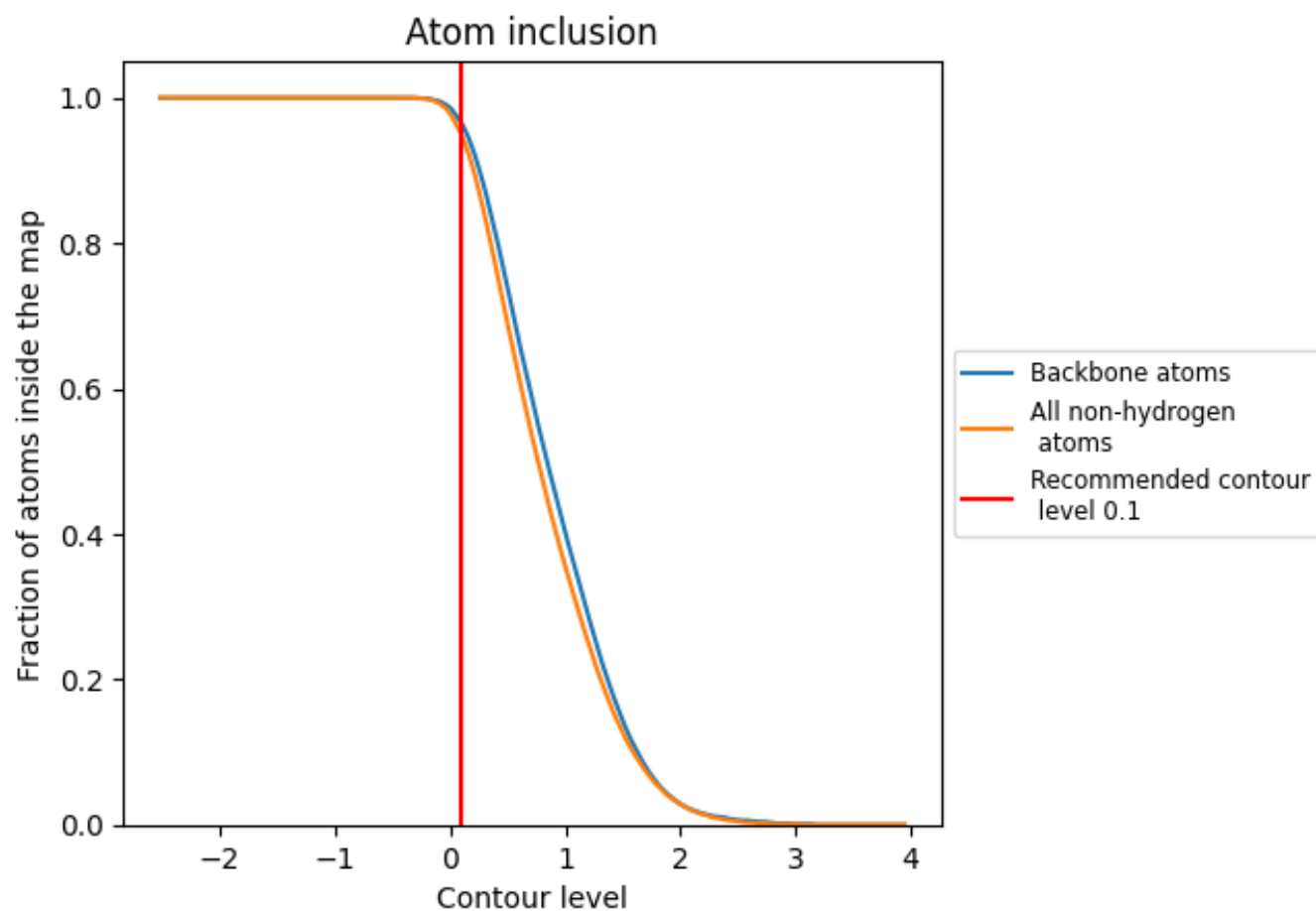
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 95% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9490	 0.4760
0	 0.9710	 0.5520
1	 0.9800	 0.5400
2	 0.9890	 0.6120
3	 0.9800	 0.6010
4	 0.9850	 0.5770
5	 0.9800	 0.5460
6	 0.9740	 0.4960
7	 0.9730	 0.4940
8	 0.8810	 0.3550
9	 0.9690	 0.5100
A	 0.9780	 0.5480
A0	 0.9180	 0.3160
A1	 0.9100	 0.3350
A3	 0.9660	 0.5440
A4	 0.7240	 0.1450
AA	 0.9820	 0.5150
AB	 0.9530	 0.4970
AC	 0.9520	 0.4980
AD	 0.9270	 0.4670
AE	 0.9600	 0.5180
AF	 0.9440	 0.4290
AG	 0.9160	 0.4150
AH	 0.9250	 0.4100
AI	 0.9690	 0.5050
AJ	 0.9440	 0.5000
AK	 0.9550	 0.4830
AL	 0.9450	 0.4820
AM	 0.9190	 0.4010
AN	 0.9620	 0.5150
AO	 0.9360	 0.3870
AP	 0.9620	 0.5190
AR	 0.8970	 0.3200
AS	 0.9260	 0.4230
AT	 0.9530	 0.4720



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
AU	 0.9170	 0.3730
AV	 0.8620	 0.1920
AW	 0.9610	 0.4740
AX	 0.9210	 0.3380
AY	 0.8220	 0.2690
AZ	 0.9210	 0.4100
Aw	 0.8220	 0.3210
Ax	 0.9280	 0.4060
Az	 0.9060	 0.4350
B	 0.9650	 0.3370
C	 0.9770	 0.5510
D	 0.9880	 0.5880
E	 0.9830	 0.5660
F	 0.9820	 0.5610
G	 0.9290	 0.4360
H	 0.7960	 0.2620
I	 0.9330	 0.3630
J	 0.8490	 0.2230
L	 0.9780	 0.5650
M	 0.9840	 0.5620
N	 0.9750	 0.5540
O	 0.9840	 0.5760
P	 0.9860	 0.5530
Q	 0.9740	 0.5310
R	 0.9870	 0.5820
S	 0.9850	 0.5660
T	 0.9900	 0.5870
U	 0.9340	 0.5090
V	 0.9310	 0.4630
W	 0.9900	 0.5950
X	 0.9720	 0.5360
Y	 0.9770	 0.5580
Z	 0.9820	 0.5820
a	 0.9560	 0.5280
b	 0.9830	 0.5700
c	 0.9770	 0.5240
d	 0.9240	 0.4330
e	 0.9140	 0.2940
f	 0.8940	 0.4120
g	 0.9830	 0.5410
h	 0.9280	 0.4300
i	 0.9900	 0.5940

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
j	 0.9680	 0.5280
k	 0.9860	 0.5790
l	 0.9040	 0.3070
m	 0.8830	 0.3130
n	 0.9120	 0.3540
o	 0.9800	 0.5910
p	 0.9270	 0.4450
q	 0.9510	 0.4700
r	 0.9780	 0.5340
s	 0.9810	 0.5560