



Full wwPDB EM Validation Report ⓘ

Jun 23, 2026 – 11:39 AM EDT

PDB ID : 6OM7 / pdb_00006om7
EMDB ID : EMD-0597
Title : Human ribosome nascent chain complex (PCSK9-RNC) stalled by a drug-like small molecule with AA and PE tRNAs
Authors : Li, W.; Cate, J.H.D.
Deposited on : 2019-04-18
Resolution : 3.70 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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
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) : 2.49

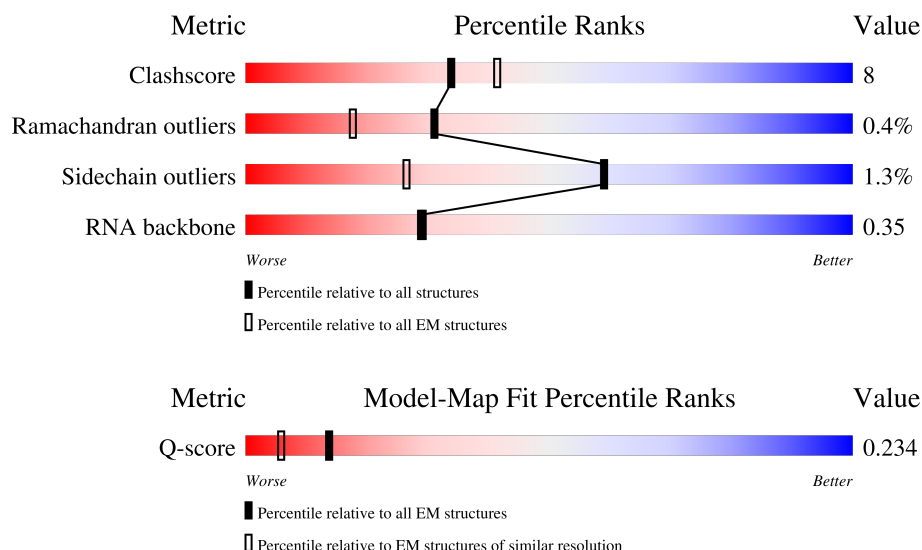
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 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	10474 (3.22 - 4.22)

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	S2	1714	16% 50% 38% 11%
2	SA	221	67% 76% 22%
3	SB	214	39% 78% 21%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	SD	226	
5	SE	259	
6	SF	189	
7	SH	189	
8	SI	204	
9	SK	98	
10	SL	153	
11	SP	127	
12	SQ	146	
13	SR	134	
14	SS	145	
15	ST	143	
16	SU	104	
17	SV	82	
18	SX	141	
19	Sa	102	
20	Sc	64	
21	Sd	55	
22	Sg	312	
23	SC	220	
24	SG	237	
25	SJ	185	
26	SM	118	
27	SN	150	
28	SO	137	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	SW	129	
30	SY	131	
31	SZ	73	
32	Sb	82	
33	Se	57	
34	Sf	67	
35	A	252	
36	B	397	
37	C	363	
38	D	157	
39	E	121	
40	F	294	
41	G	247	
42	H	225	
43	I	234	
44	J	191	
45	K	211	
46	L	169	
47	M	205	
48	N	139	
49	O	203	
50	P	195	
51	Q	153	
52	R	187	
53	S	181	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
54	T	175	
55	U	157	
56	V	99	
57	W	129	
58	X	121	
59	Y	117	
60	Z	134	
61	a	134	
62	b	147	
63	c	121	
64	d	103	
65	e	106	
66	f	129	
67	g	109	
68	h	114	
69	i	122	
70	j	97	
71	k	84	
72	l	69	
73	m	50	
74	n	50	
75	o	25	
76	p	105	
77	q	91	
78	r	122	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
79	t	3607	15% 58% 34% 7%
80	v	76	21% 46% 39% 14%
81	w	10	60% 30% 10%
82	u	76	42% 46% 45% 9%
83	y	26	73% 46% 50% .

2 Entry composition

There are 87 unique types of molecules in this entry. The entry contains 215295 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	S2	1714	Total	C	N	O	P	0	0
			36501	16306	6533	11949	1713		

- Molecule 2 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	SA	221	Total	C	N	O	S	0	0
			1741	1106	305	322	8		

- Molecule 3 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	SB	214	Total	C	N	O	S	0	0
			1738	1103	310	311	14		

- Molecule 4 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	SD	226	Total	C	N	O	S	0	0
			1757	1120	316	314	7		

- Molecule 5 is a protein called 40S ribosomal protein S4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	SE	259	Total	C	N	O	S	0	0
			2059	1316	383	352	8		

- Molecule 6 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	SF	189	Total	C	N	O	S	0	0
			1495	934	284	270	7		

- Molecule 7 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	SH	186	Total	C	N	O	S	0	0
			1497	956	274	266	1		

- Molecule 8 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	SI	204	Total	C	N	O	S	0	0
			1673	1050	329	289	5		

- Molecule 9 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	SK	98	Total	C	N	O	S	0	0
			827	539	148	134	6		

- Molecule 10 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	SL	153	Total	C	N	O	S	0	0
			1247	793	234	214	6		

- Molecule 11 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	SP	127	Total	C	N	O	S	0	0
			1045	663	198	177	7		

- Molecule 12 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	SQ	146	Total	C	N	O	S	0	0
			1158	736	218	200	4		

- Molecule 13 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	SR	134	Total	C	N	O	S	0	0
			1082	680	201	197	4		

- Molecule 14 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	SS	145	Total	C	N	O	S	0	0
			1198	751	242	203	2		

- Molecule 15 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	ST	143	Total	C	N	O	S	0	0
			1112	697	214	198	3		

- Molecule 16 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	SU	104	Total	C	N	O	S	0	0
			821	514	155	148	4		

- Molecule 17 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	SV	82	Total	C	N	O	S	0	0
			625	384	116	120	5		

- Molecule 18 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	SX	141	Total	C	N	O	S	0	0
			1098	693	219	183	3		

- Molecule 19 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Sa	102	Total	C	N	O	S	0	0
			821	512	171	133	5		

- Molecule 20 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Sc	64	Total	C	N	O	S	0	0
			506	308	102	94	2		

- Molecule 21 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Sd	55	Total	C	N	O	S	0	0
			459	286	94	74	5		

- Molecule 22 is a protein called Receptor of activated protein C kinase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Sg	312	Total	C	N	O	S	0	0
			2429	1531	423	463	12		

- Molecule 23 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	SC	220	Total	C	N	O	S	1	0
			1715	1109	296	300	10		

- Molecule 24 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	SG	237	Total	C	N	O	S	0	0
			1923	1200	387	329	7		

- Molecule 25 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	SJ	185	Total	C	N	O	S	1	0
			1533	974	309	248	2		

- Molecule 26 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	SM	118	Total	C	N	O	S	0	0
			912	571	161	173	7		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SM	52	GLN	LEU	conflict	UNP P25398
SM	69	LEU	CYS	conflict	UNP P25398
SM	99	ASN	LYS	conflict	UNP P25398

- Molecule 27 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	SN	150	Total	C	N	O	S	0	0
			1208	773	229	205	1		

- Molecule 28 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	SO	137	Total	C	N	O	S	0	0
			1024	627	200	191	6		

- Molecule 29 is a protein called 40S ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	SW	129	Total	C	N	O	S	0	0
			1034	659	193	176	6		

- Molecule 30 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	SY	131	Total	C	N	O	S	1	0
			1073	678	212	178	5		

- Molecule 31 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	SZ	73	Total	C	N	O	S	0	0
			579	372	106	100	1		

- Molecule 32 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Sb	82	Total	C	N	O	S	0	0
			640	402	118	113	7		

- Molecule 33 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Se	57	Total	C	N	O	S	0	0
			452	281	99	71	1		

- Molecule 34 is a protein called 40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Sf	67	Total	C	N	O	S	0	0
			548	346	102	93	7		

- Molecule 35 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	A	252	Total	C	N	O	S	0	0
			1930	1209	395	320	6		

- Molecule 36 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	B	397	Total	C	N	O	S	0	0
			3202	2039	602	547	14		

- Molecule 37 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	C	363	Total	C	N	O	S	0	0
			2888	1817	577	480	14		

- Molecule 38 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	D	157	Total	C	N	O	P	0	0
			3337	1489	587	1104	157		

- Molecule 39 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	E	119	Total	C	N	O	P	0	0
			2541	1132	454	836	119		

- Molecule 40 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	F	294	Total	C	N	O	S	0	0
			2392	1510	436	432	14		

- Molecule 41 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	G	236	Total	C	N	O	S	0	0
			1904	1222	361	317	4		

- Molecule 42 is a protein called 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	H	225	Total	C	N	O	S	0	0
			1870	1202	358	301	9		

- Molecule 43 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	I	234	Total	C	N	O	S	0	0
			1880	1197	362	317	4		

- Molecule 44 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	J	191	Total	C	N	O	S	0	0
			1526	960	285	275	6		

- Molecule 45 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	K	208	Total	C	N	O	S	0	0
			1692	1074	327	278	13		

- Molecule 46 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	L	169	Total	C	N	O	S	0	0
			1353	855	252	240	6		

- Molecule 47 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	M	205	Total	C	N	O	S	0	0
			1657	1036	344	273	4		

- Molecule 48 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	N	139	Total	C	N	O	S	0	0
			1138	730	218	183	7		

- Molecule 49 is a protein called 60S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	O	203	Total	C	N	O	S	0	0
			1701	1072	359	266	4		

- Molecule 50 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	P	195	Total	C	N	O	S	0	0
			1606	1034	315	252	5		

- Molecule 51 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	Q	153	Total	C	N	O	S	0	0
			1242	776	241	216	9		

- Molecule 52 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	R	187	Total	C	N	O	S	0	0
			1513	944	314	250	5		

- Molecule 53 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	S	181	Total	C	N	O	S	0	0
			1517	938	329	241	9		

- Molecule 54 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	T	175	Total	C	N	O	S	0	0
			1449	921	283	234	11		

- Molecule 55 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	U	157	Total	C	N	O	S	0	0
			1284	815	250	214	5		

- Molecule 56 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	V	99	Total	C	N	O	S	0	0
			808	518	141	147	2		

- Molecule 57 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	W	129	Total	C	N	O	S	0	0
			969	613	182	169	5		

- Molecule 58 is a protein called 60S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	X	121	Total	C	N	O	S	0	0
			989	617	202	167	3		

- Molecule 59 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	Y	117	Total	C	N	O	S	0	0
			958	612	180	165	1		

- Molecule 60 is a protein called 60S ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	Z	134	Total	C	N	O	S	0	0
			1115	700	226	186	3		

- Molecule 61 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	a	134	Total	C	N	O	S	0	0
			1103	712	207	181	3		

- Molecule 62 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	b	147	Total	C	N	O	S	0	0
			1162	736	237	186	3		

- Molecule 63 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	c	100	Total	C	N	O	S	0	0
			814	506	179	125	4		

- Molecule 64 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	d	103	Total	C	N	O	S	0	0
			801	508	141	145	7		

- Molecule 65 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	e	106	Total	C	N	O	S	0	0
			879	555	170	152	2		

- Molecule 66 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	f	129	Total	C	N	O	S	0	0
			1064	673	220	166	5		

- Molecule 67 is a protein called 60S ribosomal protein L35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	g	109	Total	C	N	O	S	0	0
			876	555	174	144	3		

- Molecule 68 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	h	114	Total	C	N	O	S	0	0
			906	566	187	147	6		

- Molecule 69 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	i	122	Total	C	N	O	S	0	0
			1015	641	205	168	1		

- Molecule 70 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	j	97	Total	C	N	O	S	0	0
			794	497	168	124	5		

- Molecule 71 is a protein called 60S ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	k	84	Total	C	N	O	S	0	0
			689	423	152	109	5		

- Molecule 72 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	l	69	Total	C	N	O	S	0	0
			569	366	103	99	1		

- Molecule 73 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	m	50	Total	C	N	O	S	0	0
			444	281	98	64	1		

- Molecule 74 is a protein called 60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	n	50	Total	C	N	O	S	0	0
			411	254	87	64	6		

- Molecule 75 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	o	25	Total	C	N	O	S	0	0
			240	145	64	28	3		

- Molecule 76 is a protein called 60S ribosomal protein L36a.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	p	105	Total	C	N	O	S	0	0
			863	542	175	140	6		

- Molecule 77 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	q	91	Total	C	N	O	S	0	0
			708	445	136	120	7		

- Molecule 78 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	r	122	Total	C	N	O	S	0	0
			980	607	204	165	4		

- Molecule 79 is a RNA chain called 28S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	t	3607	Total	C	N	O	P	0	0
			77332	34436	14150	25139	3607		

- Molecule 80 is a RNA chain called P/E site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	v	76	Total	C	N	O	P	0	0
			1618	721	287	534	76		

- Molecule 81 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	w	10	Total	C	N	O	P	0	0
			213	95	37	72	9		

- Molecule 82 is a RNA chain called A/A site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	u	76	Total	C	N	O	P	0	0
			1613	720	283	535	75		

- Molecule 83 is a protein called Proprotein convertase subtilisin/kexin type 9.

Mol	Chain	Residues	Atoms				AltConf	Trace
83	y	26	Total	C	N	O	0	0
			128	76	26	26		

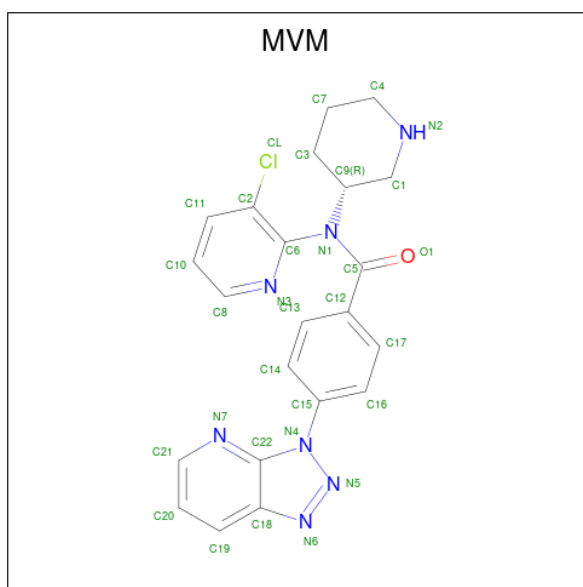
- Molecule 84 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
84	S2	1	Total	Zn	0
			1	1	
84	Sa	1	Total	Zn	0
			1	1	
84	Sf	1	Total	Zn	0
			1	1	
84	k	1	Total	Zn	0
			1	1	
84	p	1	Total	Zn	0
			1	1	
84	q	1	Total	Zn	0
			1	1	

- Molecule 85 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
85	S2	3	Total	Mg	0
			3	3	
85	D	6	Total	Mg	0
			6	6	
85	E	9	Total	Mg	0
			9	9	
85	b	1	Total	Mg	0
			1	1	
85	f	1	Total	Mg	0
			1	1	
85	t	11	Total	Mg	0
			11	11	

- Molecule 86 is N-(3-chloropyridin-2-yl)-N-[(3R)-piperidin-3-yl]-4-(3H-[1,2,3]triazolo[4,5-b]pyridin-3-yl)benzamide (CCD ID: MVM) (formula: C₂₂H₂₀ClN₇O).



Mol	Chain	Residues	Atoms					AltConf
86	t	1	Total	C	Cl	N	O	0
			31	22	1	7	1	

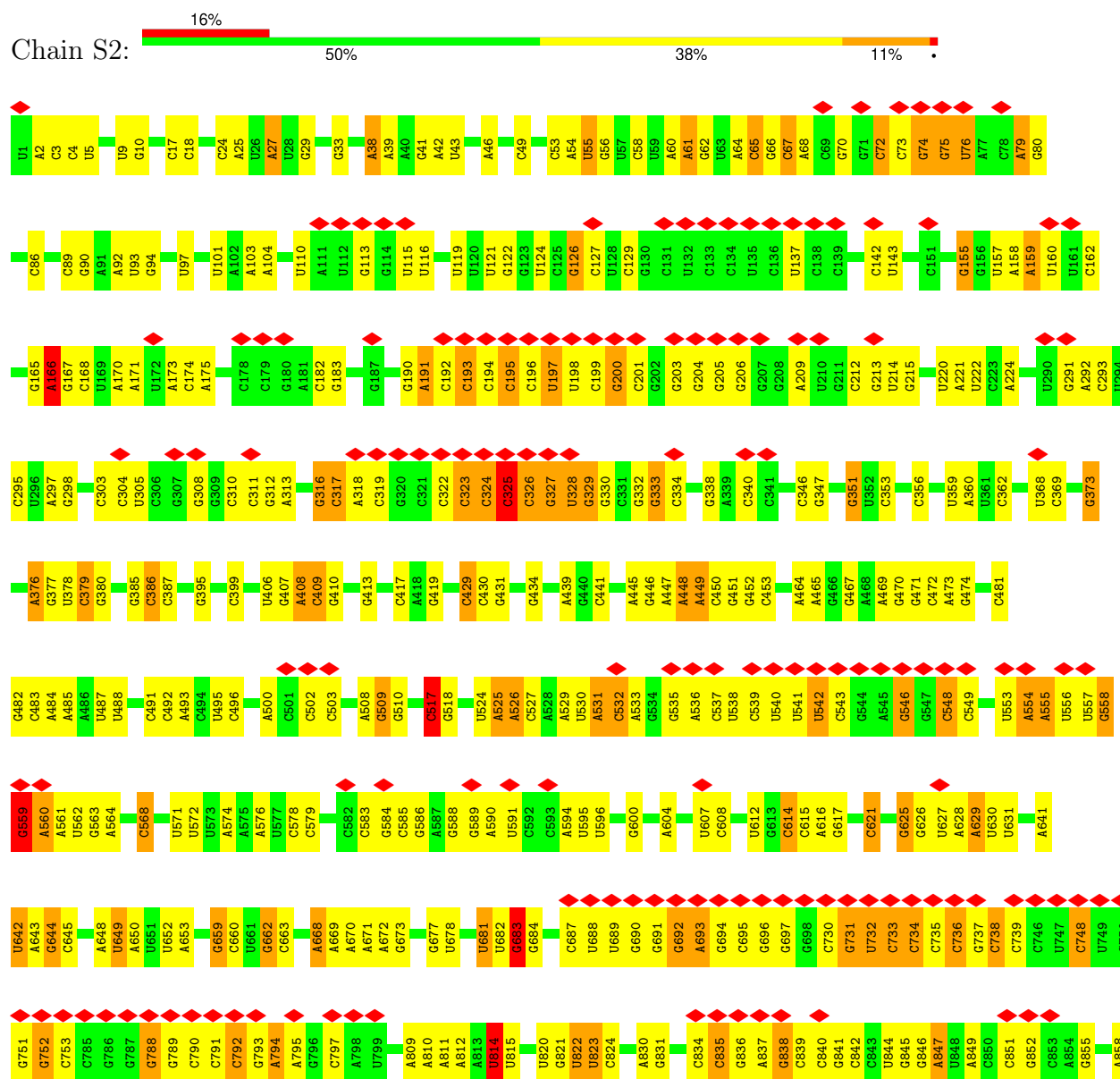
- Molecule 87 is water.

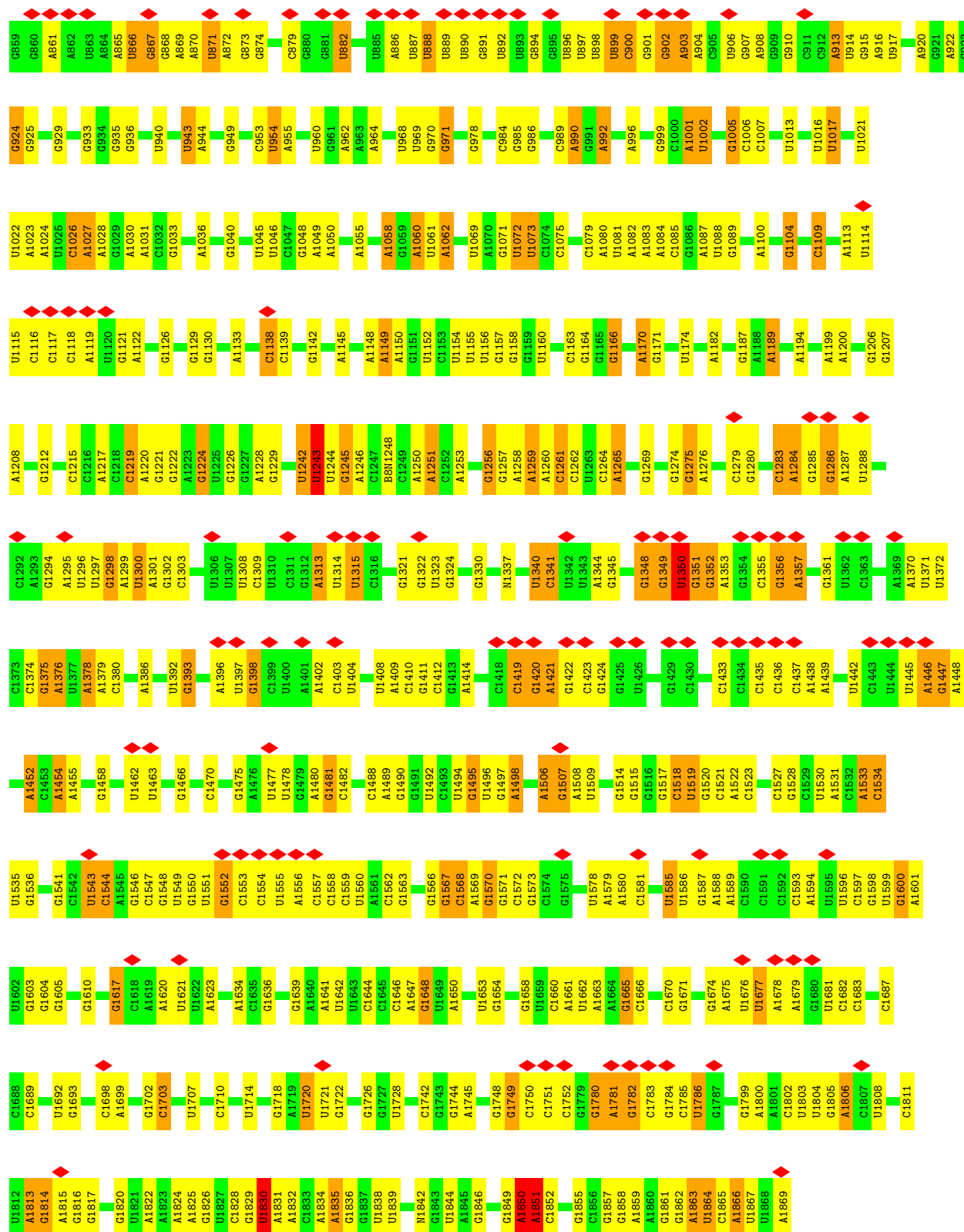
Mol	Chain	Residues	Atoms		AltConf
87	S2	6	Total	O	0
			6	6	
87	SP	1	Total	O	0
			1	1	
87	SQ	1	Total	O	0
			1	1	
87	SR	1	Total	O	0
			1	1	
87	SS	1	Total	O	0
			1	1	
87	SV	1	Total	O	0
			1	1	
87	Sb	1	Total	O	0
			1	1	
87	Sf	1	Total	O	0
			1	1	
87	u	1	Total	O	0
			1	1	

3 Residue-property plots

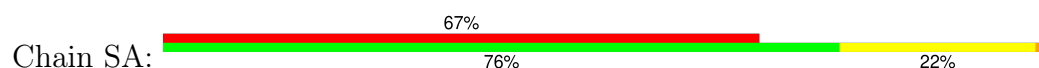
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

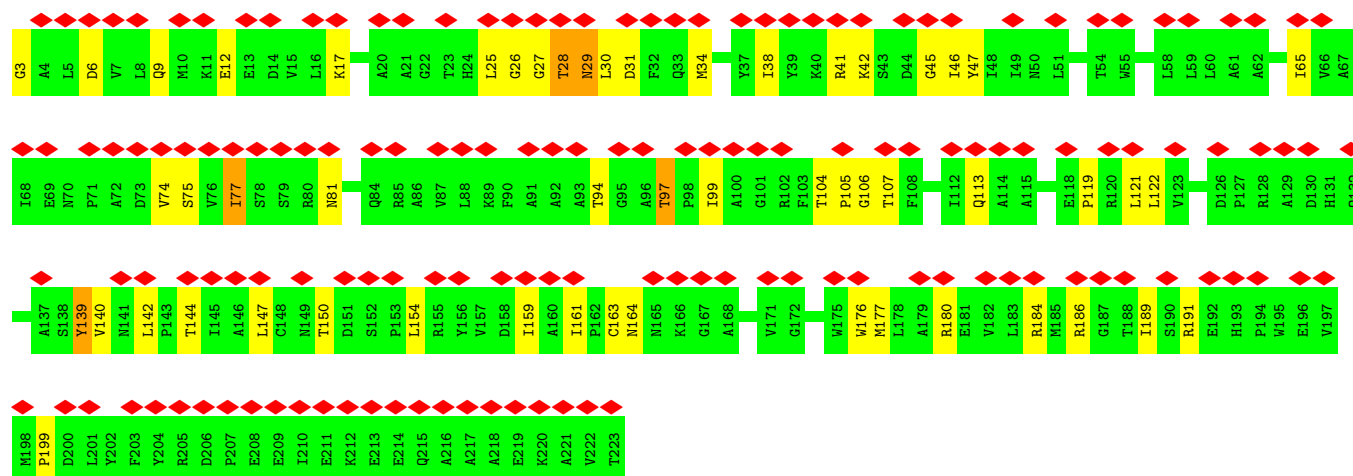
• Molecule 1: 18S ribosomal RNA





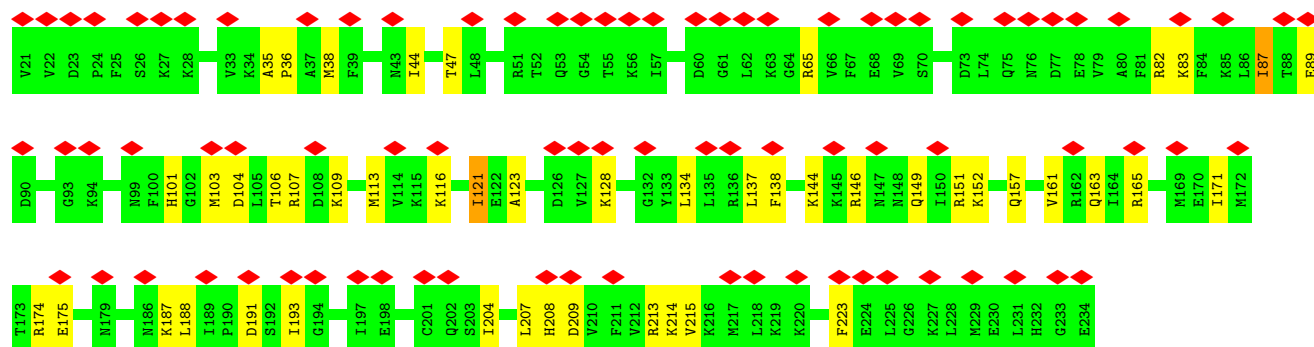
• Molecule 2: 40S ribosomal protein SA





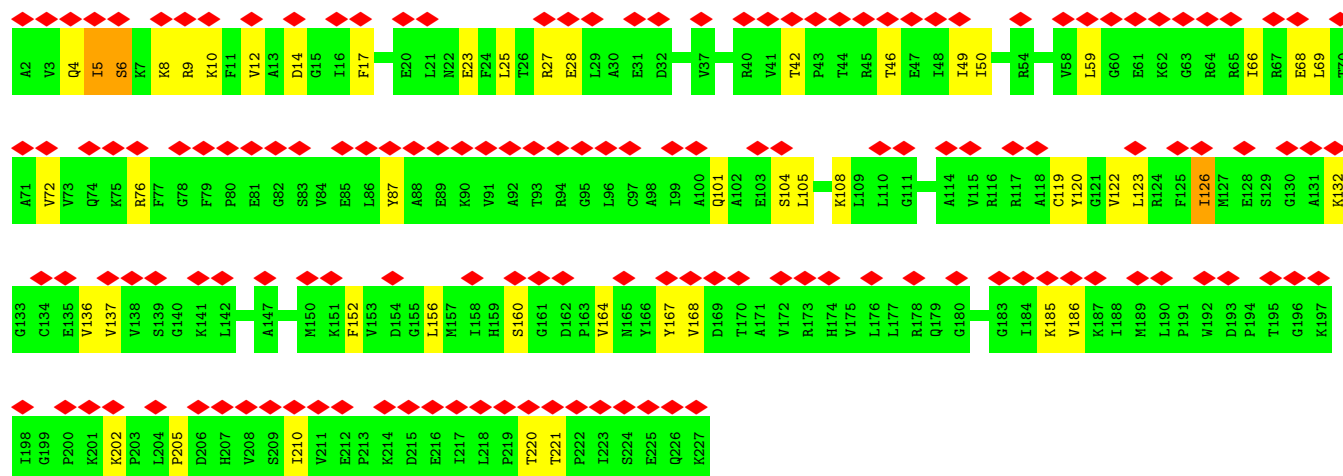
• Molecule 3: 40S ribosomal protein S3a

Chain SB:

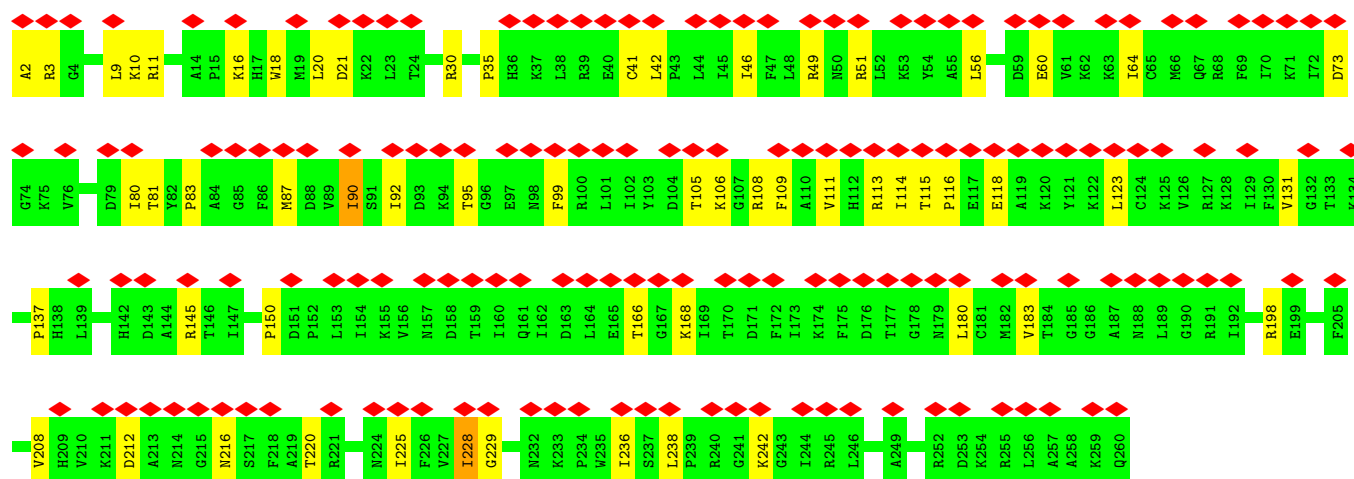
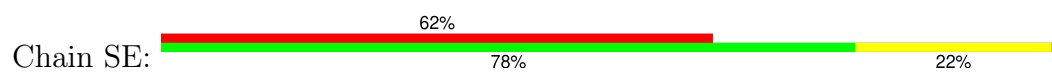


• Molecule 4: 40S ribosomal protein S3

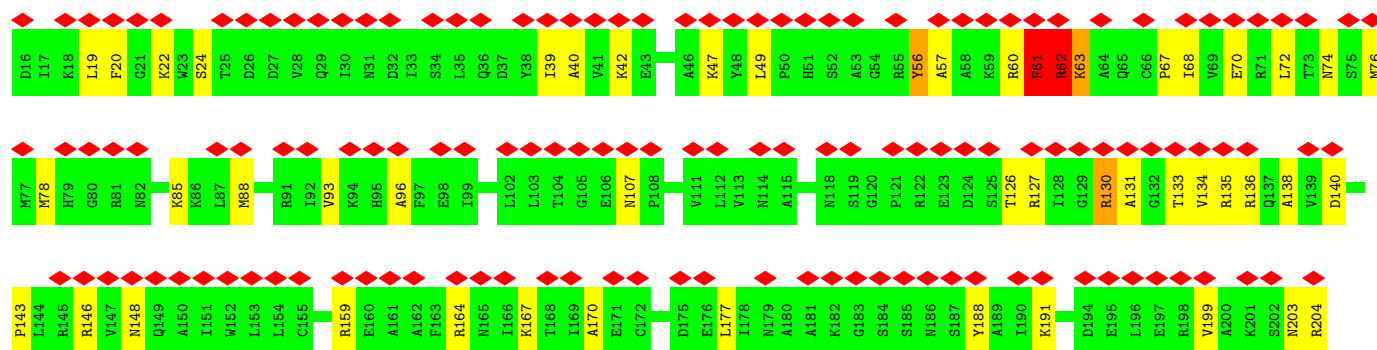
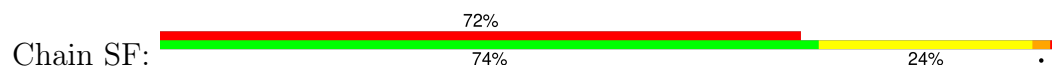
Chain SD:



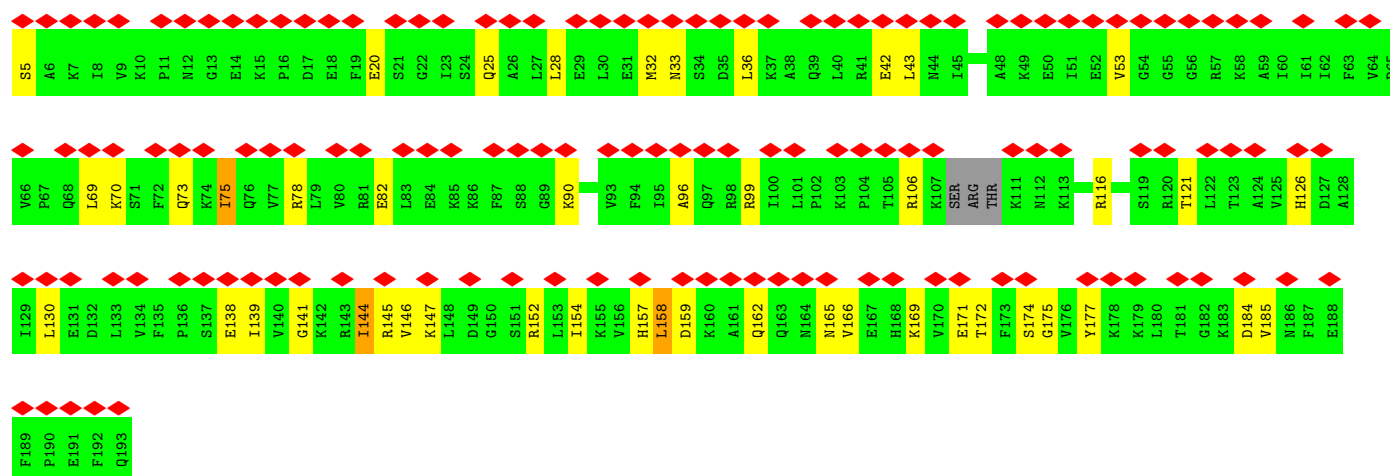
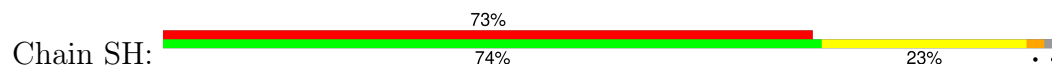
• Molecule 5: 40S ribosomal protein S4, X isoform



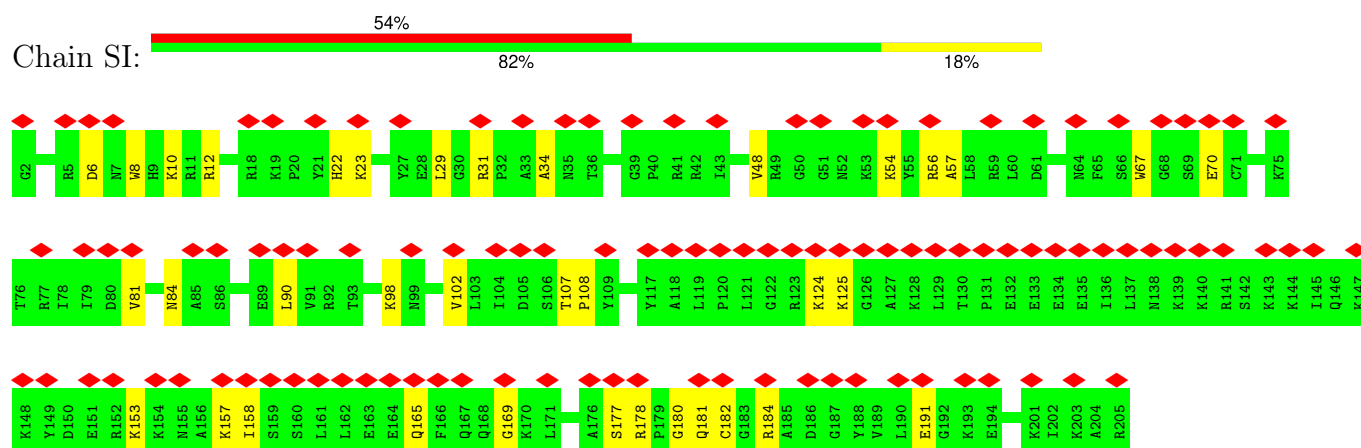
• Molecule 6: 40S ribosomal protein S5



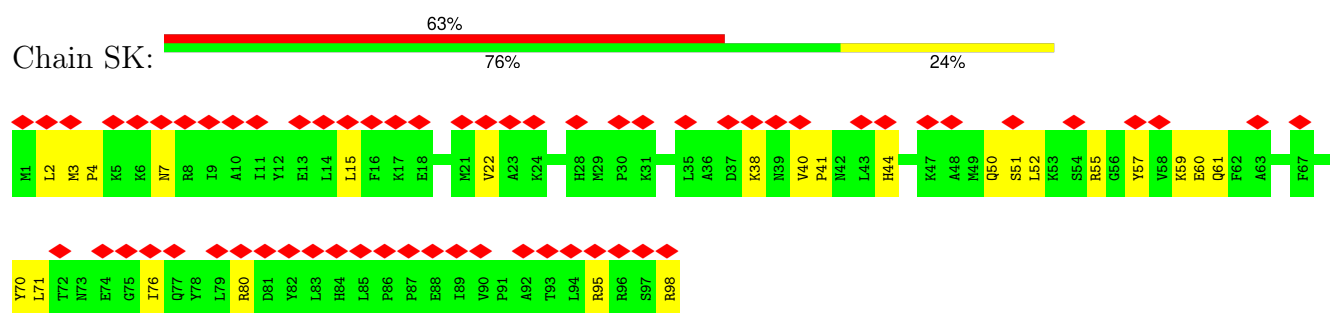
• Molecule 7: 40S ribosomal protein S7



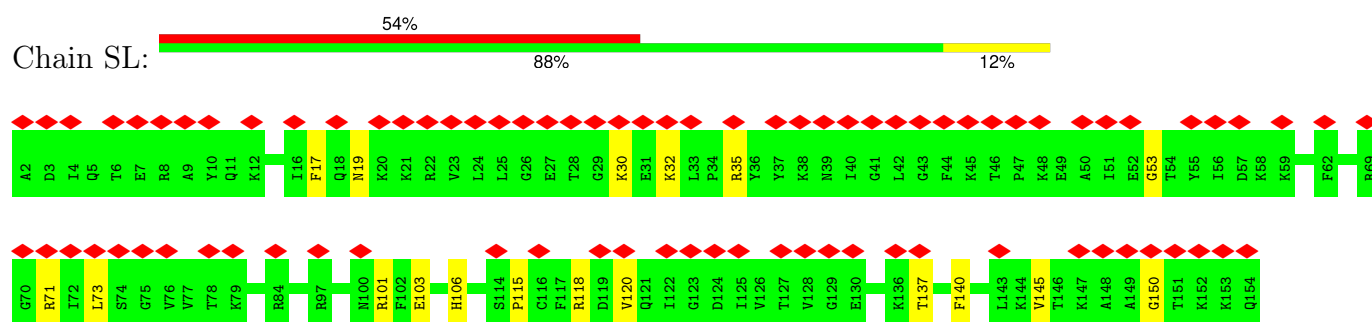
- Molecule 8: 40S ribosomal protein S8



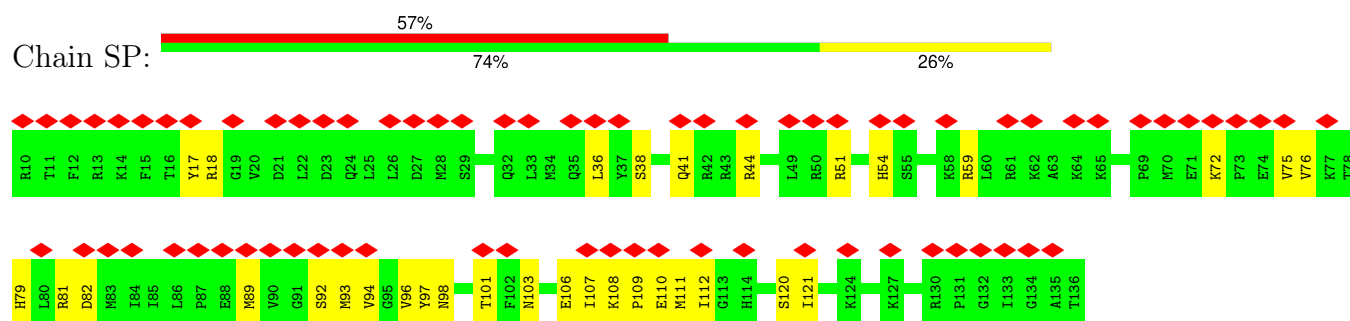
- Molecule 9: 40S ribosomal protein S10



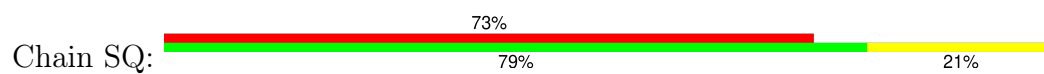
- Molecule 10: 40S ribosomal protein S11



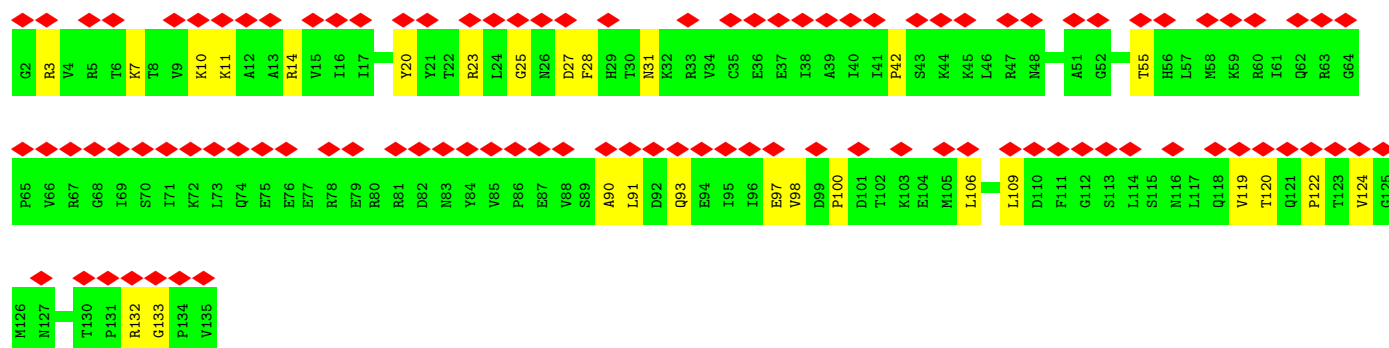
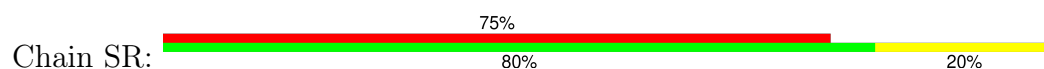
- Molecule 11: 40S ribosomal protein S15



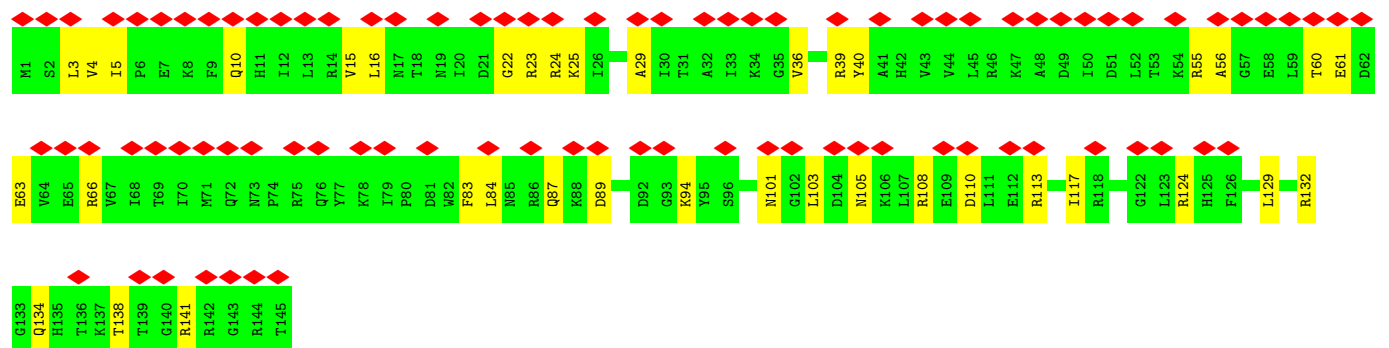
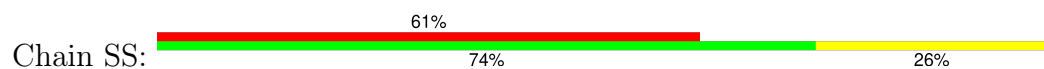
- Molecule 12: 40S ribosomal protein S16



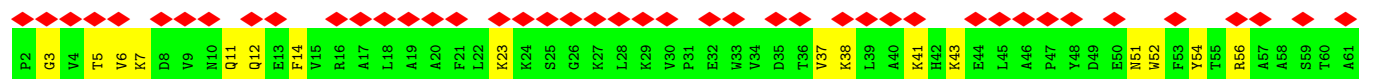
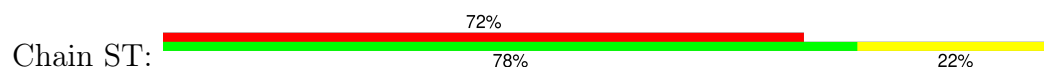
• Molecule 13: 40S ribosomal protein S17

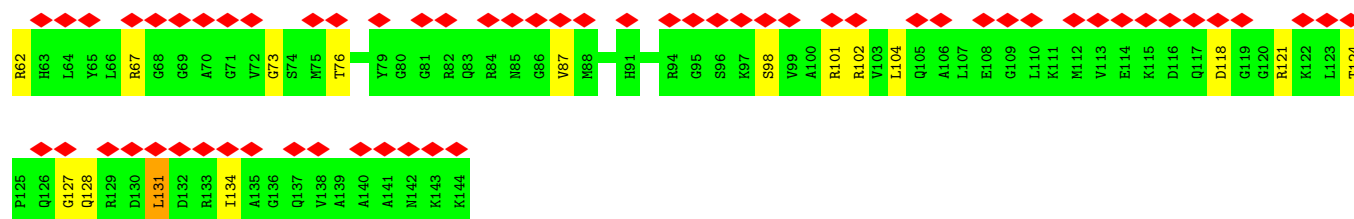


• Molecule 14: 40S ribosomal protein S18

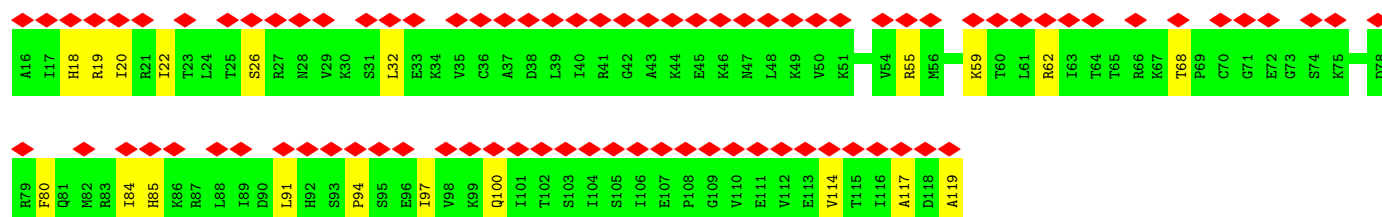
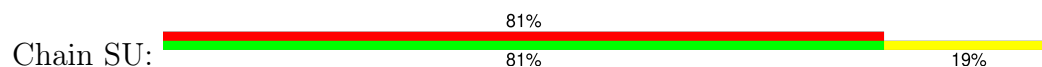


• Molecule 15: 40S ribosomal protein S19

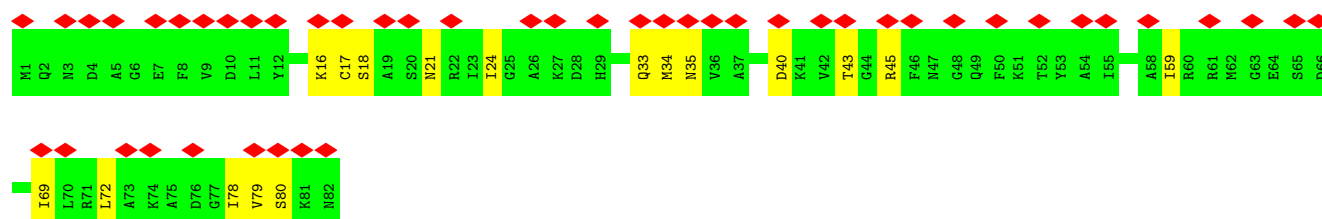
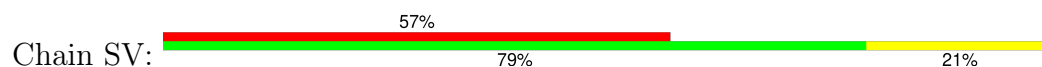




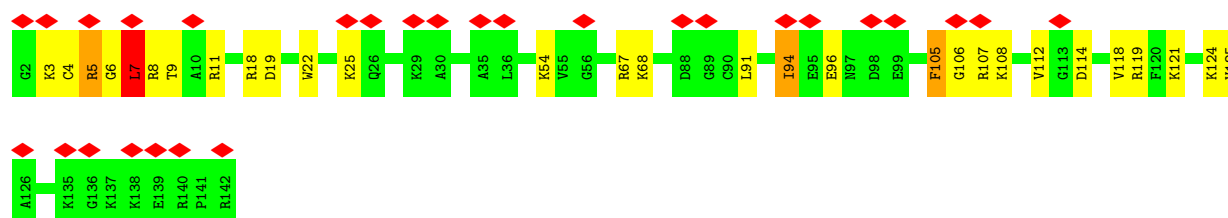
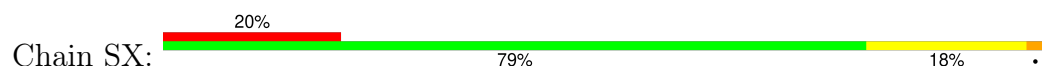
• Molecule 16: 40S ribosomal protein S20



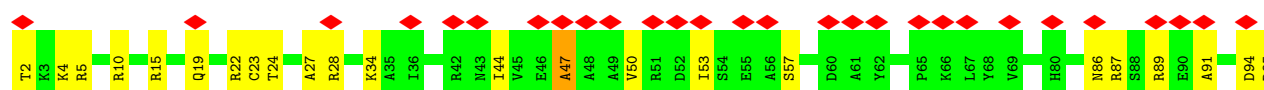
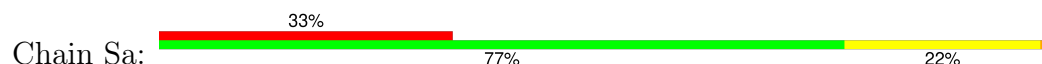
• Molecule 17: 40S ribosomal protein S21

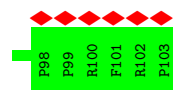


• Molecule 18: 40S ribosomal protein S23

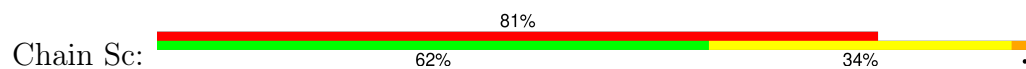


• Molecule 19: 40S ribosomal protein S26





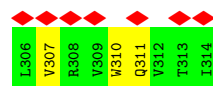
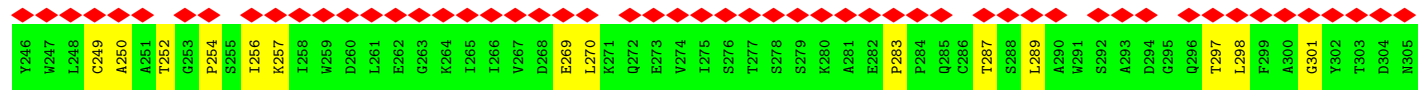
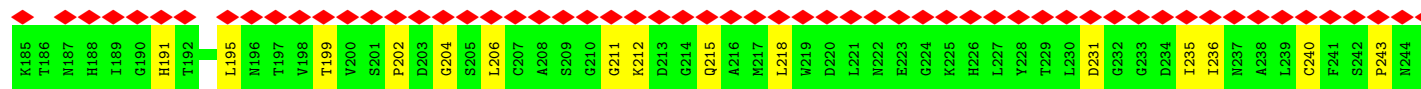
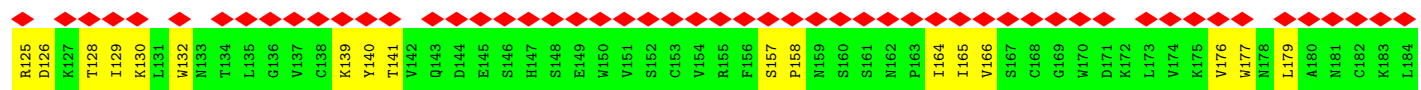
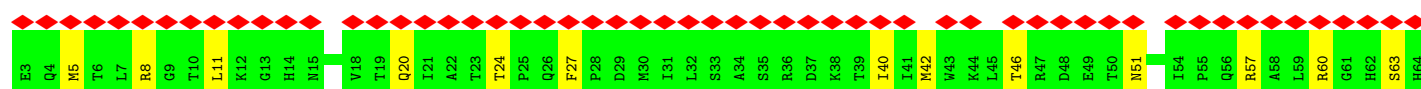
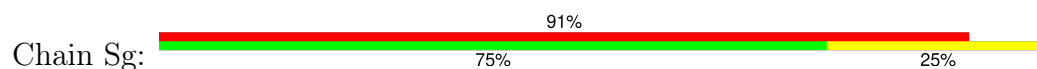
- Molecule 20: 40S ribosomal protein S28



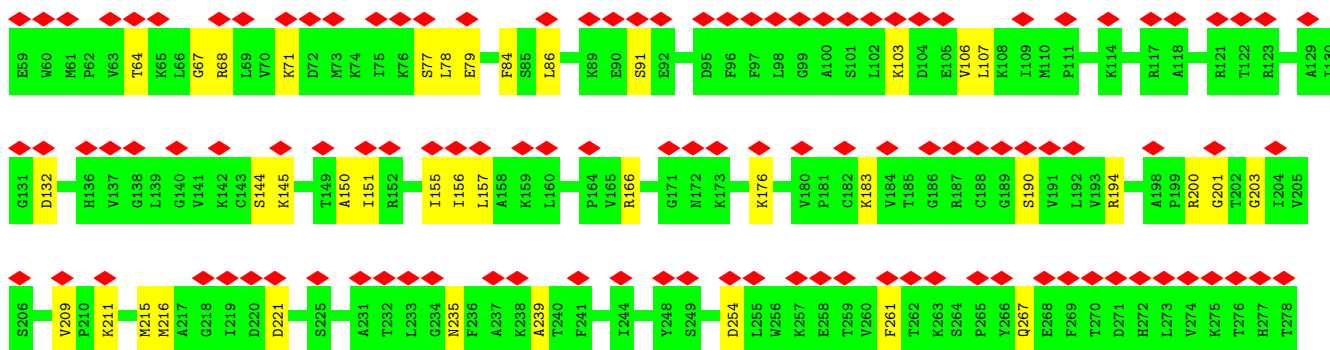
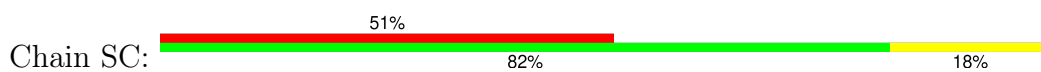
- Molecule 21: 40S ribosomal protein S29



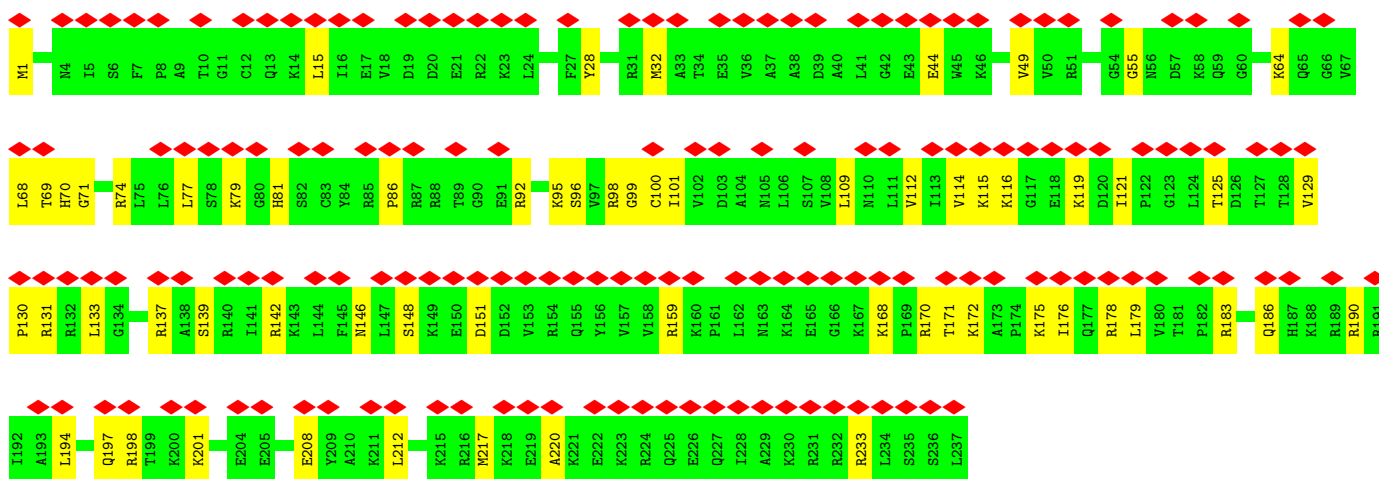
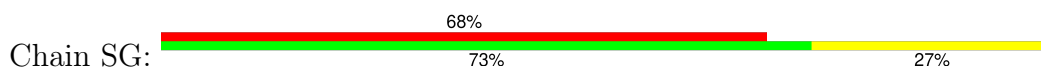
- Molecule 22: Receptor of activated protein C kinase 1



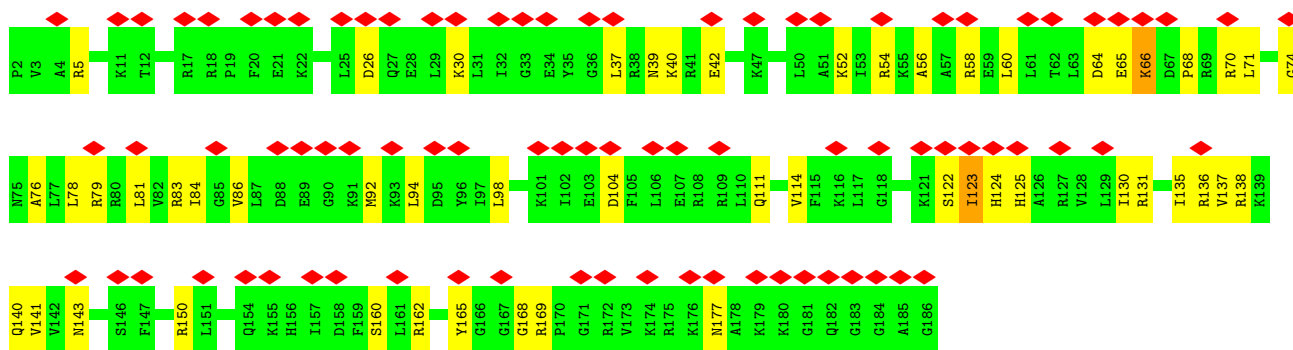
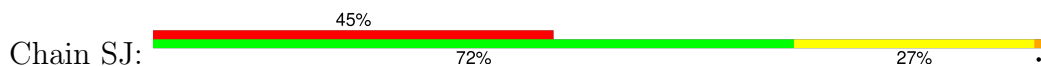
- Molecule 23: 40S ribosomal protein S2



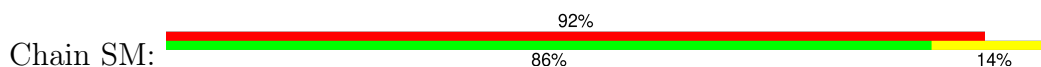
• Molecule 24: 40S ribosomal protein S6

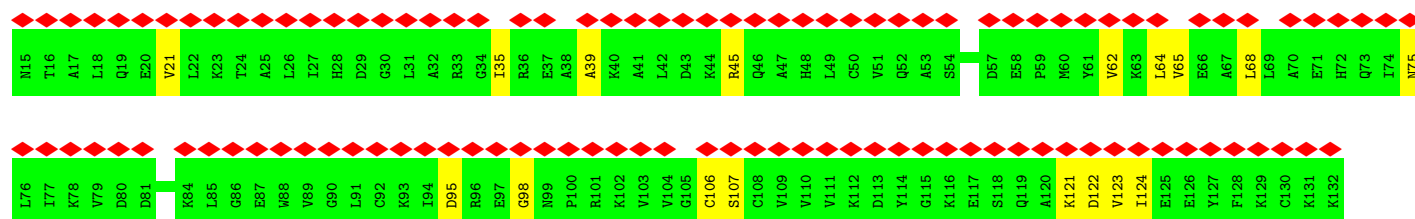


• Molecule 25: 40S ribosomal protein S9

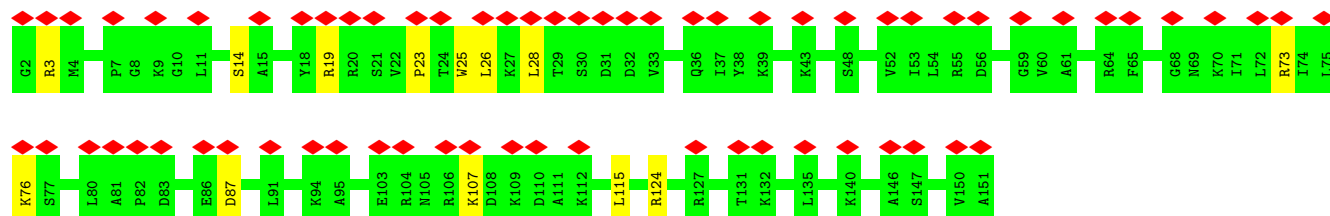


• Molecule 26: 40S ribosomal protein S12

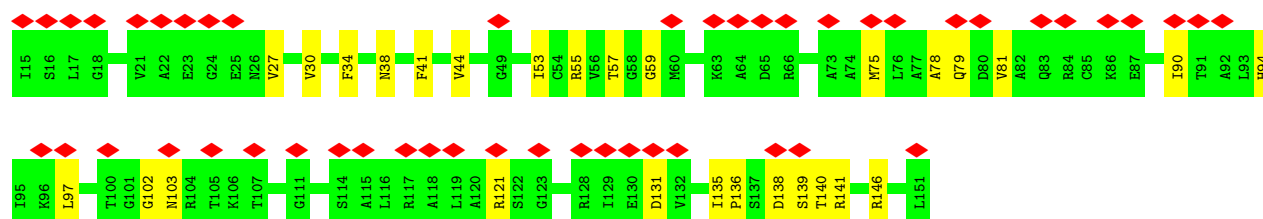
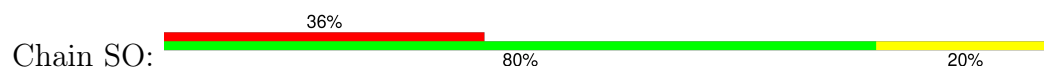




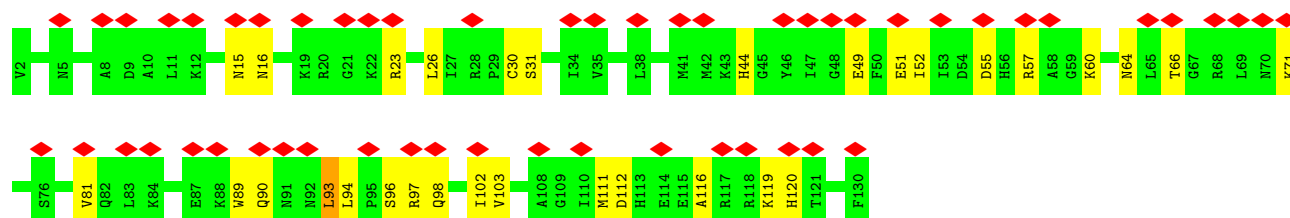
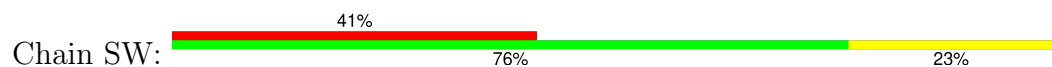
• Molecule 27: 40S ribosomal protein S13



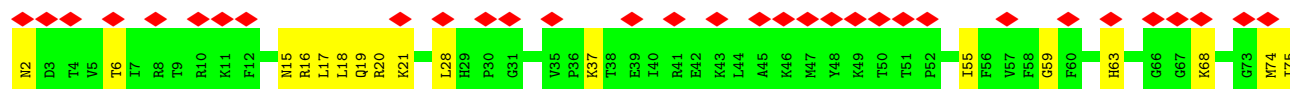
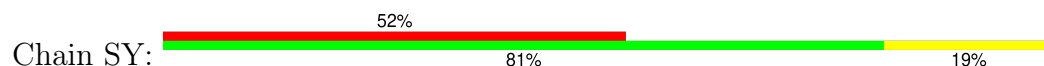
• Molecule 28: 40S ribosomal protein S14

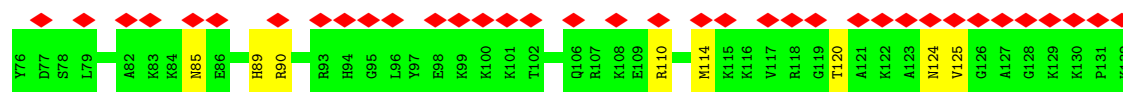


• Molecule 29: 40S ribosomal protein S15a

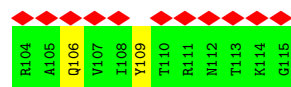
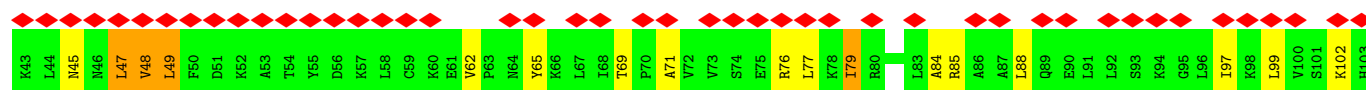
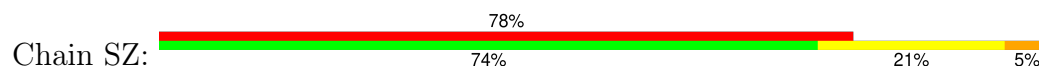


• Molecule 30: 40S ribosomal protein S24

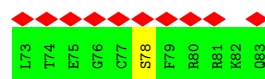
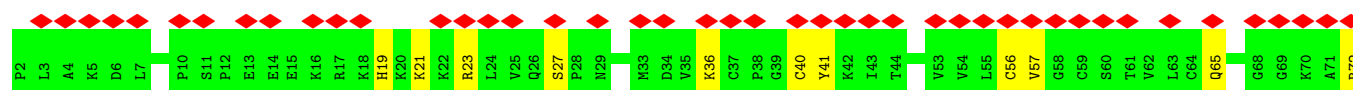
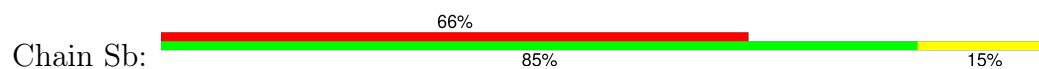




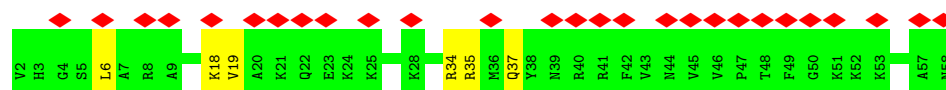
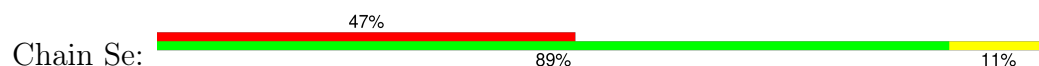
- Molecule 31: 40S ribosomal protein S25



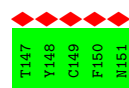
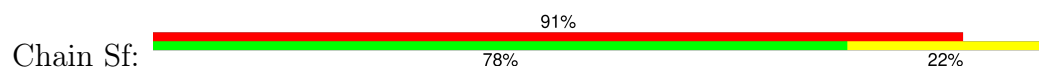
- Molecule 32: 40S ribosomal protein S27



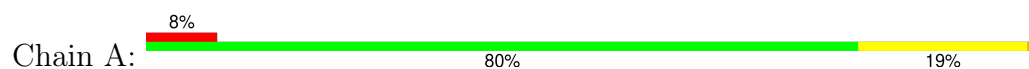
- Molecule 33: 40S ribosomal protein S30

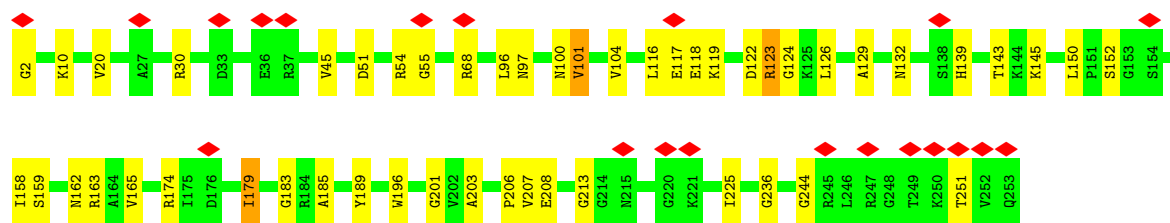


- Molecule 34: 40S ribosomal protein S27a

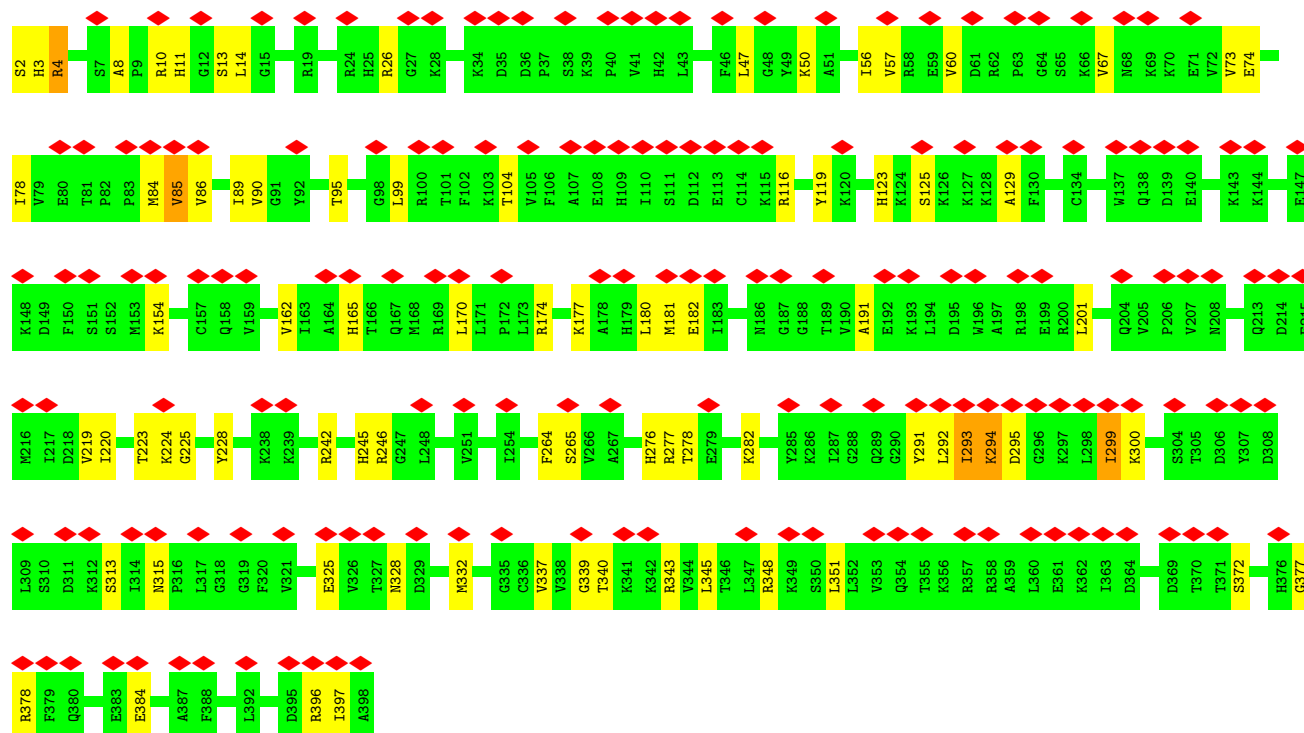
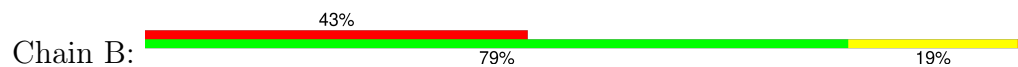


- Molecule 35: 60S ribosomal protein L8

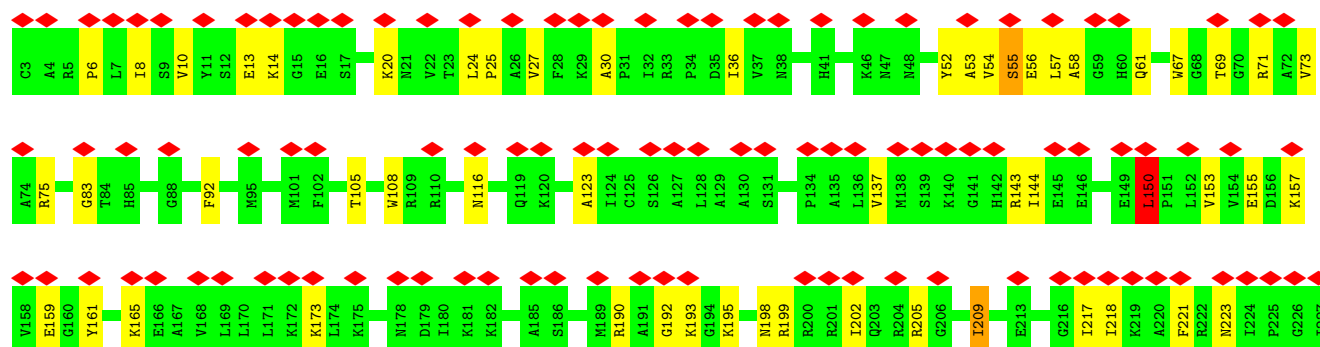
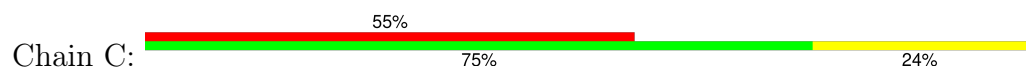


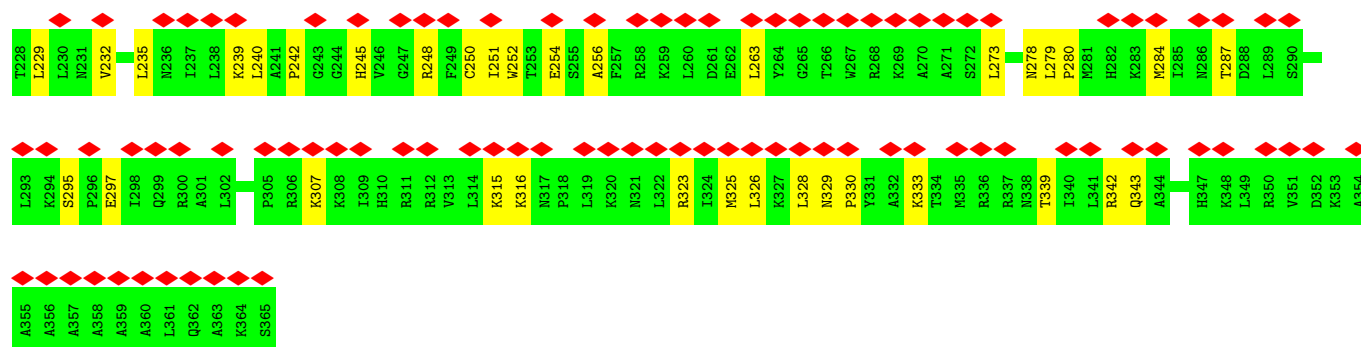


• Molecule 36: 60S ribosomal protein L3

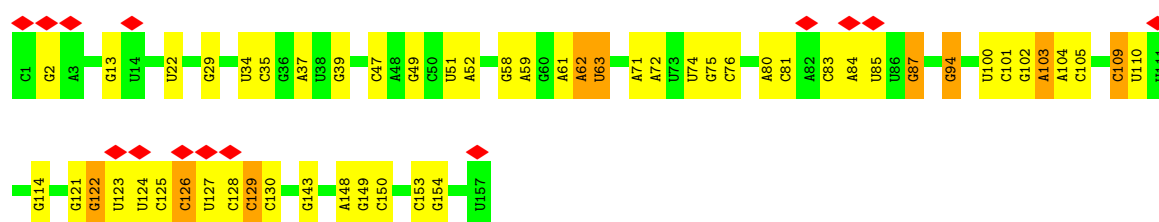


• Molecule 37: 60S ribosomal protein L4

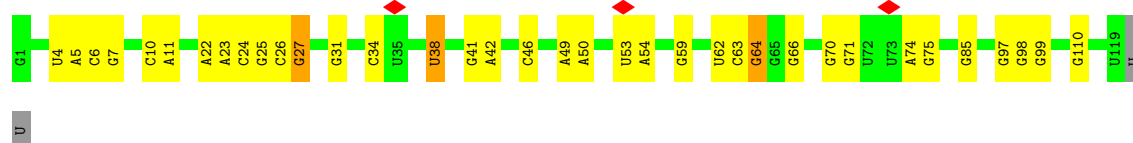




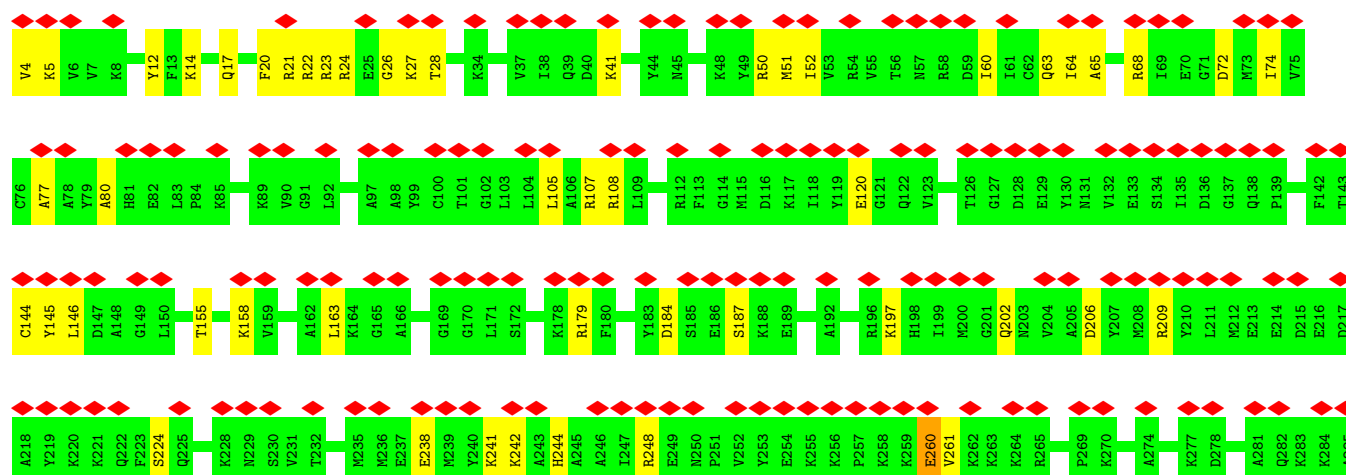
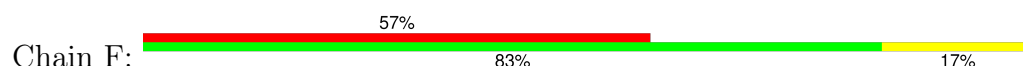
• Molecule 38: 5.8S ribosomal RNA

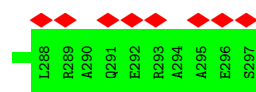


• Molecule 39: 5S ribosomal RNA

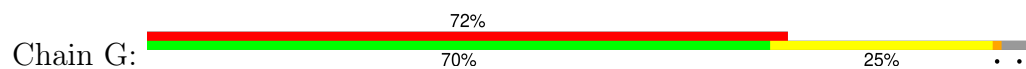


• Molecule 40: 60S ribosomal protein L5

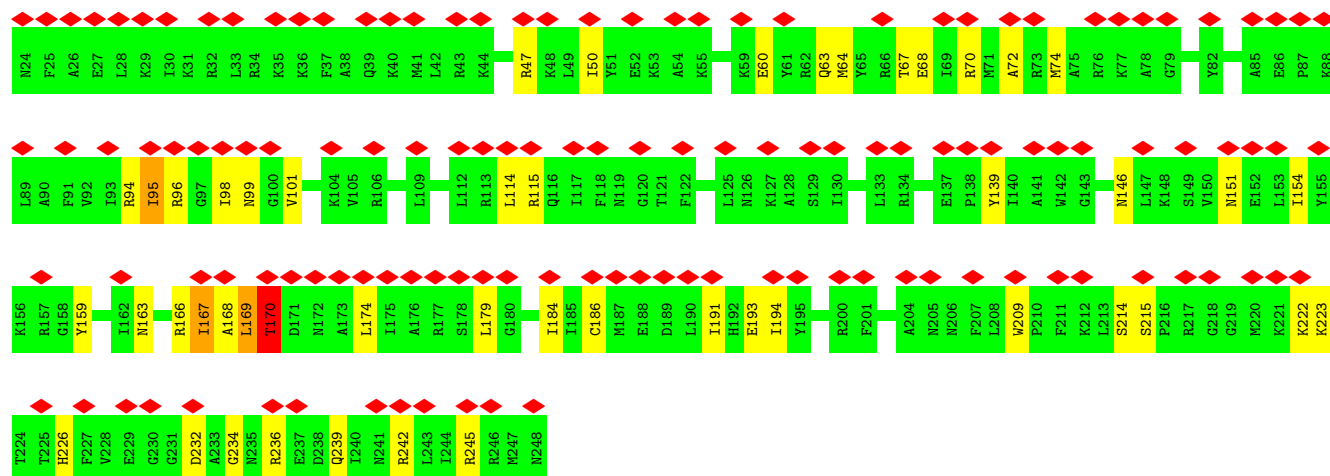
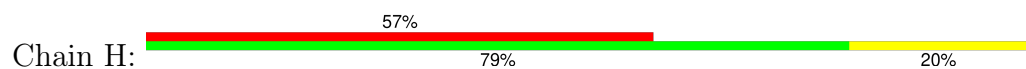




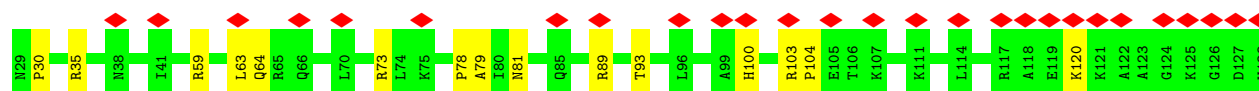
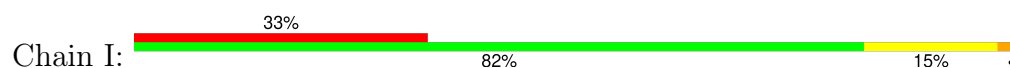
• Molecule 41: 60S ribosomal protein L6

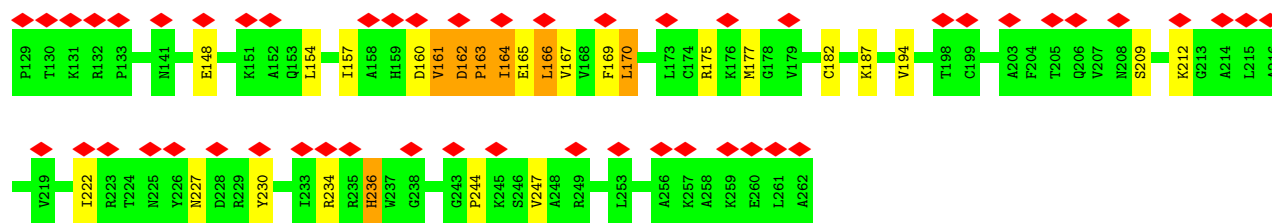


• Molecule 42: 60S ribosomal protein L7

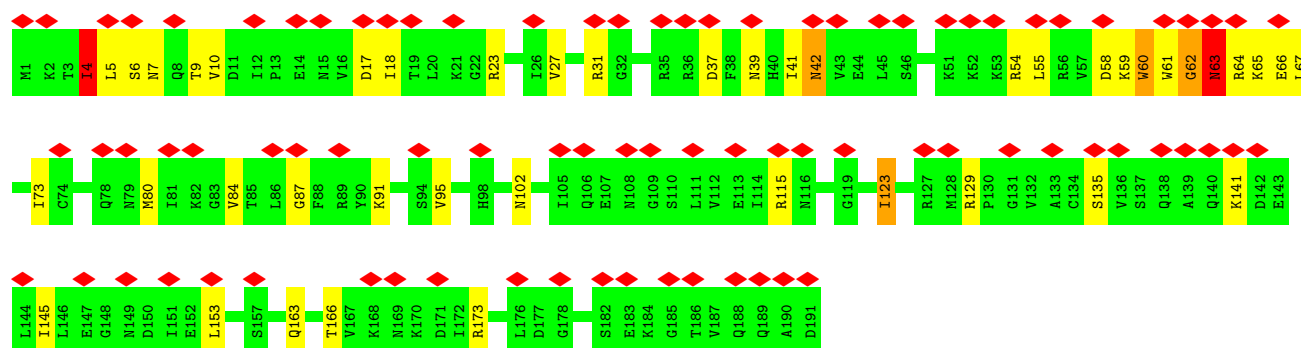
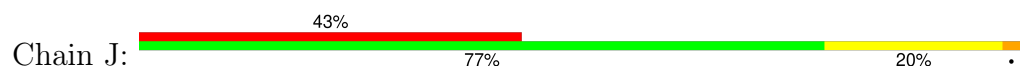


• Molecule 43: 60S ribosomal protein L7a

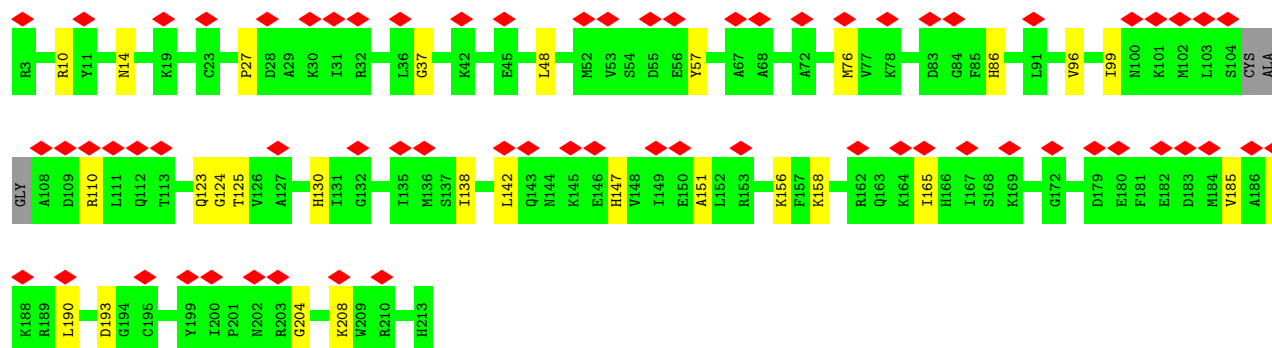
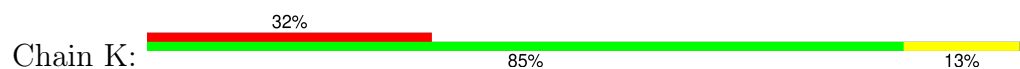




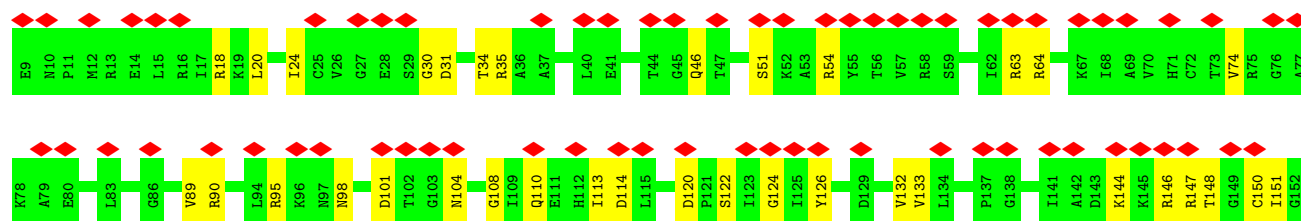
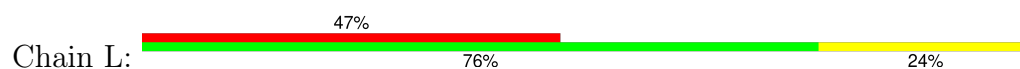
• Molecule 44: 60S ribosomal protein L9

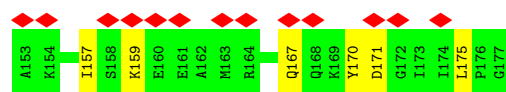


• Molecule 45: 60S ribosomal protein L10

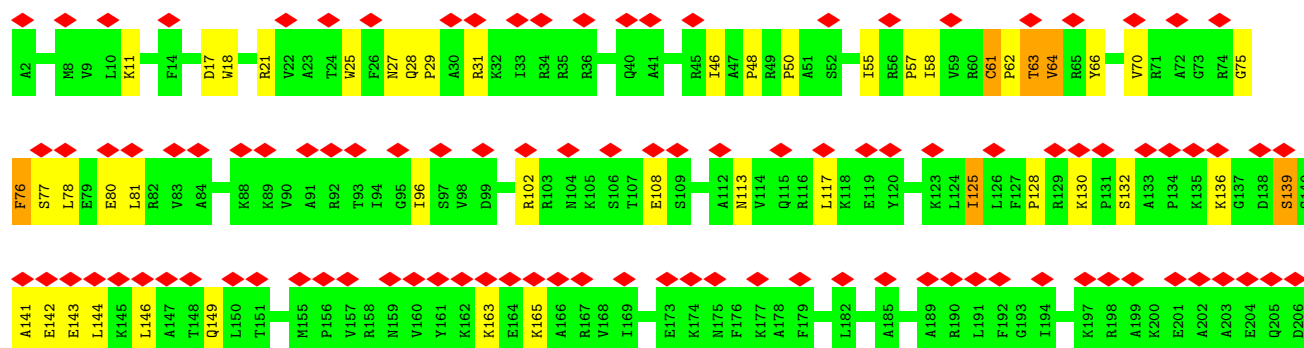
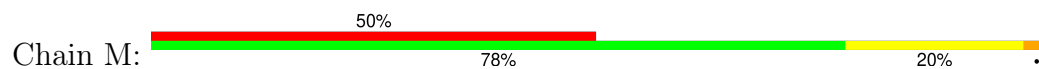


• Molecule 46: 60S ribosomal protein L11

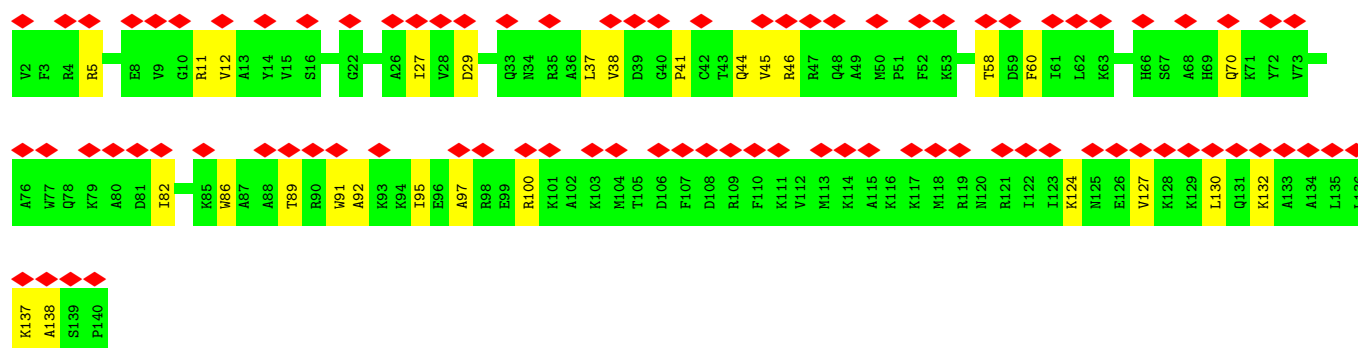
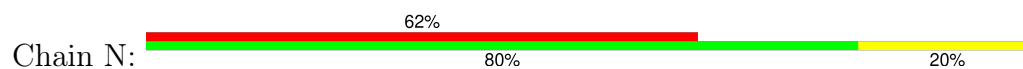




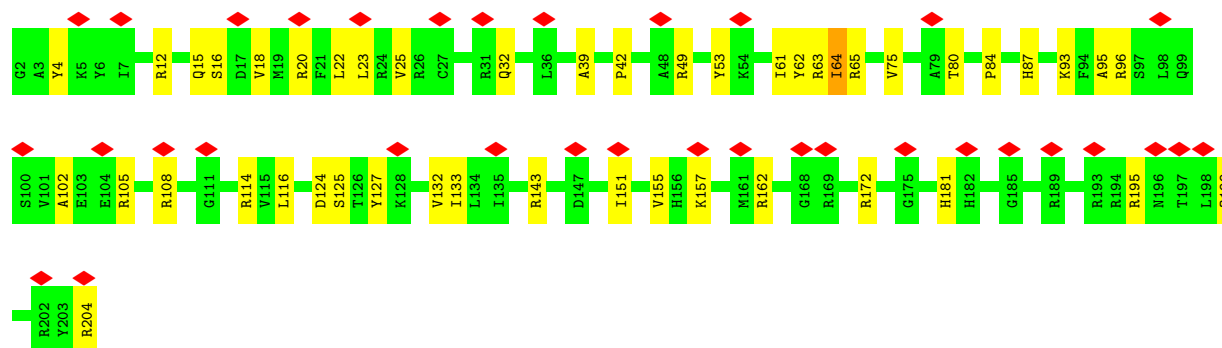
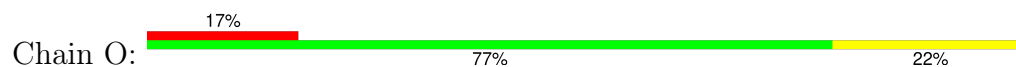
• Molecule 47: 60S ribosomal protein L13



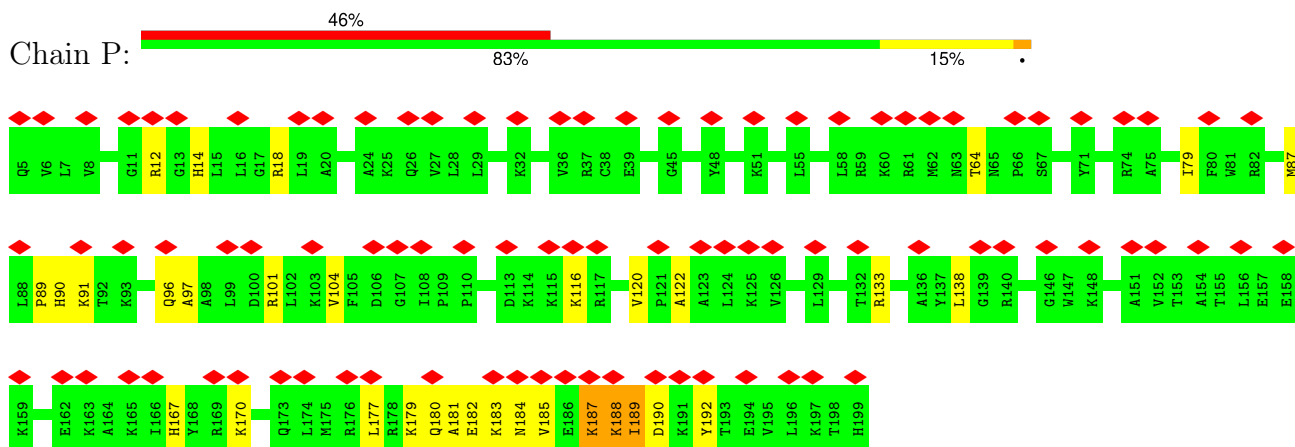
• Molecule 48: 60S ribosomal protein L14



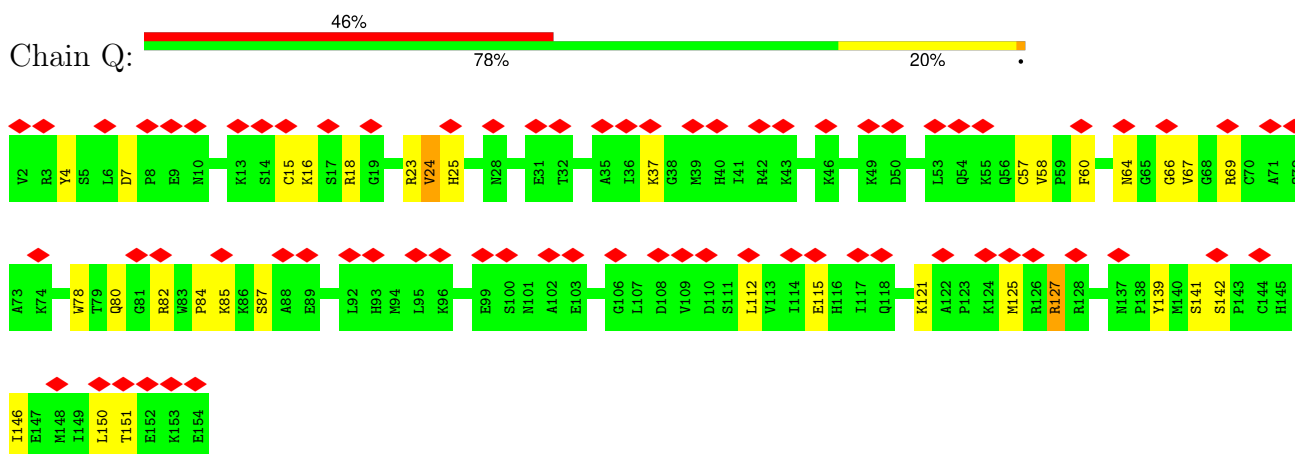
• Molecule 49: 60S ribosomal protein L15



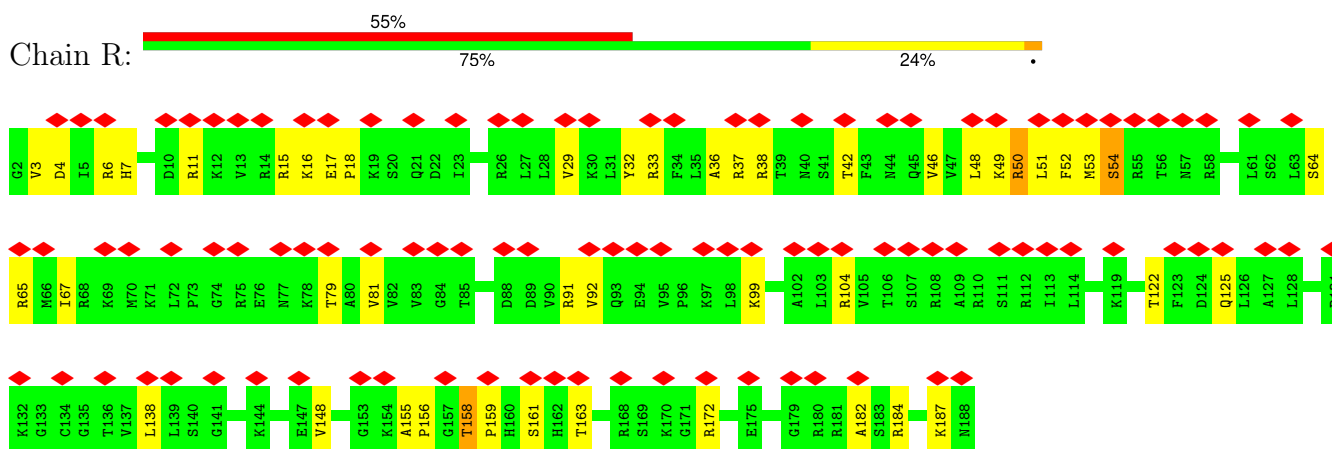
• Molecule 50: 60S ribosomal protein L13a



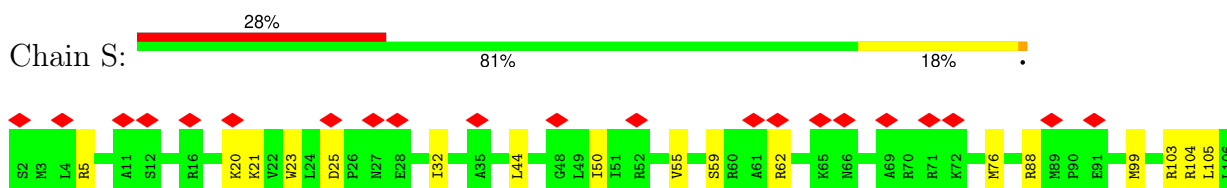
• Molecule 51: 60S ribosomal protein L17

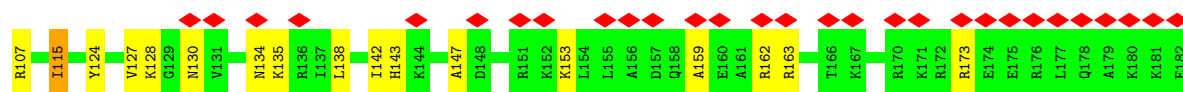


• Molecule 52: 60S ribosomal protein L18



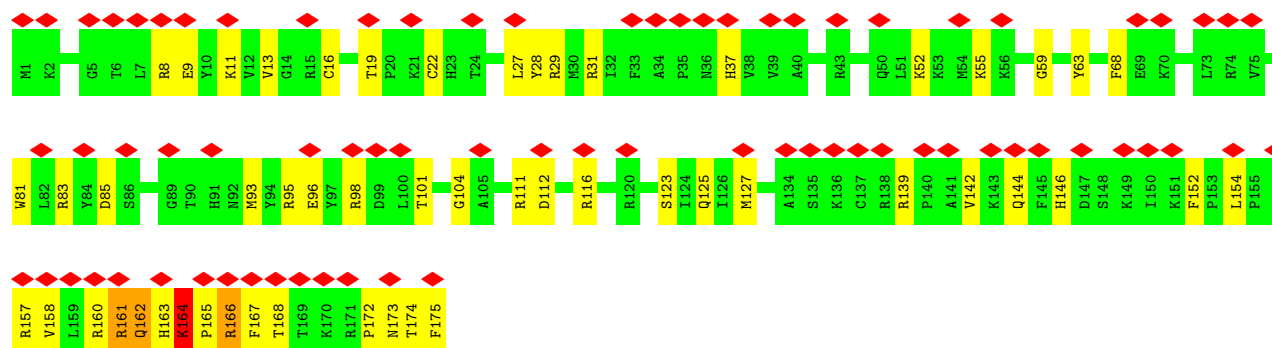
• Molecule 53: 60S ribosomal protein L19





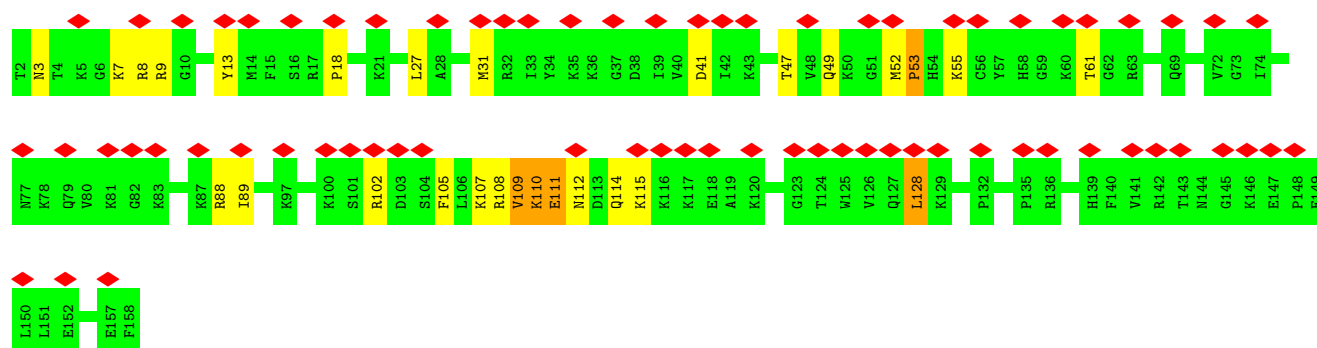
- Molecule 54: 60S ribosomal protein L18a

Chain T: 42% 70% 28%



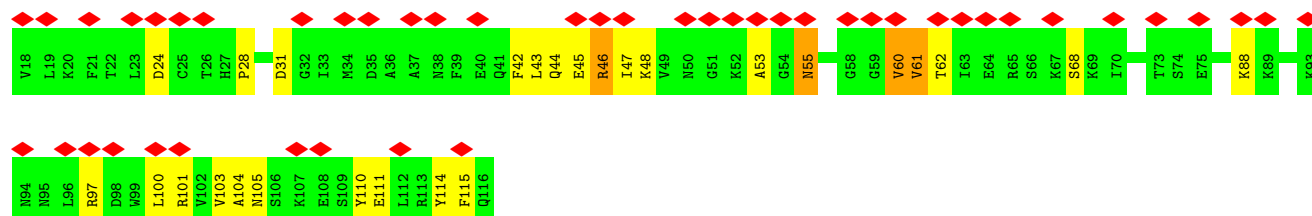
- Molecule 55: 60S ribosomal protein L21

Chain U: 45% 82% 15%



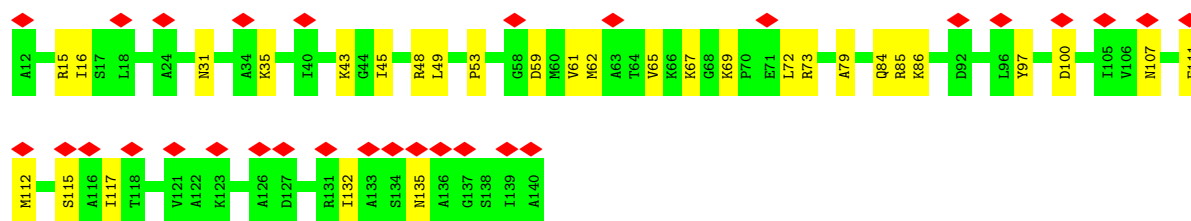
- Molecule 56: 60S ribosomal protein L22

Chain V: 46% 73% 23%

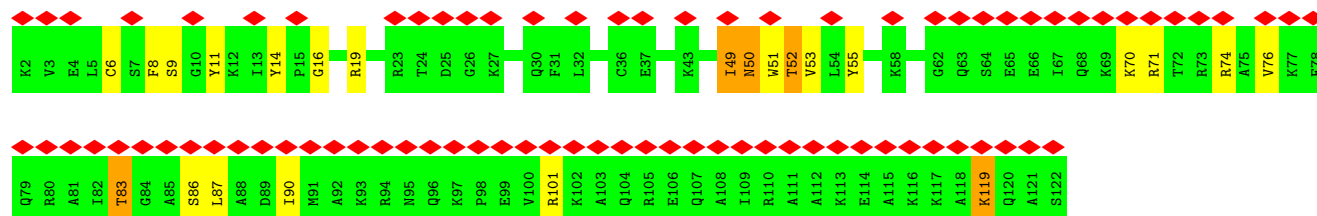
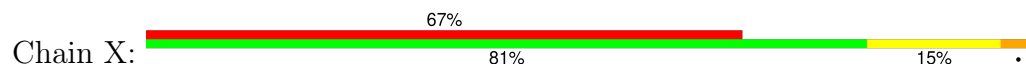


- Molecule 57: 60S ribosomal protein L23

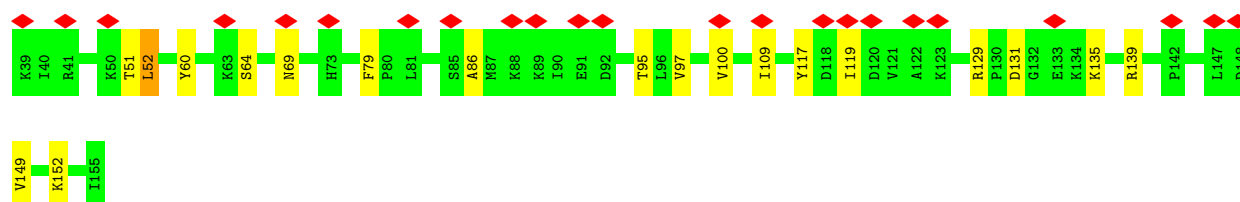
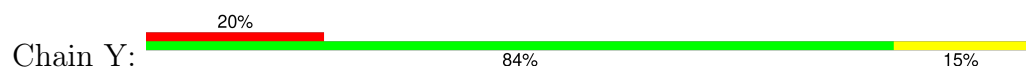
Chain W: 23% 77% 23%



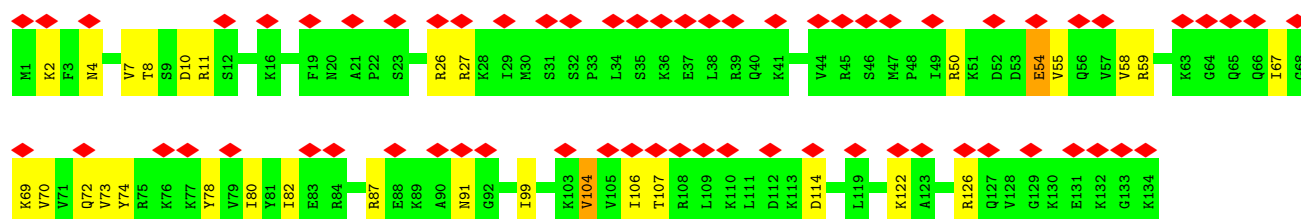
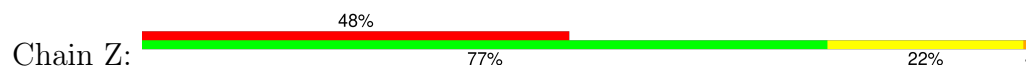
• Molecule 58: 60S ribosomal protein L24



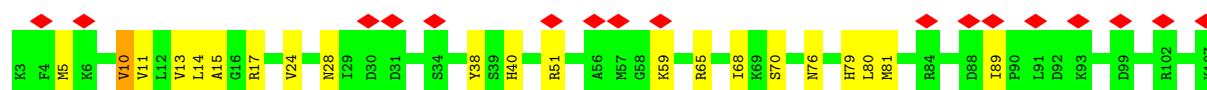
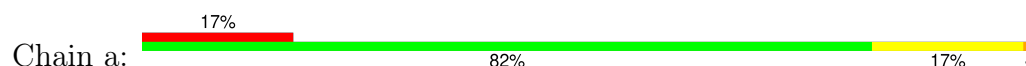
• Molecule 59: 60S ribosomal protein L23a

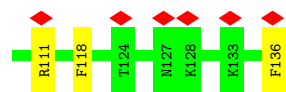


• Molecule 60: 60S ribosomal protein L26

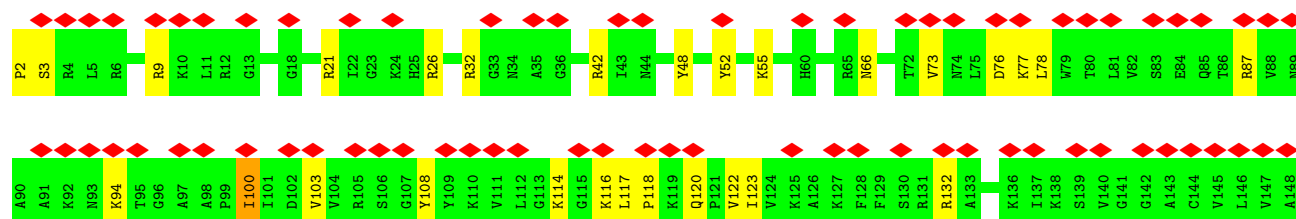
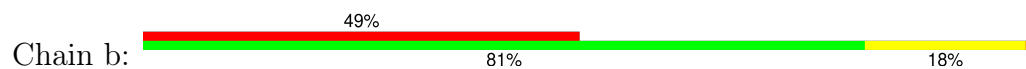


• Molecule 61: 60S ribosomal protein L27

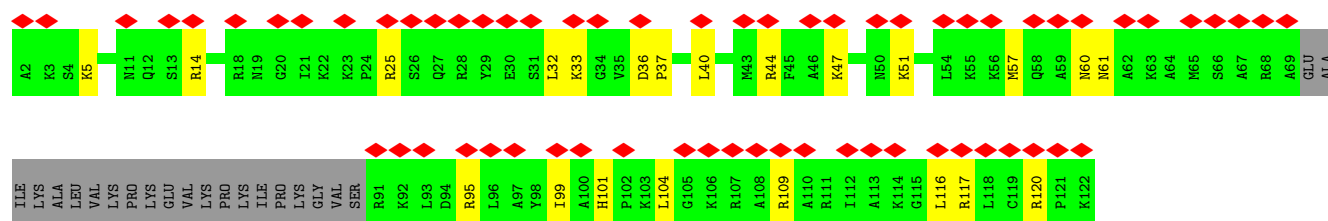




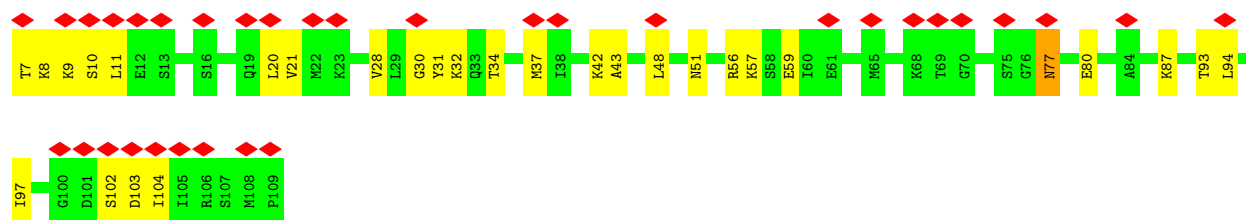
- Molecule 62: 60S ribosomal protein L27a



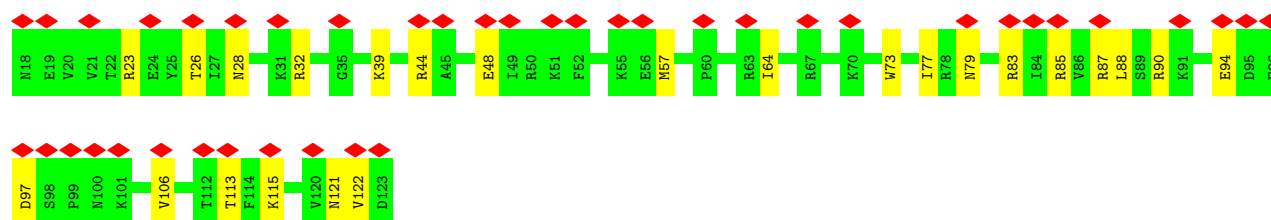
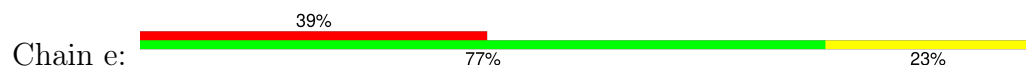
- Molecule 63: 60S ribosomal protein L29



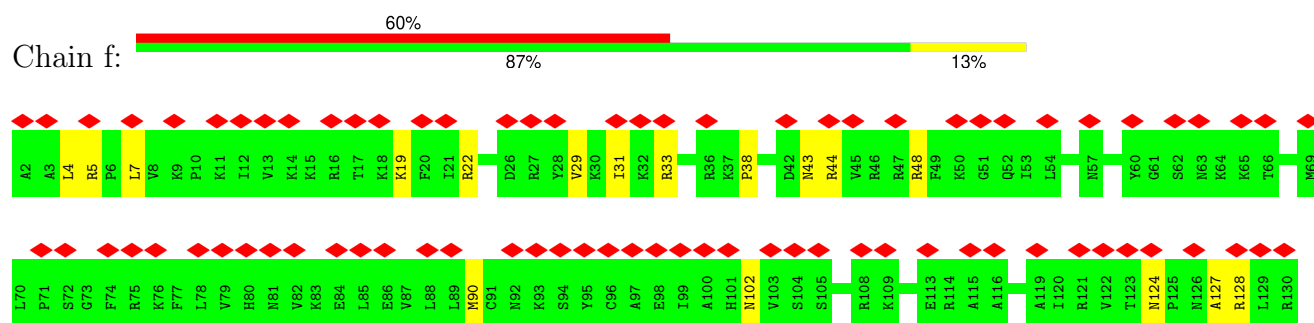
- Molecule 64: 60S ribosomal protein L30



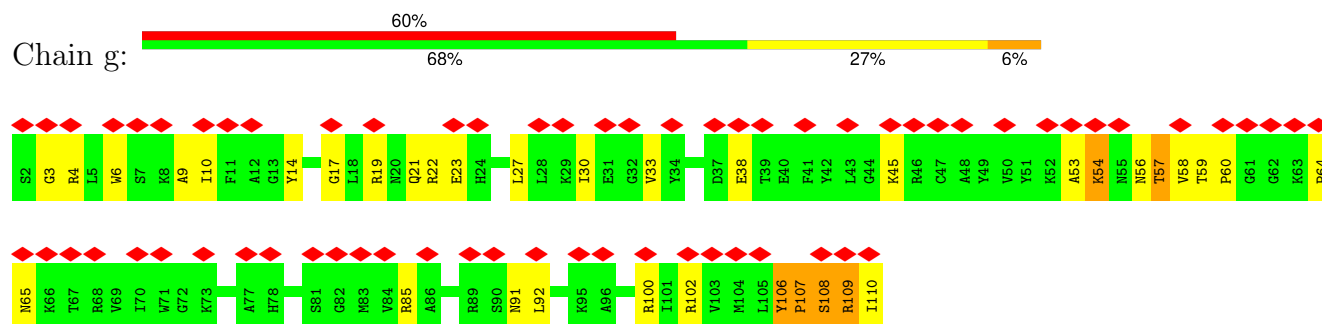
- Molecule 65: 60S ribosomal protein L31



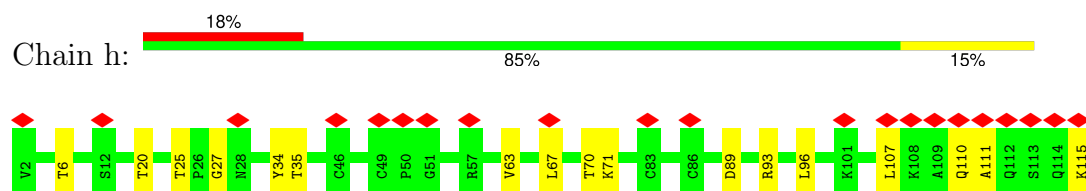
- Molecule 66: 60S ribosomal protein L32



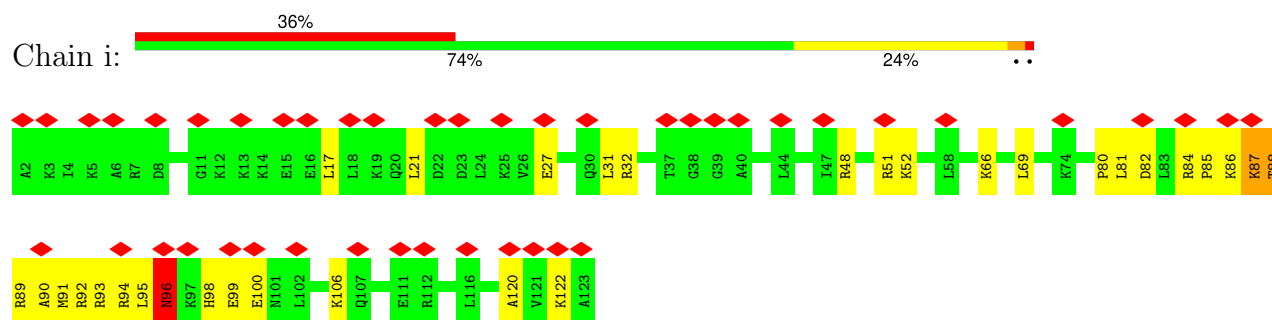
• Molecule 67: 60S ribosomal protein L35a



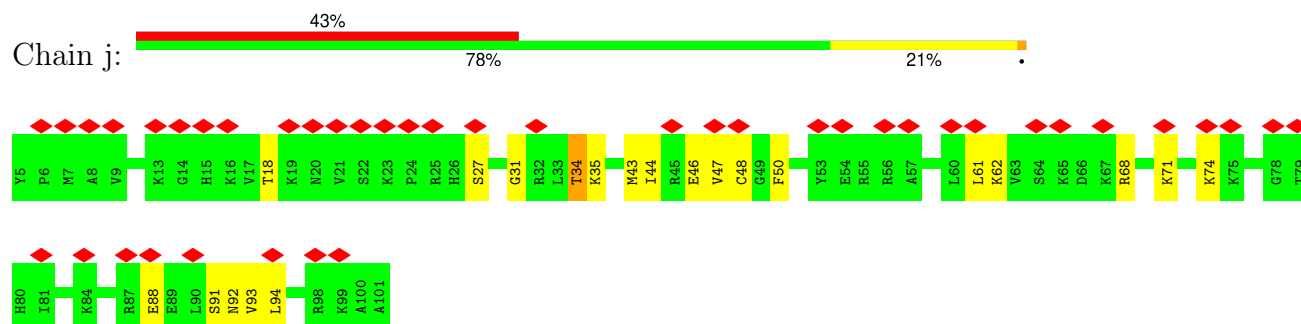
• Molecule 68: 60S ribosomal protein L34



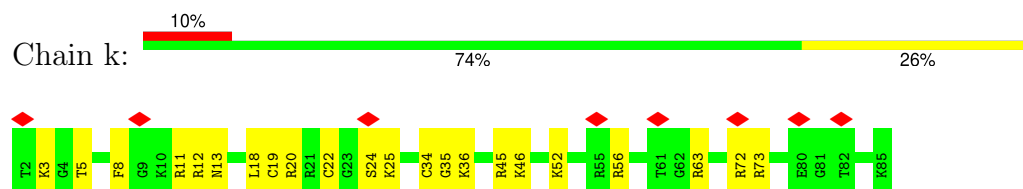
• Molecule 69: 60S ribosomal protein L35



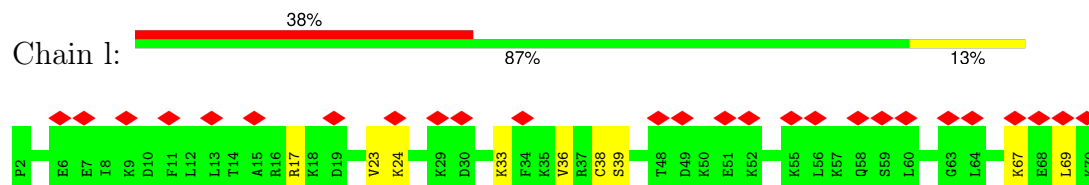
• Molecule 70: 60S ribosomal protein L36



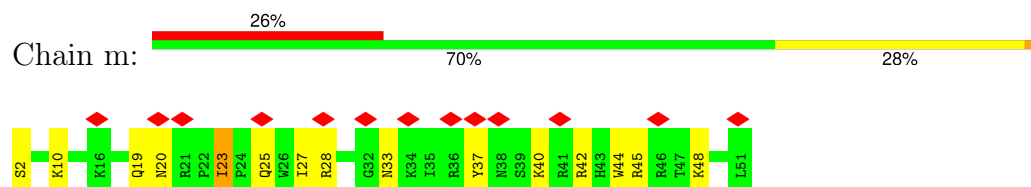
- Molecule 71: 60S ribosomal protein L37



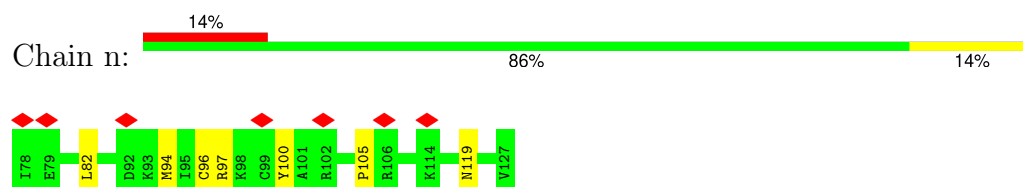
- Molecule 72: 60S ribosomal protein L38



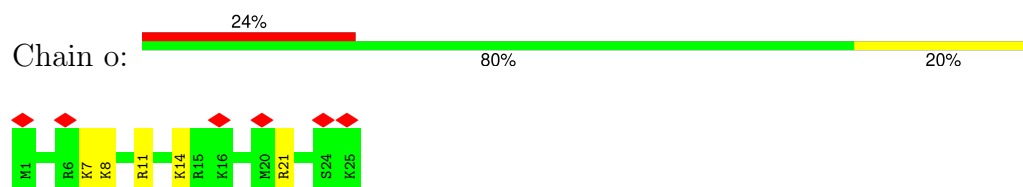
- Molecule 73: 60S ribosomal protein L39



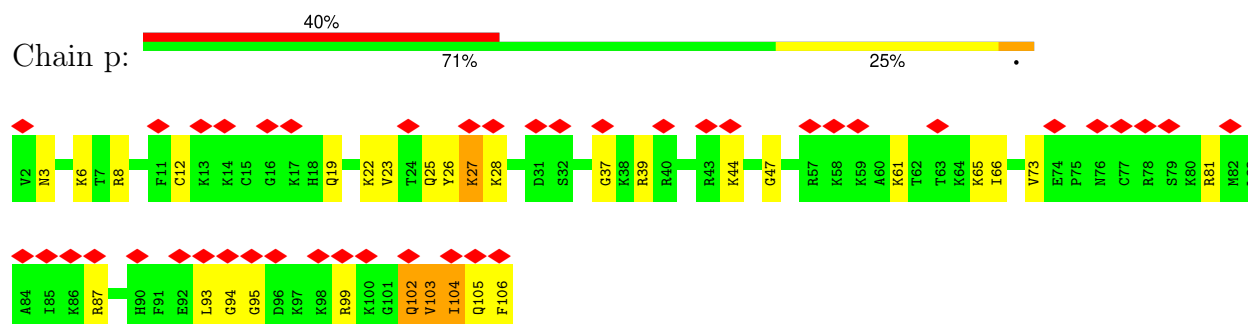
- Molecule 74: 60S ribosomal protein L40



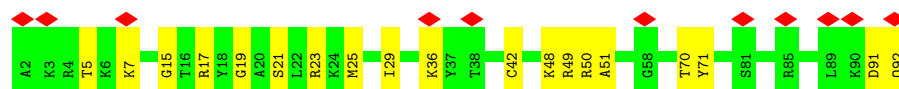
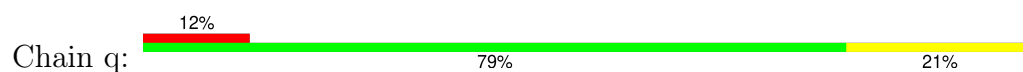
- Molecule 75: 60S ribosomal protein L41



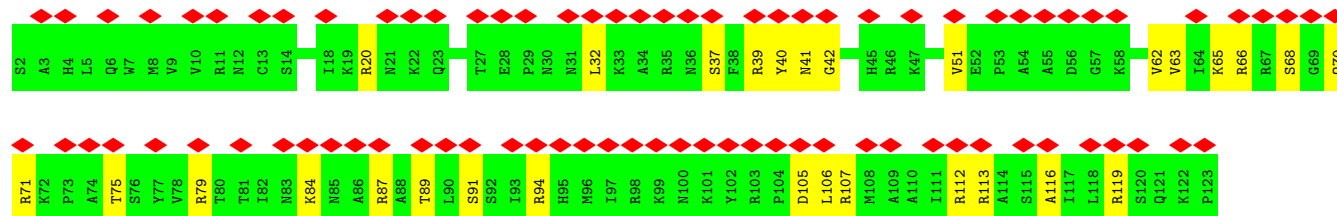
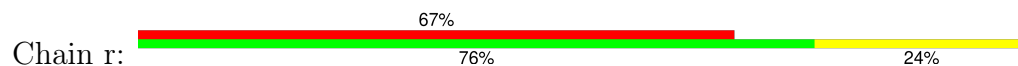
- Molecule 76: 60S ribosomal protein L36a



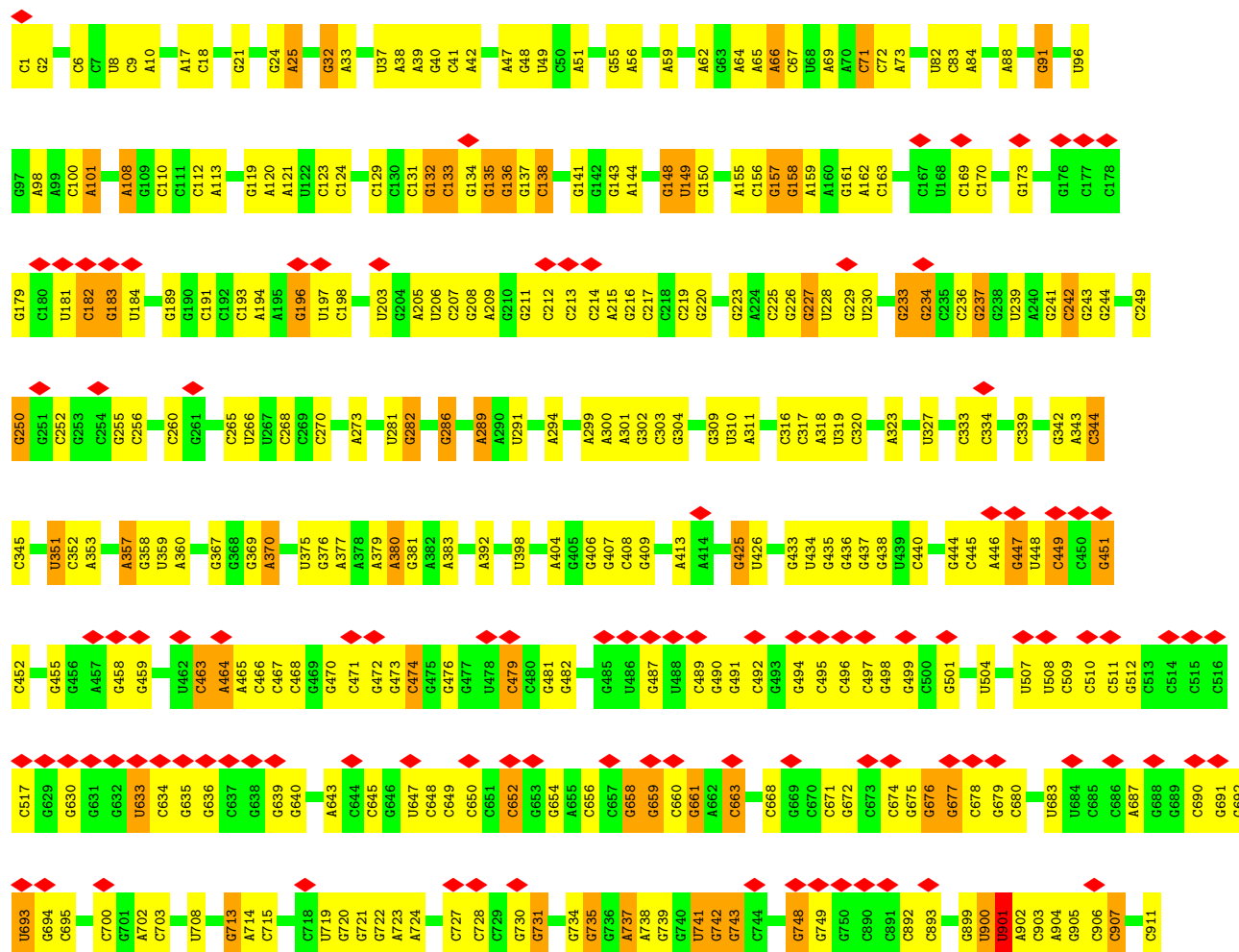
- Molecule 77: 60S ribosomal protein L37a

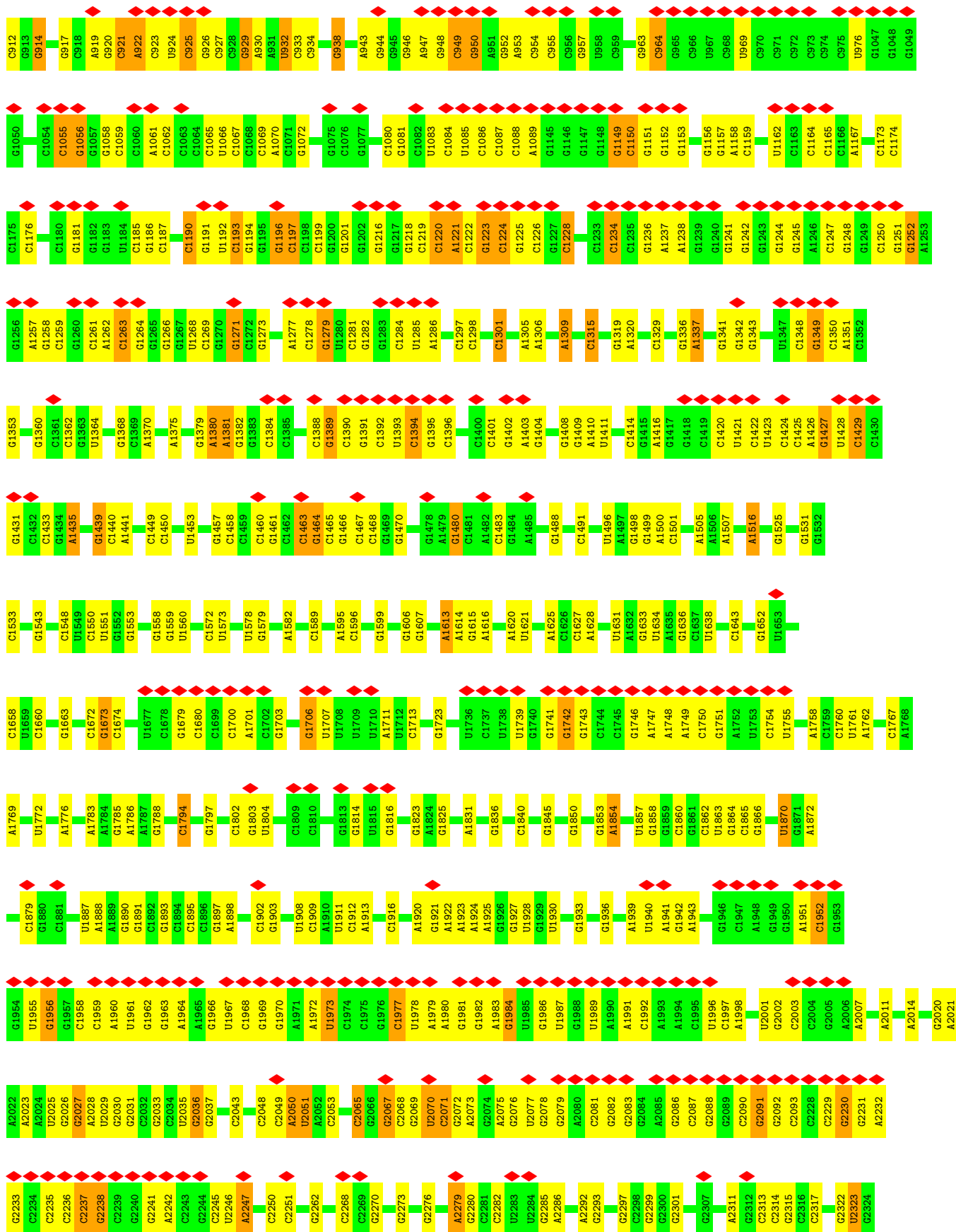


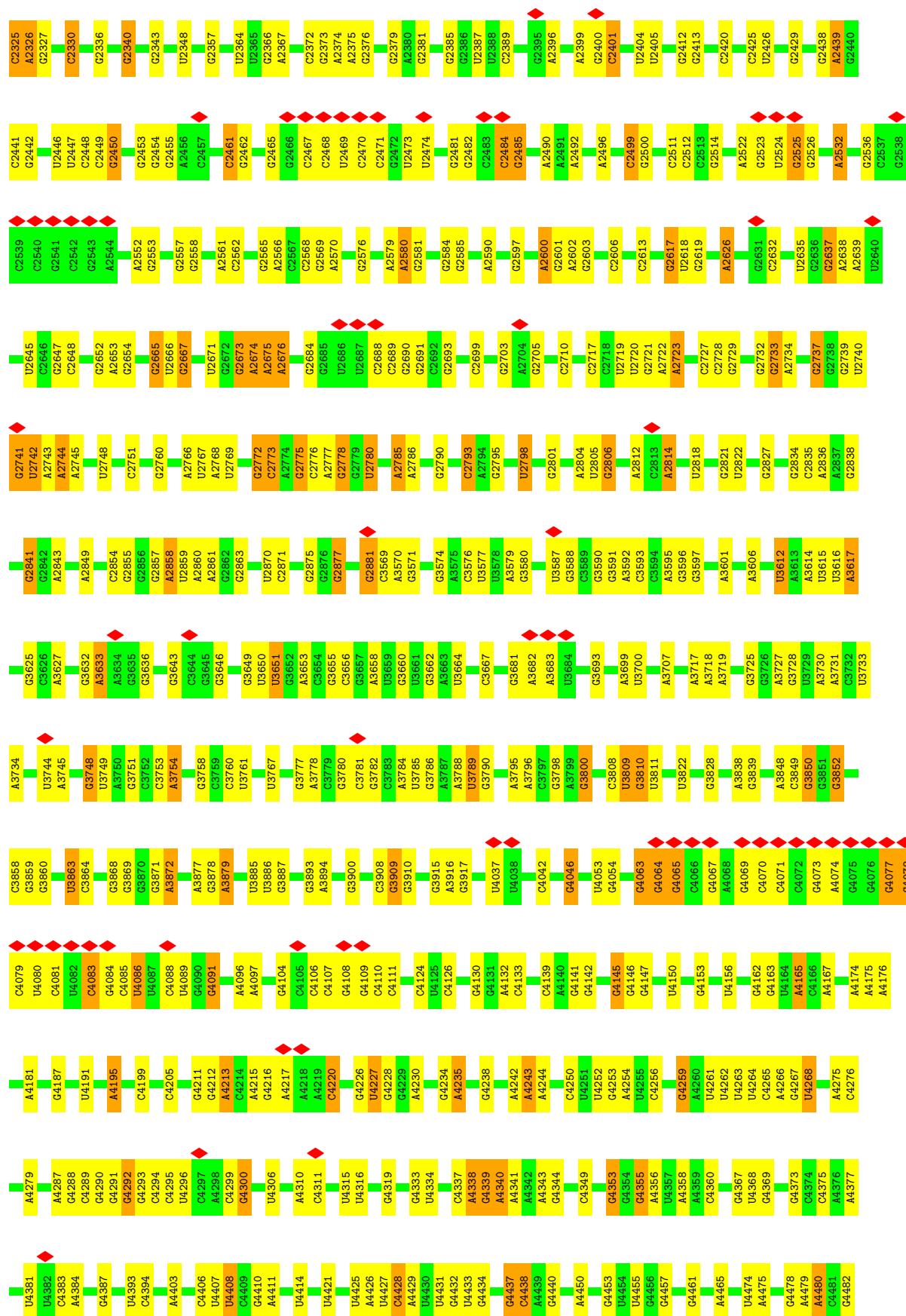
• Molecule 78: 60S ribosomal protein L28

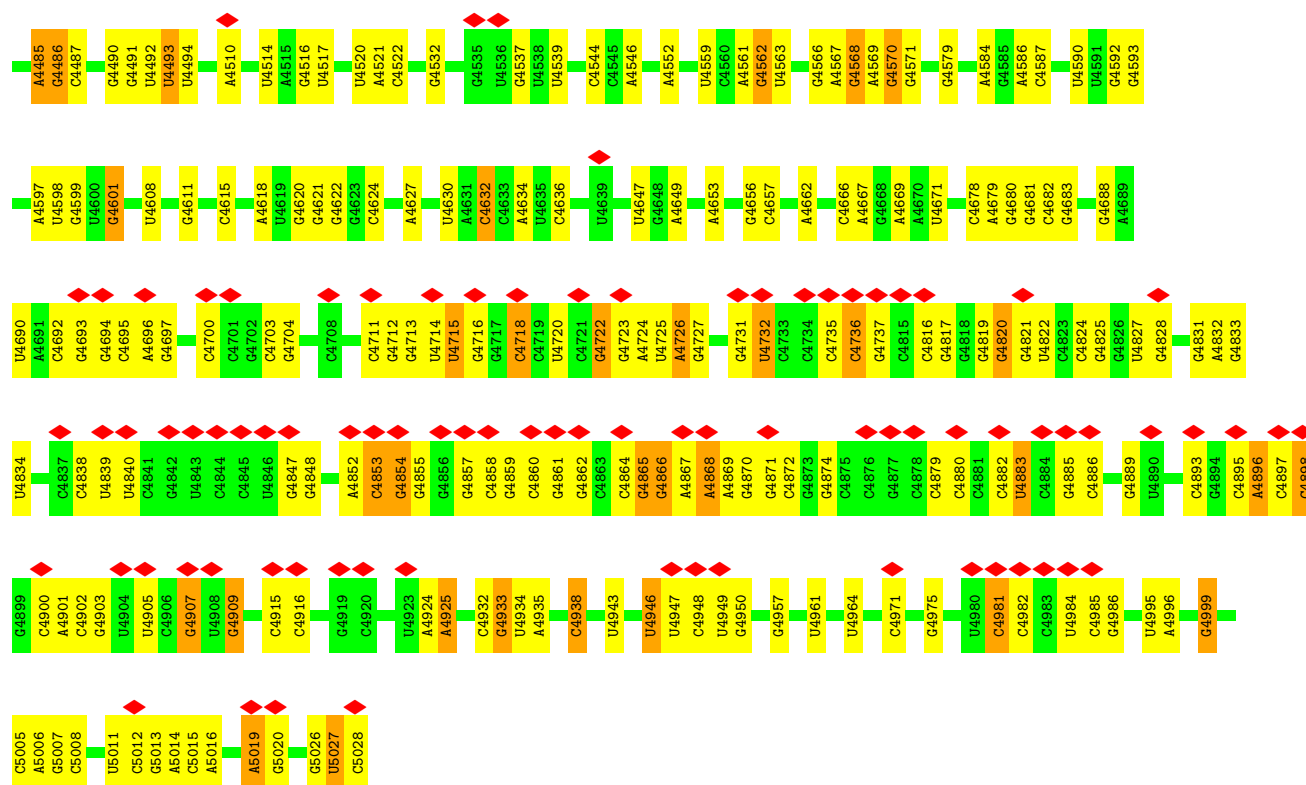


• Molecule 79: 28S ribosomal RNA

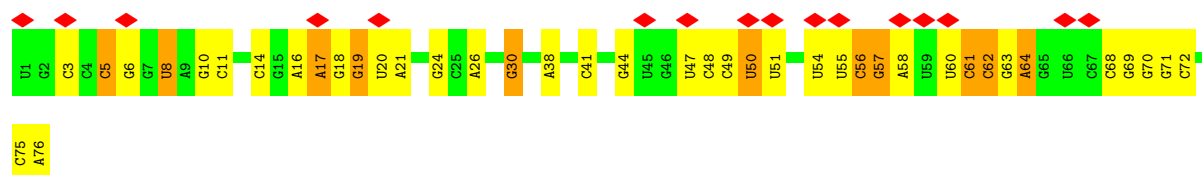








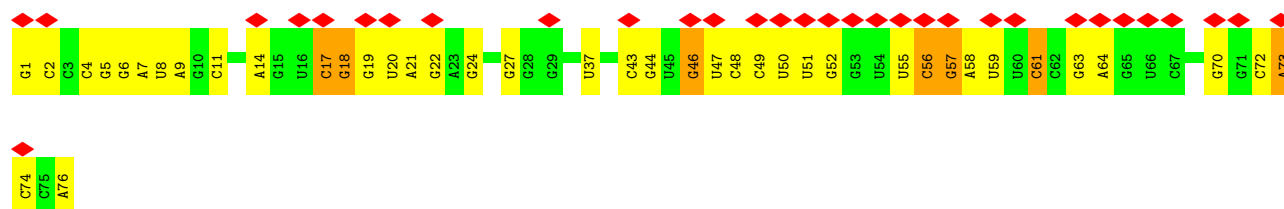
• Molecule 80: P/E site tRNA



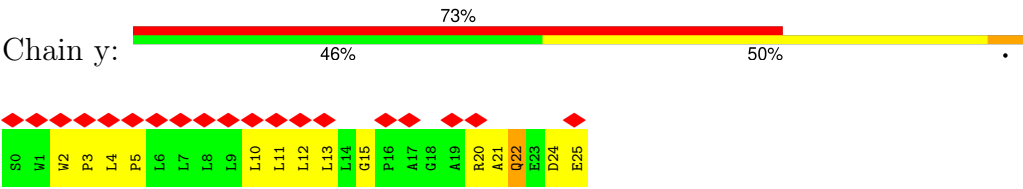
• Molecule 81: mRNA



• Molecule 82: A/A site tRNA



● Molecule 83: Proprotein convertase subtilisin/kexin type 9



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	9564	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.113	Depositor
Minimum map value	-0.062	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.022	Depositor
Map size ($\text{\AA}$)	524.60004, 524.60004, 524.60004	wwPDB
Map dimensions	430, 430, 430	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.22, 1.22, 1.22	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: E3C, OMG, OMU, B8Q, PSU, 5MU, ZN, 6MZ, MG, UR3, MA6, MVM, B8N, 5MC, OMC, 4AC, M7A, A2M

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	S2	0.42	8/39949 (0.0%)	0.48	9/62213 (0.0%)
2	SA	0.39	0/1778	0.77	5/2416 (0.2%)
3	SB	0.35	0/1765	0.61	0/2362
4	SD	0.35	0/1785	0.75	2/2404 (0.1%)
5	SE	0.33	0/2099	0.67	1/2822 (0.0%)
6	SF	0.43	0/1514	0.89	7/2031 (0.3%)
7	SH	0.33	0/1518	0.72	0/2029
8	SI	0.34	0/1702	0.70	0/2271
9	SK	0.32	0/851	0.73	2/1147 (0.2%)
10	SL	0.36	0/1266	0.63	0/1690
11	SP	0.32	0/1065	0.65	0/1423
12	SQ	0.34	0/1177	0.81	0/1575
13	SR	0.33	0/1097	0.78	0/1474
14	SS	0.30	0/1216	0.66	0/1628
15	ST	0.31	0/1131	0.68	0/1515
16	SU	0.33	0/831	0.75	0/1115
17	SV	0.36	0/631	0.69	0/844
18	SX	0.38	0/1116	0.79	4/1490 (0.3%)
19	Sa	0.41	0/836	0.70	0/1121
20	Sc	0.36	0/508	0.91	1/680 (0.1%)
21	Sd	0.36	0/470	0.85	0/623
22	Sg	0.31	0/2486	0.74	2/3384 (0.1%)
23	SC	0.38	0/1753	0.75	1/2365 (0.0%)
24	SG	0.29	0/1946	0.69	0/2590
25	SJ	0.49	1/1561 (0.1%)	0.84	1/2083 (0.0%)
26	SM	0.27	0/922	0.69	0/1238
27	SN	0.35	0/1232	0.60	0/1656
28	SO	0.34	0/1037	0.70	0/1391
29	SW	0.41	0/1051	0.69	0/1406
30	SY	0.32	0/1094	0.64	0/1452
31	SZ	0.64	1/585 (0.2%)	1.14	5/785 (0.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Sb	0.31	0/653	0.60	0/876
33	Se	0.30	0/458	0.73	0/604
34	Sf	0.29	0/560	0.81	0/745
35	A	0.46	0/1968	0.73	2/2639 (0.1%)
36	B	0.42	0/3270	0.79	4/4377 (0.1%)
37	C	0.46	0/2942	0.73	3/3951 (0.1%)
38	D	0.40	0/3726	0.44	0/5804
39	E	0.37	0/2839	0.41	0/4425
40	F	0.38	0/2437	0.71	0/3262
41	G	0.37	0/1942	0.80	2/2606 (0.1%)
42	H	0.47	0/1905	0.81	1/2539 (0.0%)
43	I	0.38	0/1913	0.77	1/2576 (0.0%)
44	J	0.37	0/1545	0.79	8/2077 (0.4%)
45	K	0.37	0/1730	0.67	1/2311 (0.0%)
46	L	0.33	0/1376	0.70	2/1841 (0.1%)
47	M	0.43	0/1688	0.93	5/2260 (0.2%)
48	N	0.38	0/1161	0.66	1/1554 (0.1%)
49	O	0.46	0/1746	0.73	0/2338
50	P	0.44	0/1638	0.75	2/2191 (0.1%)
51	Q	0.44	0/1268	0.66	0/1701
52	R	0.45	0/1537	0.83	6/2052 (0.3%)
53	S	0.40	0/1533	0.71	0/2025
54	T	0.44	0/1488	0.71	1/1997 (0.1%)
55	U	0.40	0/1312	0.73	0/1753
56	V	0.36	0/822	0.76	1/1103 (0.1%)
57	W	0.40	0/983	0.60	0/1319
58	X	3.42	1/1004 (0.1%)	0.80	3/1332 (0.2%)
59	Y	0.37	0/975	0.69	0/1312
60	Z	0.41	0/1132	0.70	0/1504
61	a	0.37	0/1126	0.70	0/1502
62	b	0.47	0/1191	0.76	0/1591
63	c	0.36	0/826	0.74	0/1088
64	d	0.39	0/812	0.72	1/1089 (0.1%)
65	e	0.43	0/894	0.76	2/1204 (0.2%)
66	f	0.45	0/1082	0.75	0/1443
67	g	0.49	0/895	0.96	8/1198 (0.7%)
68	h	0.44	0/916	0.82	3/1220 (0.2%)
69	i	0.37	0/1023	0.80	1/1351 (0.1%)
70	j	0.34	0/805	0.73	0/1065
71	k	0.46	0/703	0.69	0/929
72	l	0.34	0/575	0.66	0/761
73	m	0.43	0/454	0.71	0/599
74	n	0.37	0/417	0.76	0/553

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	o	0.44	0/241	0.82	0/305
76	p	0.41	0/877	0.82	2/1156 (0.2%)
77	q	0.42	0/718	0.80	4/953 (0.4%)
78	r	0.48	0/995	0.85	3/1334 (0.2%)
79	t	0.39	0/86502	0.46	2/134927 (0.0%)
80	v	0.30	0/1802	0.52	2/2797 (0.1%)
81	w	0.35	0/235	0.58	0/365
82	u	0.27	0/1800	0.50	0/2804
83	y	0.35	0/127	1.74	4/175 (2.3%)
All	All	0.45	11/230539 (0.0%)	0.59	115/338706 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
9	SK	0	1
30	SY	0	1
47	M	0	2
58	X	0	1
64	d	0	1
All	All	0	6

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	X	119	LYS	CD-CE	107.68	4.75	1.52
1	S2	325	C	N1-C2	19.50	1.79	1.40
1	S2	325	C	C2-N3	18.64	1.73	1.35
1	S2	325	C	N3-C4	17.83	1.69	1.33
1	S2	325	C	N1-C6	17.07	1.71	1.37
1	S2	325	C	C4-C5	14.79	1.72	1.43
1	S2	325	C	C5-C6	13.51	1.61	1.34
25	SJ	66	LYS	C-N	10.79	1.48	1.33
31	SZ	47	LEU	CG-CD1	7.05	1.75	1.52
1	S2	484	A2M	O3'-P	5.48	1.61	1.56
1	S2	1678	A2M	O3'-P	5.17	1.61	1.56

All (115) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
83	y	4	LEU	CA-C-N	11.95	134.78	119.84
83	y	4	LEU	C-N-CA	11.95	134.78	119.84
67	g	54	LYS	N-CA-C	11.90	124.26	111.28
47	M	61	CYS	CA-C-N	11.13	131.40	119.05
47	M	61	CYS	C-N-CA	11.13	131.40	119.05
68	h	70	THR	N-CA-C	-10.53	102.61	114.62
44	J	60	TRP	N-CA-C	10.36	122.16	111.07
1	S2	1351	G	O3'-P-O5'	10.13	119.19	104.00
6	SF	63	LYS	CA-CB-CG	10.13	134.35	114.10
67	g	106	TYR	CA-C-N	-9.93	107.43	119.84
67	g	106	TYR	C-N-CA	-9.93	107.43	119.84
50	P	189	ILE	N-CA-C	9.41	120.22	110.62
47	M	64	VAL	N-CA-C	-9.14	101.30	110.62
50	P	188	LYS	N-CA-C	8.95	121.12	111.36
76	p	103	VAL	N-CA-C	-8.23	99.01	109.30
31	SZ	77	LEU	CB-CG-CD1	7.55	133.34	110.70
47	M	61	CYS	N-CA-C	7.45	119.10	109.64
1	S2	1350	U	O3'-P-O5'	7.40	115.10	104.00
47	M	76	PHE	N-CA-C	-7.38	97.96	109.25
76	p	102	GLN	N-CA-C	7.35	120.88	110.23
6	SF	133	THR	N-CA-C	-7.29	100.29	110.35
31	SZ	77	LEU	CB-CG-CD2	-7.27	88.90	110.70
56	V	60	VAL	N-CA-C	7.24	118.01	110.62
58	X	50	ASN	N-CA-C	7.13	119.05	111.28
1	S2	1352	G	O5'-P-OP1	-6.97	87.09	108.00
42	H	170	THR	N-CA-C	6.96	125.63	110.80
1	S2	1350	U	P-O3'-C3'	6.83	130.45	120.20
36	B	294	LYS	CA-C-N	6.66	134.27	121.54
36	B	294	LYS	C-N-CA	6.66	134.27	121.54
58	X	49	ILE	N-CA-C	-6.65	97.94	107.98
22	Sg	93	THR	CA-C-N	6.61	134.17	121.54
22	Sg	93	THR	C-N-CA	6.61	134.17	121.54
64	d	80	GLU	N-CA-C	-6.60	107.10	114.62
44	J	62	GLY	N-CA-C	6.45	118.91	111.36
1	S2	1349	G	P-O3'-C3'	6.36	129.74	120.20
44	J	63	ASN	CA-C-N	-6.31	109.48	121.54
44	J	63	ASN	C-N-CA	-6.31	109.48	121.54
44	J	7	ASN	N-CA-C	6.29	118.86	108.99
83	y	15	GLY	CA-C-N	6.21	127.60	119.84
83	y	15	GLY	C-N-CA	6.21	127.60	119.84
52	R	54	SER	N-CA-C	6.15	118.42	109.07
44	J	4	ILE	N-CA-C	6.12	116.30	110.42
2	SA	28	THR	N-CA-C	6.12	117.95	111.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	Sc	30	VAL	N-CA-C	6.10	122.35	113.39
54	T	27	LEU	CA-CB-CG	6.09	137.62	116.30
77	q	7	LYS	CA-C-N	-6.03	116.77	123.16
77	q	7	LYS	C-N-CA	-6.03	116.77	123.16
6	SF	56	TYR	CA-CB-CG	6.00	124.70	113.90
31	SZ	79	ILE	N-CA-C	5.97	117.19	108.53
67	g	109	ARG	N-CA-C	5.96	117.85	111.36
69	i	86	LYS	N-CA-C	5.96	117.85	111.36
43	I	236	HIS	N-CA-C	5.87	118.73	110.23
5	SE	64	ILE	N-CA-C	-5.86	107.05	113.43
6	SF	61	PHE	N-CA-C	5.83	119.23	111.30
2	SA	139	TYR	CA-CB-CG	-5.77	103.52	113.90
1	S2	1351	G	OP1-P-O3'	-5.75	90.75	108.00
65	e	94	GLU	CA-C-N	5.73	130.96	122.82
65	e	94	GLU	C-N-CA	5.73	130.96	122.82
77	q	91	ASP	CA-C-N	5.72	131.99	121.70
77	q	91	ASP	C-N-CA	5.72	131.99	121.70
1	S2	1351	G	C4'-C3'-C2'	-5.71	96.89	102.60
41	G	233	PHE	CA-C-N	5.69	132.40	121.54
41	G	233	PHE	C-N-CA	5.69	132.40	121.54
79	t	901	U	P-O3'-C3'	5.65	128.68	120.20
1	S2	1351	G	P-O3'-C3'	5.63	128.65	120.20
4	SD	4	GLN	N-CA-C	5.56	118.02	109.07
31	SZ	49	LEU	CA-C-N	5.54	129.56	121.31
31	SZ	49	LEU	C-N-CA	5.54	129.56	121.31
45	K	10	ARG	N-CA-C	-5.52	99.05	110.80
35	A	179	ILE	CA-C-N	5.49	132.02	121.54
35	A	179	ILE	C-N-CA	5.49	132.02	121.54
52	R	158	THR	CA-C-N	5.49	125.75	119.83
52	R	158	THR	C-N-CA	5.49	125.75	119.83
2	SA	140	VAL	CA-C-N	5.43	130.12	122.46
2	SA	140	VAL	C-N-CA	5.43	130.12	122.46
78	r	106	LEU	CA-CB-CG	5.42	135.28	116.30
18	SX	7	LEU	N-CA-C	5.41	117.25	111.36
78	r	20	ARG	CA-C-N	5.37	129.98	122.08
78	r	20	ARG	C-N-CA	5.37	129.98	122.08
80	v	61	C	C2-N1-C1'	5.32	134.77	118.80
67	g	57	THR	CA-CB-CG2	5.26	119.44	110.50
6	SF	61	PHE	CA-C-N	-5.23	113.12	121.44
6	SF	61	PHE	C-N-CA	-5.23	113.12	121.44
52	R	50	ARG	N-CA-C	-5.21	106.93	113.28
58	X	119	LYS	CG-CD-CE	5.20	123.26	111.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	SC	190	SER	N-CA-C	-5.19	106.75	114.64
37	C	150	LEU	CA-C-N	-5.16	113.39	119.84
37	C	150	LEU	C-N-CA	-5.16	113.39	119.84
1	S2	559	G	P-O3'-C3'	5.15	127.92	120.20
52	R	54	SER	CA-C-N	5.15	128.84	120.60
52	R	54	SER	C-N-CA	5.15	128.84	120.60
68	h	27	GLY	CA-C-N	5.14	131.36	121.54
68	h	27	GLY	C-N-CA	5.14	131.36	121.54
36	B	4	ARG	CA-C-N	5.13	131.34	121.54
36	B	4	ARG	C-N-CA	5.13	131.34	121.54
80	v	50	U	P-O3'-C3'	5.13	127.89	120.20
18	SX	105	PHE	N-CA-C	5.12	116.93	108.49
4	SD	6	SER	N-CA-C	5.11	117.71	110.50
37	C	92	PHE	N-CA-C	5.11	116.89	110.24
48	N	132	LYS	N-CA-C	-5.11	108.79	114.62
79	t	4946	U	P-O3'-C3'	5.11	127.87	120.20
67	g	59	THR	N-CA-C	5.10	121.09	109.81
46	L	170	TYR	CA-C-N	5.10	131.29	121.54
46	L	170	TYR	C-N-CA	5.10	131.29	121.54
25	SJ	66	LYS	CA-CB-CG	5.10	124.30	114.10
18	SX	96	GLU	CA-C-N	5.09	131.26	121.54
18	SX	96	GLU	C-N-CA	5.09	131.26	121.54
6	SF	62	ARG	NE-CZ-NH2	5.06	123.75	119.20
9	SK	38	LYS	CA-C-N	5.05	129.58	122.46
9	SK	38	LYS	C-N-CA	5.05	129.58	122.46
67	g	53	ALA	CA-C-N	5.03	127.02	120.28
67	g	53	ALA	C-N-CA	5.03	127.02	120.28
2	SA	25	LEU	N-CA-C	5.03	117.10	108.90
44	J	141	LYS	CA-C-N	5.02	131.12	121.54
44	J	141	LYS	C-N-CA	5.02	131.12	121.54

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
47	M	139	SER	Peptide
47	M	142	GLU	Peptide
9	SK	60	GLU	Peptide
30	SY	2	ASN	Peptide
58	X	90	ILE	Peptide
64	d	87	LYS	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	S2	36501	0	18416	405	0
2	SA	1741	0	1746	41	0
3	SB	1738	0	1809	29	0
4	SD	1757	0	1853	40	0
5	SE	2059	0	2162	36	0
6	SF	1495	0	1547	55	0
7	SH	1497	0	1590	32	0
8	SI	1673	0	1756	26	0
9	SK	827	0	854	13	0
10	SL	1247	0	1321	21	0
11	SP	1045	0	1095	41	0
12	SQ	1158	0	1232	22	0
13	SR	1082	0	1137	17	0
14	SS	1198	0	1261	37	0
15	ST	1112	0	1146	25	0
16	SU	821	0	883	15	0
17	SV	625	0	628	12	0
18	SX	1098	0	1161	64	0
19	Sa	821	0	871	18	0
20	Sc	506	0	536	47	0
21	Sd	459	0	452	38	0
22	Sg	2429	0	2386	48	0
23	SC	1715	0	1802	23	0
24	SG	1923	0	2089	45	0
25	SJ	1533	0	1653	41	0
26	SM	912	0	930	12	0
27	SN	1208	0	1294	10	0
28	SO	1024	0	1050	33	0
29	SW	1034	0	1080	19	0
30	SY	1073	0	1155	20	0
31	SZ	579	0	639	17	0
32	Sb	640	0	665	6	0
33	Se	452	0	498	3	0
34	Sf	548	0	552	12	0
35	A	1930	0	2029	35	0
36	B	3202	0	3343	60	0
37	C	2888	0	3063	80	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	D	3337	0	1692	25	0
39	E	2541	0	1285	14	0
40	F	2392	0	2425	37	0
41	G	1904	0	2055	46	0
42	H	1870	0	1996	42	0
43	I	1880	0	2018	78	0
44	J	1526	0	1605	57	0
45	K	1692	0	1744	16	0
46	L	1353	0	1386	24	0
47	M	1657	0	1764	53	0
48	N	1138	0	1204	16	0
49	O	1701	0	1749	50	0
50	P	1606	0	1743	37	0
51	Q	1242	0	1269	22	0
52	R	1513	0	1628	79	0
53	S	1517	0	1670	28	0
54	T	1449	0	1491	86	0
55	U	1284	0	1352	31	0
56	V	808	0	831	26	0
57	W	969	0	1031	20	0
58	X	989	0	1041	48	0
59	Y	958	0	1029	14	0
60	Z	1115	0	1205	31	0
61	a	1103	0	1179	14	0
62	b	1162	0	1213	27	0
63	c	814	0	880	16	0
64	d	801	0	845	22	0
65	e	879	0	924	15	0
66	f	1064	0	1160	15	0
67	g	876	0	910	65	0
68	h	906	0	1002	10	0
69	i	1015	0	1147	60	0
70	j	794	0	870	22	0
71	k	689	0	717	25	0
72	l	569	0	637	6	0
73	m	444	0	483	20	0
74	n	411	0	443	6	0
75	o	240	0	289	4	0
76	p	863	0	930	36	0
77	q	708	0	757	12	0
78	r	980	0	1041	17	0
79	t	77332	0	39072	633	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
80	v	1618	0	826	14	0
81	w	213	0	109	2	0
82	u	1613	0	821	7	0
83	y	128	0	62	25	0
84	S2	1	0	0	0	0
84	Sa	1	0	0	0	0
84	Sf	1	0	0	0	0
84	k	1	0	0	0	0
84	p	1	0	0	0	0
84	q	1	0	0	0	0
85	D	6	0	0	0	0
85	E	9	0	0	0	0
85	S2	3	0	0	0	0
85	b	1	0	0	0	0
85	f	1	0	0	0	0
85	t	11	0	0	0	0
86	t	31	0	0	0	0
87	S2	6	0	0	0	0
87	SP	1	0	0	0	0
87	SQ	1	0	0	0	0
87	SR	1	0	0	0	0
87	SS	1	0	0	0	0
87	SV	1	0	0	0	0
87	Sb	1	0	0	0	0
87	Sf	1	0	0	0	0
87	u	1	0	0	0	0
All	All	215295	0	159214	2717	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 (2717) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:814:5MU:C4	1:S2:814:5MU:C5	1.82	1.63
43:I:164:ILE:CG2	49:O:22:LEU:HD13	1.31	1.60
1:S2:325:C:C4	1:S2:325:C:N3	1.69	1.59
31:SZ:47:LEU:CD1	31:SZ:47:LEU:CG	1.75	1.59
1:S2:325:C:C6	1:S2:325:C:N1	1.71	1.57
73:m:37:TYR:HB2	83:y:2:TRP:CB	1.28	1.55
1:S2:325:C:N3	1:S2:325:C:C2	1.73	1.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
73:m:37:TYR:CB	83:y:2:TRP:CB	1.76	1.53
1:S2:325:C:N1	1:S2:325:C:C2	1.79	1.49
10:SL:101:ARG:NH2	18:SX:5:ARG:HH12	1.09	1.43
52:R:18:PRO:HD3	52:R:52:PHE:CD1	1.51	1.42
43:I:163:PRO:HG2	43:I:166:LEU:CG	1.48	1.41
43:I:164:ILE:CG2	49:O:22:LEU:CD1	2.00	1.37
67:g:45:LYS:NZ	67:g:109:ARG:NH2	1.73	1.36
67:g:54:LYS:CD	79:t:437:G:H5'	1.35	1.35
1:S2:650:A:OP2	18:SX:108:LYS:CE	1.71	1.35
10:SL:101:ARG:NH2	18:SX:5:ARG:NH1	1.74	1.34
28:SO:140:THR:CG2	28:SO:141:ARG:H	1.37	1.34
50:P:179:LYS:HA	50:P:182:GLU:CD	1.49	1.34
76:p:28:LYS:NZ	79:t:4306:U:O4'	1.59	1.32
54:T:164:LYS:HB2	54:T:165:PRO:CD	1.47	1.31
43:I:78:PRO:HB3	43:I:236:HIS:O	1.25	1.30
52:R:15:ARG:CD	52:R:53:MET:HA	1.63	1.29
52:R:53:MET:CG	79:t:1674:C:OP1	1.80	1.29
54:T:160:ARG:HD3	54:T:163:HIS:CD2	1.67	1.28
52:R:158:THR:OG1	52:R:159:PRO:HD2	1.30	1.28
67:g:54:LYS:CD	79:t:437:G:C5'	1.78	1.28
43:I:234:ARG:NH2	70:j:46:GLU:O	1.64	1.27
50:P:179:LYS:CA	50:P:182:GLU:OE2	1.81	1.27
54:T:174:THR:HG21	79:t:4724:A:O2'	1.12	1.25
67:g:45:LYS:HZ1	67:g:109:ARG:CZ	1.49	1.25
67:g:45:LYS:NZ	67:g:109:ARG:CZ	1.99	1.24
6:SF:130:ARG:O	6:SF:136:ARG:HD2	1.08	1.24
56:V:43:LEU:O	56:V:47:ILE:HG12	1.30	1.23
43:I:160:ASP:O	43:I:187:LYS:HD3	1.32	1.23
67:g:54:LYS:HD3	79:t:437:G:C5'	1.23	1.22
54:T:160:ARG:CD	54:T:163:HIS:CD2	2.22	1.22
37:C:328:LEU:HD11	42:H:170:THR:O	1.27	1.22
1:S2:985:G:H4'	28:SO:138:ASP:OD2	1.33	1.21
76:p:103:VAL:O	76:p:105:GLN:OE1	1.59	1.21
20:Sc:28:THR:O	20:Sc:46:VAL:N	1.71	1.21
43:I:163:PRO:CG	43:I:166:LEU:CD1	2.18	1.20
44:J:63:ASN:OD1	44:J:65:LYS:HG2	1.40	1.19
58:X:49:ILE:CD1	58:X:52:THR:CG2	2.21	1.19
73:m:37:TYR:CG	83:y:2:TRP:CB	2.25	1.18
69:i:87:LYS:HA	71:k:73:ARG:NH2	1.55	1.18
43:I:163:PRO:CG	43:I:166:LEU:HG	1.73	1.18
43:I:164:ILE:HG21	49:O:22:LEU:CD1	1.65	1.15

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:I:163:PRO:HG2	43:I:166:LEU:CD1	1.75	1.15
28:SO:140:THR:HG22	28:SO:141:ARG:N	1.57	1.14
58:X:49:ILE:HD12	58:X:52:THR:HG22	1.26	1.14
52:R:18:PRO:HD3	52:R:52:PHE:CE1	1.83	1.14
54:T:165:PRO:O	54:T:167:PHE:N	1.81	1.14
6:SF:130:ARG:O	6:SF:136:ARG:CD	1.95	1.13
58:X:49:ILE:HD11	58:X:52:THR:CG2	1.78	1.13
6:SF:131:ALA:CB	6:SF:136:ARG:HG3	1.78	1.12
4:SD:5:ILE:CB	4:SD:9:ARG:HD2	1.79	1.11
52:R:18:PRO:CD	52:R:52:PHE:CD1	2.32	1.11
43:I:234:ARG:HH21	70:j:46:GLU:C	1.59	1.11
54:T:174:THR:CG2	79:t:4724:A:O2'	1.99	1.10
6:SF:130:ARG:NH2	6:SF:136:ARG:HH12	1.48	1.10
20:Sc:29:GLN:HG2	20:Sc:45:ASN:CB	1.81	1.10
52:R:15:ARG:HD3	52:R:53:MET:H	1.07	1.10
11:SP:111:MET:HE2	14:SS:117:ILE:CD1	1.81	1.09
20:Sc:29:GLN:HA	20:Sc:45:ASN:HA	1.25	1.09
54:T:164:LYS:HB2	54:T:165:PRO:HD3	1.21	1.09
67:g:45:LYS:HZ2	67:g:109:ARG:NH2	1.34	1.09
20:Sc:30:VAL:HG23	20:Sc:32:VAL:HG13	1.33	1.08
50:P:179:LYS:HA	50:P:182:GLU:OE2	0.90	1.08
52:R:15:ARG:HD2	52:R:53:MET:HA	1.16	1.08
4:SD:5:ILE:HB	4:SD:9:ARG:HD2	1.10	1.08
11:SP:111:MET:HE2	14:SS:117:ILE:HD13	1.36	1.08
47:M:77:SER:HB2	47:M:102:ARG:HB3	1.36	1.07
55:U:105:PHE:O	55:U:109:VAL:HG12	1.53	1.07
20:Sc:29:GLN:CG	20:Sc:45:ASN:HB3	1.83	1.07
54:T:165:PRO:HG2	54:T:168:THR:HB	1.14	1.07
79:t:1582:A:N6	83:y:12:LEU:CB	2.18	1.06
28:SO:140:THR:CG2	28:SO:141:ARG:N	2.07	1.06
73:m:37:TYR:HB3	83:y:2:TRP:CB	1.83	1.06
37:C:55:SER:CB	79:t:351:U:OP1	2.04	1.06
67:g:56:ASN:CG	67:g:64:PRO:HB2	1.76	1.06
67:g:54:LYS:CG	79:t:437:G:OP1	2.04	1.06
44:J:6:SER:HB3	44:J:67:LEU:HD11	1.35	1.05
55:U:107:LYS:O	55:U:111:GLU:CG	2.04	1.05
43:I:163:PRO:CG	43:I:166:LEU:CG	2.31	1.05
43:I:164:ILE:HG23	49:O:22:LEU:CD1	1.87	1.04
52:R:15:ARG:HD3	52:R:53:MET:N	1.71	1.04
11:SP:110:GLU:OE2	14:SS:113:ARG:HD3	1.57	1.04
1:S2:650:A:OP2	18:SX:108:LYS:HE2	1.51	1.04

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:R:15:ARG:CD	52:R:53:MET:CA	2.36	1.04
58:X:49:ILE:HD11	58:X:52:THR:HG21	1.37	1.04
20:Sc:28:THR:N	20:Sc:46:VAL:O	1.90	1.03
58:X:50:ASN:OD1	58:X:55:TYR:CE2	2.11	1.03
37:C:55:SER:HA	79:t:351:U:OP1	1.58	1.03
1:S2:649:U:P	18:SX:108:LYS:HD2	1.98	1.03
56:V:48:LYS:HE3	56:V:53:ALA:HB2	1.39	1.03
47:M:63:THR:HG23	79:t:101:A:O2'	1.58	1.02
52:R:29:VAL:HA	52:R:51:LEU:HD13	1.41	1.02
54:T:164:LYS:CB	54:T:165:PRO:CD	2.36	1.02
18:SX:5:ARG:O	18:SX:9:THR:HG21	1.58	1.02
67:g:106:TYR:CB	67:g:107:PRO:HD2	1.89	1.02
52:R:53:MET:HG2	79:t:1674:C:OP1	0.84	1.02
56:V:46:ARG:HA	56:V:46:ARG:HE	1.20	1.02
1:S2:621:C:H5'	18:SX:107:ARG:HH22	1.20	1.02
11:SP:110:GLU:OE2	14:SS:113:ARG:CG	2.07	1.01
2:SA:27:GLY:HA2	2:SA:46:ILE:CA	1.89	1.01
2:SA:27:GLY:CA	2:SA:46:ILE:HA	1.91	1.00
28:SO:140:THR:HG22	28:SO:141:ARG:H	1.11	1.00
56:V:48:LYS:CE	56:V:53:ALA:HB2	1.91	1.00
67:g:106:TYR:HB3	67:g:107:PRO:HD2	1.42	1.00
28:SO:140:THR:HG23	28:SO:141:ARG:H	1.20	0.99
58:X:50:ASN:OD1	58:X:55:TYR:CD2	2.14	0.99
1:S2:1219:B8Q:C4'	20:Sc:24:GLN:OE1	2.10	0.99
1:S2:650:A:OP2	18:SX:108:LYS:HE3	1.62	0.99
76:p:28:LYS:NZ	79:t:4306:U:C1'	2.25	0.98
37:C:55:SER:CA	79:t:351:U:OP1	2.10	0.98
43:I:78:PRO:CB	43:I:236:HIS:O	2.11	0.98
79:t:1582:A:H61	83:y:12:LEU:CB	1.73	0.98
43:I:162:ASP:CG	43:I:163:PRO:HD3	1.88	0.98
44:J:42:ASN:O	44:J:59:LYS:NZ	1.97	0.98
54:T:165:PRO:CG	54:T:168:THR:HB	1.94	0.98
44:J:4:ILE:O	44:J:60:TRP:O	1.82	0.98
43:I:163:PRO:HG2	43:I:166:LEU:HG	0.99	0.97
52:R:15:ARG:CD	52:R:53:MET:H	1.78	0.97
6:SF:131:ALA:CA	6:SF:136:ARG:HG3	1.93	0.97
58:X:49:ILE:HD12	58:X:52:THR:CG2	1.89	0.97
67:g:109:ARG:HD3	67:g:110:ILE:HD12	1.45	0.97
11:SP:110:GLU:OE2	14:SS:113:ARG:CD	2.11	0.97
4:SD:5:ILE:HB	4:SD:9:ARG:CD	1.95	0.97
1:S2:649:U:O5'	18:SX:108:LYS:HD2	1.64	0.96

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:J:6:SER:HB3	44:J:67:LEU:CD1	1.96	0.96
47:M:77:SER:OG	47:M:102:ARG:O	1.82	0.96
54:T:164:LYS:HB2	54:T:165:PRO:HD2	1.41	0.95
6:SF:131:ALA:HA	6:SF:136:ARG:HG3	1.48	0.95
67:g:109:ARG:CD	67:g:110:ILE:HD12	1.96	0.95
6:SF:131:ALA:HA	6:SF:136:ARG:CG	1.95	0.95
11:SP:108:LYS:HB2	11:SP:109:PRO:HD2	1.49	0.95
54:T:174:THR:HG21	79:t:4724:A:HO2'	1.25	0.94
44:J:62:GLY:O	44:J:67:LEU:HD23	1.67	0.93
18:SX:5:ARG:O	18:SX:9:THR:CG2	2.17	0.93
43:I:163:PRO:HG3	43:I:166:LEU:HD11	1.51	0.93
11:SP:111:MET:HB3	14:SS:117:ILE:HD13	1.50	0.93
69:i:87:LYS:HA	71:k:73:ARG:HH22	1.22	0.93
44:J:6:SER:CB	44:J:67:LEU:CD1	2.46	0.93
44:J:5:LEU:HD12	44:J:60:TRP:CZ3	2.03	0.93
58:X:49:ILE:CD1	58:X:52:THR:HB	1.99	0.92
21:Sd:46:TYR:O	21:Sd:49:ASP:N	2.00	0.92
67:g:54:LYS:HD3	79:t:437:G:P	2.10	0.92
10:SL:101:ARG:HH22	18:SX:5:ARG:NH1	1.50	0.92
54:T:163:HIS:HD2	54:T:164:LYS:NZ	1.68	0.92
1:S2:621:C:H5'	18:SX:107:ARG:NH2	1.85	0.92
67:g:54:LYS:HG3	79:t:437:G:OP1	1.69	0.91
52:R:29:VAL:HA	52:R:51:LEU:CD1	2.01	0.91
52:R:29:VAL:HG22	52:R:51:LEU:HD13	1.53	0.91
1:S2:986:G:O4'	28:SO:138:ASP:OD1	1.89	0.91
2:SA:27:GLY:HA2	2:SA:46:ILE:HA	0.94	0.91
43:I:164:ILE:HG23	49:O:22:LEU:HD13	1.45	0.90
58:X:49:ILE:CD1	58:X:52:THR:CB	2.50	0.90
50:P:122:ALA:HB2	54:T:162:GLN:OE1	1.70	0.90
47:M:63:THR:HG21	62:b:66:ASN:ND2	1.87	0.90
54:T:173:ASN:HA	79:t:4724:A:C2	2.07	0.90
43:I:163:PRO:CD	43:I:166:LEU:HD12	2.03	0.89
52:R:18:PRO:CD	52:R:52:PHE:HD1	1.77	0.89
10:SL:101:ARG:HH21	18:SX:5:ARG:HH12	0.93	0.89
58:X:49:ILE:HD11	58:X:52:THR:CB	2.02	0.89
6:SF:130:ARG:HH21	6:SF:136:ARG:HH12	0.90	0.89
69:i:91:MET:HE2	69:i:94:ARG:NH2	1.87	0.89
47:M:55:ILE:HG12	47:M:76:PHE:HZ	1.39	0.88
52:R:18:PRO:CD	52:R:52:PHE:CE1	2.56	0.88
43:I:81:ASN:ND2	43:I:236:HIS:CD2	2.42	0.88
11:SP:110:GLU:HB3	14:SS:117:ILE:HG21	1.56	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:t:3879:A:N7	83:y:22:GLN:CB	2.36	0.88
1:S2:1160:U:OP2	18:SX:4:CYS:O	1.93	0.87
6:SF:130:ARG:NH2	6:SF:136:ARG:NH1	2.21	0.87
52:R:15:ARG:CD	52:R:53:MET:N	2.33	0.87
69:i:81:LEU:HD23	69:i:84:ARG:CZ	2.05	0.87
67:g:106:TYR:O	67:g:107:PRO:C	2.12	0.87
54:T:160:ARG:HD2	54:T:163:HIS:CD2	2.08	0.86
6:SF:131:ALA:HB2	6:SF:136:ARG:HG3	1.57	0.86
43:I:163:PRO:CG	43:I:166:LEU:HD12	2.01	0.86
43:I:165:GLU:O	43:I:167:VAL:N	2.08	0.86
44:J:4:ILE:HD12	44:J:4:ILE:H	1.38	0.86
56:V:42:PHE:O	56:V:46:ARG:HB2	1.76	0.86
76:p:28:LYS:O	79:t:4306:U:O2'	1.94	0.85
21:Sd:46:TYR:HB3	21:Sd:49:ASP:HB2	1.56	0.85
40:F:4:VAL:N	79:t:1760:C:HO2'	1.74	0.85
44:J:63:ASN:O	44:J:64:ARG:C	2.16	0.85
69:i:91:MET:CE	69:i:94:ARG:NH2	2.40	0.84
54:T:165:PRO:O	54:T:166:ARG:C	2.20	0.84
20:Sc:31:ARG:HA	20:Sc:43:ILE:HA	1.59	0.84
44:J:6:SER:CB	44:J:67:LEU:HD11	2.08	0.84
6:SF:130:ARG:HH21	6:SF:136:ARG:NH1	1.73	0.83
44:J:63:ASN:OD1	44:J:65:LYS:NZ	2.09	0.83
76:p:27:LYS:H	76:p:27:LYS:HD2	1.43	0.83
43:I:163:PRO:HG3	43:I:166:LEU:CD1	2.05	0.83
50:P:187:LYS:NZ	50:P:187:LYS:HB3	1.92	0.83
67:g:56:ASN:CG	67:g:64:PRO:CB	2.42	0.83
21:Sd:38:MET:CE	21:Sd:43:PHE:HD1	1.91	0.83
43:I:163:PRO:CG	43:I:166:LEU:HD11	2.05	0.83
67:g:56:ASN:CB	67:g:64:PRO:HB2	2.09	0.83
11:SP:111:MET:HE2	14:SS:117:ILE:HD12	1.60	0.82
20:Sc:30:VAL:CG2	20:Sc:32:VAL:HG13	2.08	0.82
55:U:107:LYS:O	55:U:111:GLU:CB	2.28	0.82
37:C:328:LEU:CD1	42:H:170:THR:O	2.22	0.82
43:I:160:ASP:O	43:I:187:LYS:CD	2.24	0.82
67:g:45:LYS:HZ1	67:g:109:ARG:NH2	1.54	0.82
67:g:54:LYS:HD3	79:t:437:G:O5'	1.78	0.82
67:g:109:ARG:HE	67:g:109:ARG:H	1.26	0.82
79:t:161:G:H1	79:t:266:U:H3	1.28	0.82
50:P:179:LYS:CA	50:P:182:GLU:CD	2.39	0.81
54:T:163:HIS:CD2	54:T:164:LYS:NZ	2.48	0.81
69:i:91:MET:SD	69:i:94:ARG:NE	2.53	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Sc:14:VAL:CG1	20:Sc:30:VAL:HB	2.09	0.81
21:Sd:43:PHE:HZ	21:Sd:52:PHE:HD2	1.28	0.81
1:S2:649:U:H5''	18:SX:108:LYS:CE	2.10	0.81
21:Sd:39:CYS:O	21:Sd:42:CYS:SG	2.38	0.81
58:X:51:TRP:CD1	58:X:52:THR:N	2.49	0.81
46:L:63:ARG:HD3	76:p:104:ILE:HB	1.63	0.80
43:I:162:ASP:N	79:t:148:G:C6	2.40	0.80
37:C:83:GLY:H	83:y:10:LEU:CB	1.94	0.80
52:R:48:LEU:O	52:R:51:LEU:HB2	1.82	0.80
47:M:77:SER:CB	47:M:102:ARG:HB3	2.12	0.80
54:T:160:ARG:HD2	54:T:164:LYS:HZ3	1.45	0.80
67:g:45:LYS:HZ2	67:g:109:ARG:HH22	1.29	0.80
4:SD:5:ILE:CG2	4:SD:9:ARG:HD2	2.12	0.79
21:Sd:30:LEU:HA	21:Sd:39:CYS:HA	1.64	0.79
47:M:63:THR:CG2	62:b:66:ASN:ND2	2.44	0.79
52:R:16:LYS:O	52:R:52:PHE:CZ	2.35	0.79
69:i:89:ARG:CZ	69:i:93:ARG:HH22	1.96	0.79
54:T:161:ARG:HB3	54:T:162:GLN:NE2	1.97	0.79
54:T:161:ARG:HB3	54:T:162:GLN:HE22	1.48	0.79
2:SA:27:GLY:HA3	2:SA:46:ILE:CD1	2.12	0.79
49:O:143:ARG:HD3	69:i:99:GLU:OE1	1.82	0.79
44:J:63:ASN:OD1	44:J:65:LYS:CG	2.28	0.79
54:T:163:HIS:HD2	54:T:164:LYS:HZ3	1.27	0.78
69:i:87:LYS:CA	71:k:73:ARG:HH22	1.93	0.78
44:J:6:SER:OG	44:J:67:LEU:HD13	1.84	0.78
16:SU:68:THR:O	21:Sd:40:ARG:NH2	2.15	0.78
67:g:54:LYS:HD3	79:t:437:G:H5'	0.88	0.78
69:i:88:THR:O	69:i:92:ARG:NE	2.16	0.78
52:R:15:ARG:CZ	52:R:53:MET:O	2.32	0.78
1:S2:649:U:O5'	18:SX:108:LYS:CD	2.30	0.78
54:T:165:PRO:C	54:T:167:PHE:N	2.41	0.77
58:X:50:ASN:CG	58:X:55:TYR:CE2	2.63	0.77
54:T:163:HIS:CD2	54:T:164:LYS:HZ2	2.02	0.77
52:R:18:PRO:HD3	52:R:52:PHE:HD1	1.04	0.77
52:R:29:VAL:CA	52:R:51:LEU:HD13	2.13	0.77
50:P:179:LYS:O	50:P:182:GLU:HG2	1.85	0.77
56:V:46:ARG:HA	56:V:46:ARG:NE	2.00	0.77
58:X:49:ILE:CD1	58:X:52:THR:HG21	2.04	0.77
79:t:2618:U:HO2'	79:t:2673:G:H1	1.31	0.77
43:I:164:ILE:HG23	49:O:22:LEU:HD11	1.67	0.77
79:t:4493:U:C5	83:y:25:GLU:N	2.53	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Sc:29:GLN:CA	20:Sc:45:ASN:HA	2.13	0.77
56:V:45:GLU:OE1	56:V:46:ARG:NH1	2.18	0.76
54:T:160:ARG:HD2	54:T:163:HIS:HD2	1.47	0.76
76:p:28:LYS:O	76:p:28:LYS:HD3	1.84	0.76
44:J:5:LEU:HD12	44:J:60:TRP:CE3	2.20	0.76
55:U:107:LYS:O	55:U:111:GLU:HG3	1.83	0.76
69:i:91:MET:SD	69:i:94:ARG:CZ	2.74	0.76
20:Sc:29:GLN:HG2	20:Sc:45:ASN:HB3	0.89	0.76
20:Sc:14:VAL:HG12	20:Sc:30:VAL:HB	1.68	0.76
44:J:63:ASN:ND2	44:J:64:ARG:N	2.34	0.76
69:i:87:LYS:HA	71:k:73:ARG:HH21	1.51	0.76
55:U:111:GLU:O	55:U:114:GLN:HG3	1.86	0.76
67:g:109:ARG:HD2	67:g:110:ILE:H	1.50	0.75
73:m:37:TYR:CD2	83:y:2:TRP:CB	2.68	0.75
2:SA:27:GLY:HA3	2:SA:46:ILE:HD12	1.67	0.75
43:I:163:PRO:HG2	43:I:166:LEU:HD12	1.67	0.75
67:g:54:LYS:HG2	79:t:437:G:OP1	1.85	0.75
37:C:55:SER:HB3	79:t:351:U:OP1	1.84	0.75
54:T:160:ARG:HD2	54:T:164:LYS:NZ	2.01	0.75
1:S2:1033:G:H1	1:S2:1080:A:HO2'	1.33	0.75
43:I:164:ILE:HG21	49:O:22:LEU:HD13	0.75	0.75
41:G:141:ARG:HD2	67:g:109:ARG:O	1.87	0.75
69:i:91:MET:HA	69:i:94:ARG:HG3	1.67	0.75
58:X:50:ASN:HA	58:X:55:TYR:CD1	2.22	0.74
79:t:3879:A:N1	83:y:20:ARG:CA	2.50	0.74
44:J:4:ILE:HD12	44:J:4:ILE:N	2.03	0.74
31:SZ:47:LEU:CD1	31:SZ:47:LEU:HG	2.11	0.74
40:F:22:ARG:HD2	40:F:27:LYS:HB2	1.68	0.74
54:T:164:LYS:CB	54:T:165:PRO:HD2	2.12	0.74
55:U:107:LYS:O	55:U:111:GLU:HG2	1.87	0.74
58:X:49:ILE:HD11	58:X:52:THR:HB	1.67	0.74
67:g:109:ARG:H	67:g:109:ARG:NE	1.85	0.74
47:M:63:THR:OG1	47:M:66:TYR:HD2	1.71	0.74
69:i:81:LEU:HD23	69:i:84:ARG:NE	2.02	0.74
67:g:54:LYS:CD	79:t:437:G:H5''	1.54	0.74
36:B:291:TYR:CE1	36:B:300:LYS:HA	2.23	0.73
10:SL:101:ARG:HH22	18:SX:5:ARG:HH12	1.08	0.73
54:T:165:PRO:HB2	54:T:167:PHE:O	1.88	0.73
52:R:158:THR:CB	52:R:159:PRO:HD2	2.18	0.73
52:R:16:LYS:O	52:R:52:PHE:CE2	2.41	0.73
56:V:43:LEU:O	56:V:47:ILE:CG1	2.25	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:X:50:ASN:HA	58:X:55:TYR:CG	2.23	0.73
67:g:45:LYS:HZ1	67:g:109:ARG:NE	1.87	0.73
10:SL:101:ARG:HH21	18:SX:5:ARG:NH1	1.53	0.73
43:I:163:PRO:HD2	43:I:166:LEU:HD12	1.70	0.73
58:X:51:TRP:CG	58:X:52:THR:N	2.57	0.73
56:V:48:LYS:HE2	56:V:53:ALA:HB2	1.70	0.73
41:G:141:ARG:CD	67:g:109:ARG:O	2.37	0.72
67:g:56:ASN:ND2	67:g:65:ASN:O	2.12	0.72
79:t:3879:A:N1	83:y:20:ARG:HA	2.04	0.72
11:SP:106:GLU:OE2	11:SP:107:ILE:O	2.07	0.72
79:t:2617:G:H1	79:t:2676:A:H61	1.37	0.72
2:SA:27:GLY:CA	2:SA:46:ILE:HD13	2.19	0.72
43:I:164:ILE:HD12	43:I:164:ILE:O	1.90	0.72
67:g:109:ARG:HD3	67:g:110:ILE:CD1	2.20	0.72
18:SX:5:ARG:HG2	18:SX:5:ARG:HH11	1.53	0.71
20:Sc:26:GLN:O	20:Sc:47:LYS:HB2	1.90	0.71
20:Sc:31:ARG:HB2	20:Sc:43:ILE:HD13	1.72	0.71
38:D:149:G:H21	43:I:64:GLN:HE22	1.38	0.71
44:J:62:GLY:C	44:J:67:LEU:HD23	2.15	0.71
1:S2:325:C:C6	1:S2:325:C:C1'	2.74	0.71
1:S2:663:C:OP2	18:SX:3:LYS:NZ	2.21	0.71
54:T:161:ARG:C	54:T:162:GLN:HE21	1.97	0.71
76:p:99:ARG:O	76:p:102:GLN:HG2	1.90	0.71
79:t:703:C:H42	79:t:943:A:H61	1.36	0.71
52:R:29:VAL:CG2	52:R:51:LEU:HD13	2.20	0.71
69:i:81:LEU:CD2	69:i:84:ARG:CZ	2.68	0.71
20:Sc:18:LEU:HD22	20:Sc:18:LEU:N	2.05	0.71
69:i:89:ARG:O	69:i:93:ARG:HD3	1.89	0.71
76:p:105:GLN:OE1	76:p:105:GLN:N	2.23	0.71
79:t:2536:G:N7	79:t:2741:G:N2	2.39	0.71
42:H:98:ILE:HD11	52:R:3:VAL:HA	1.71	0.71
50:P:122:ALA:CB	54:T:162:GLN:OE1	2.39	0.71
20:Sc:18:LEU:HG	20:Sc:43:ILE:HD11	1.73	0.71
43:I:234:ARG:NH2	70:j:46:GLU:CA	2.54	0.71
43:I:234:ARG:HH21	70:j:46:GLU:CA	2.04	0.71
21:Sd:43:PHE:HZ	21:Sd:52:PHE:CD2	2.08	0.71
50:P:180:GLN:O	50:P:183:LYS:HB3	1.90	0.71
67:g:56:ASN:HB3	67:g:64:PRO:HB2	1.72	0.71
47:M:63:THR:HG23	79:t:101:A:HO2'	1.56	0.70
54:T:160:ARG:HG2	54:T:163:HIS:HB3	1.71	0.70
79:t:2372:C:OP2	79:t:2373:G:N2	2.24	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:Sd:38:MET:HB3	21:Sd:42:CYS:SG	2.31	0.70
25:SJ:37:LEU:HD23	25:SJ:42:GLU:HG3	1.73	0.70
1:S2:650:A:OP2	18:SX:108:LYS:NZ	2.06	0.70
21:Sd:39:CYS:N	21:Sd:42:CYS:SG	2.64	0.70
54:T:160:ARG:HG2	54:T:163:HIS:CB	2.21	0.70
18:SX:107:ARG:CD	18:SX:112:VAL:HG12	2.20	0.70
79:t:1981:G:H5''	79:t:1982:G:H5'	1.72	0.70
22:Sg:87:LEU:HB2	22:Sg:101:PHE:HB2	1.72	0.70
1:S2:1748:G:H1	1:S2:1786:U:H3	1.38	0.70
47:M:75:GLY:O	47:M:102:ARG:NH1	2.25	0.70
52:R:46:VAL:O	52:R:50:ARG:HG3	1.91	0.70
25:SJ:60:LEU:HB3	25:SJ:70:ARG:HD2	1.73	0.70
67:g:54:LYS:HD2	79:t:437:G:H5'	1.63	0.70
69:i:88:THR:CG2	69:i:91:MET:H	2.05	0.70
5:SE:41:CYS:SG	5:SE:42:LEU:N	2.65	0.69
36:B:291:TYR:HE1	36:B:300:LYS:HA	1.57	0.69
43:I:161:VAL:HG12	43:I:163:PRO:HD2	1.73	0.69
79:t:4493:U:C5	83:y:24:ASP:C	2.69	0.69
21:Sd:38:MET:CE	21:Sd:43:PHE:CD1	2.76	0.69
67:g:106:TYR:HB3	67:g:107:PRO:CD	2.21	0.69
47:M:63:THR:CG2	79:t:101:A:O2'	2.40	0.69
11:SP:110:GLU:OE2	14:SS:113:ARG:HG3	1.92	0.69
69:i:87:LYS:CA	71:k:73:ARG:NH2	2.47	0.69
1:S2:834:C:H2'	1:S2:836:G:H1	1.57	0.69
1:S2:936:G:O6	64:d:8:LYS:NZ	2.25	0.69
1:S2:1298:G:H1'	11:SP:79:HIS:HB2	1.75	0.69
52:R:15:ARG:NE	52:R:53:MET:CA	2.55	0.69
47:M:57:PRO:HB3	47:M:76:PHE:CD1	2.28	0.69
28:SO:34:PHE:HB3	28:SO:41:PHE:HB2	1.74	0.68
55:U:108:ARG:HA	55:U:111:GLU:CG	2.23	0.68
52:R:17:GLU:HA	52:R:52:PHE:CE1	2.28	0.68
41:G:112:MET:O	78:r:87:ARG:NH1	2.27	0.68
14:SS:138:THR:HA	14:SS:141:ARG:HH11	1.59	0.68
40:F:21:ARG:HA	40:F:24:ARG:HH21	1.57	0.68
43:I:163:PRO:HD3	79:t:148:G:C2	2.21	0.68
52:R:15:ARG:NE	52:R:53:MET:N	2.41	0.68
6:SF:140:ASP:HB2	20:Sc:46:VAL:HG12	1.75	0.68
47:M:63:THR:HG1	47:M:66:TYR:HD2	1.38	0.68
54:T:160:ARG:HD3	54:T:163:HIS:NE2	2.07	0.68
69:i:88:THR:HG23	69:i:91:MET:H	1.60	0.67
1:S2:1001:A:N7	19:Sa:19:GLN:NE2	2.41	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:SB:109:LYS:NZ	3:SB:113:MET:SD	2.67	0.67
6:SF:130:ARG:HD3	6:SF:130:ARG:N	2.09	0.67
60:Z:55:VAL:HG23	60:Z:107:THR:N	2.09	0.67
11:SP:111:MET:CB	14:SS:117:ILE:HD13	2.24	0.67
44:J:5:LEU:CD1	44:J:60:TRP:CZ3	2.78	0.67
56:V:28:PRO:HG3	56:V:100:LEU:HD21	1.75	0.67
36:B:47:LEU:HD12	36:B:84:MET:HE1	1.76	0.67
52:R:15:ARG:NE	52:R:53:MET:HA	2.08	0.67
67:g:106:TYR:CB	67:g:107:PRO:CD	2.70	0.67
1:S2:925:G:H1	1:S2:1017:U:H3	1.43	0.67
20:Sc:28:THR:O	20:Sc:45:ASN:C	2.37	0.67
20:Sc:29:GLN:HB3	20:Sc:44:ARG:O	1.94	0.67
44:J:91:LYS:HG2	44:J:145:ILE:HG12	1.76	0.67
1:S2:325:C:C2	1:S2:325:C:C1'	2.76	0.66
43:I:163:PRO:CD	43:I:166:LEU:CD1	2.70	0.66
80:v:19:G:N3	80:v:57:G:N2	2.43	0.66
37:C:326:LEU:HD21	37:C:333:LYS:HD3	1.78	0.66
79:t:133:C:H41	79:t:135:G:H1'	1.60	0.66
34:Sf:109:ASP:H	34:Sf:113:LYS:HB3	1.61	0.66
55:U:107:LYS:O	55:U:111:GLU:HB3	1.94	0.66
69:i:89:ARG:CZ	69:i:93:ARG:NH2	2.58	0.66
1:S2:126:G:OP1	24:SG:198:ARG:NH1	2.28	0.66
47:M:55:ILE:HG12	47:M:76:PHE:CZ	2.27	0.66
54:T:98:ARG:HH22	79:t:737:A:H61	1.43	0.66
54:T:174:THR:O	54:T:175:PHE:HB3	1.96	0.66
22:Sg:42:MET:HB2	22:Sg:57:ARG:HB2	1.78	0.66
42:H:232:ASP:HB2	42:H:236:ARG:HH22	1.59	0.66
38:D:74:U:H3	60:Z:72:GLN:HE21	1.44	0.66
6:SF:130:ARG:HD3	6:SF:130:ARG:H	1.61	0.66
18:SX:5:ARG:HH11	18:SX:5:ARG:CG	2.08	0.66
20:Sc:17:VAL:HG12	20:Sc:19:GLY:H	1.60	0.66
1:S2:1352:G:C8	6:SF:63:LYS:HG3	2.31	0.66
4:SD:49:ILE:HG22	4:SD:87:TYR:HB2	1.78	0.66
11:SP:110:GLU:CB	14:SS:117:ILE:HG21	2.25	0.66
7:SH:32:MET:H	7:SH:36:LEU:HD13	1.61	0.65
54:T:161:ARG:HH21	54:T:161:ARG:CG	2.09	0.65
16:SU:59:LYS:HD2	16:SU:84:ILE:HD11	1.78	0.65
21:Sd:21:CYS:CB	21:Sd:39:CYS:SG	2.85	0.65
44:J:63:ASN:O	44:J:65:LYS:N	2.29	0.65
37:C:54:VAL:HG21	37:C:105:THR:O	1.96	0.65
44:J:4:ILE:H	44:J:4:ILE:CD1	2.07	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:SP:110:GLU:OE1	11:SP:110:GLU:HA	1.96	0.65
1:S2:681:U:O2'	18:SX:8:ARG:NH1	2.29	0.65
65:e:73:TRP:HZ3	65:e:77:ILE:HG12	1.62	0.65
1:S2:693:A:N6	1:S2:738:C:O2'	2.29	0.65
1:S2:1224:G:H1	1:S2:1642:U:H3	1.43	0.65
2:SA:27:GLY:CA	2:SA:46:ILE:CD1	2.73	0.65
44:J:6:SER:OG	44:J:67:LEU:CD1	2.44	0.65
47:M:61:CYS:HB2	47:M:66:TYR:O	1.97	0.65
73:m:37:TYR:CE2	83:y:3:PRO:O	2.50	0.65
76:p:39:ARG:HH11	79:t:289:A:H5'	1.62	0.65
56:V:48:LYS:HA	56:V:53:ALA:HA	1.79	0.65
1:S2:1566:G:N7	15:ST:101:ARG:NH2	2.45	0.65
5:SE:105:THR:HG23	5:SE:106:LYS:HG3	1.79	0.65
41:G:192:LYS:HD3	79:t:700:C:H5''	1.79	0.65
79:t:159:A:H61	79:t:268:C:H42	1.41	0.65
79:t:4315:U:H5'	79:t:4316:U:H5'	1.79	0.65
1:S2:1286:G:H1'	26:SM:35:ILE:HB	1.78	0.64
1:S2:1357:A:N6	25:SJ:64:ASP:OD1	2.29	0.64
2:SA:42:LYS:HD3	2:SA:46:ILE:HB	1.79	0.64
37:C:209:ILE:HG13	37:C:251:ILE:HB	1.79	0.64
63:c:57:MET:HE2	79:t:1794:C:H5'	1.79	0.64
79:t:1067:C:O2	79:t:1197:C:N4	2.29	0.64
2:SA:27:GLY:H	2:SA:47:TYR:H	1.43	0.64
38:D:63:U:OP1	69:i:48:ARG:NH2	2.30	0.64
52:R:158:THR:OG1	52:R:159:PRO:CD	2.26	0.64
1:S2:72:C:OP2	1:S2:79:A:N6	2.31	0.64
1:S2:1552:G:H5''	4:SD:5:ILE:CG2	2.28	0.64
20:Sc:31:ARG:HB2	20:Sc:43:ILE:CD1	2.27	0.64
52:R:29:VAL:HG22	52:R:51:LEU:CD1	2.24	0.64
52:R:29:VAL:CG2	52:R:51:LEU:HD22	2.26	0.64
79:t:2580:A:N6	79:t:2723:A:OP2	2.31	0.64
76:p:61:LYS:HD3	76:p:87:ARG:HH12	1.61	0.64
32:Sb:36:LYS:HB3	32:Sb:78:SER:HB3	1.80	0.64
1:S2:509:OMG:H2'	1:S2:510:G:H8	1.62	0.64
49:O:93:LYS:NZ	79:t:281:U:O2	2.31	0.64
60:Z:55:VAL:HG23	60:Z:106:ILE:C	2.21	0.64
1:S2:682:U:H5'	18:SX:8:ARG:HH11	1.63	0.64
47:M:146:LEU:HD21	69:i:122:LYS:HG3	1.79	0.64
52:R:18:PRO:N	52:R:52:PHE:CD1	2.66	0.64
64:d:37:MET:SD	64:d:42:LYS:NZ	2.70	0.64
1:S2:649:U:OP1	18:SX:108:LYS:HA	1.98	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:992:A:N7	19:Sa:15:ARG:NH2	2.44	0.63
18:SX:8:ARG:HD3	18:SX:8:ARG:H	1.63	0.63
79:t:2065:C:H42	79:t:2251:C:H42	1.46	0.63
47:M:125:ILE:HG21	47:M:141:ALA:HB2	1.81	0.63
52:R:15:ARG:HD3	52:R:53:MET:CA	2.14	0.63
76:p:81:ARG:HH22	79:t:4256:C:H5''	1.63	0.63
1:S2:1357:A:N7	25:SJ:66:LYS:N	2.45	0.63
60:Z:8:THR:O	79:t:223:G:N2	2.31	0.63
52:R:65:ARG:NH2	79:t:1441:A:OP1	2.32	0.63
1:S2:986:G:C4'	28:SO:138:ASP:OD1	2.46	0.63
10:SL:101:ARG:NE	18:SX:6:GLY:O	2.28	0.63
79:t:226:G:O6	79:t:227:G:N2	2.32	0.63
1:S2:940:U:H3	1:S2:1002:U:H3	1.46	0.63
16:SU:18:HIS:ND1	16:SU:117:ALA:O	2.31	0.63
56:V:46:ARG:HE	56:V:46:ARG:CA	2.06	0.63
54:T:165:PRO:C	54:T:167:PHE:H	2.07	0.63
69:i:87:LYS:C	71:k:73:ARG:HH22	2.06	0.63
79:t:445:C:H5''	79:t:447:G:H8	1.64	0.63
79:t:1072:G:N2	79:t:1190:C:O2	2.32	0.63
1:S2:814:5MU:C4	1:S2:814:5MU:C6	2.59	0.63
54:T:93:MET:HG3	79:t:1933:G:H4'	1.81	0.63
1:S2:1780:G:H3'	1:S2:1781:A:H4'	1.80	0.63
39:E:85:G:OP1	42:H:222:LYS:NZ	2.31	0.63
11:SP:111:MET:CE	14:SS:117:ILE:HD13	2.20	0.62
1:S2:1414:A:O2'	15:ST:128:GLN:NE2	2.31	0.62
41:G:101:ASN:HD21	41:G:105:ARG:HH22	1.47	0.62
53:S:115:ILE:HG12	53:S:142:ILE:HD11	1.81	0.62
79:t:3758:G:H21	79:t:3760:C:H42	1.44	0.62
79:t:742:G:N2	79:t:743:G:O6	2.32	0.62
79:t:1319:G:N2	79:t:2330:C:N3	2.47	0.62
23:SC:68:ARG:HH21	23:SC:71:LYS:HZ3	1.48	0.62
36:B:10:ARG:NH1	36:B:11:HIS:O	2.32	0.62
36:B:116:ARG:HG2	36:B:177:LYS:HG2	1.80	0.62
50:P:179:LYS:CB	50:P:182:GLU:OE2	2.47	0.62
51:Q:80:GLN:NE2	79:t:3863:U:O2'	2.32	0.62
71:k:5:THR:O	79:t:2778:G:N2	2.30	0.62
1:S2:621:C:C5'	18:SX:107:ARG:HH22	2.05	0.62
11:SP:108:LYS:HB2	11:SP:109:PRO:CD	2.28	0.62
40:F:23:ARG:NH2	79:t:4242:A:OP2	2.31	0.62
50:P:179:LYS:O	50:P:182:GLU:CG	2.47	0.62
69:i:91:MET:CE	69:i:94:ARG:CZ	2.77	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:SJ:54:ARG:NH2	25:SJ:98:LEU:O	2.31	0.62
36:B:26:ARG:NH1	36:B:180:LEU:O	2.32	0.62
71:k:19:CYS:SG	71:k:20:ARG:N	2.73	0.62
79:t:137:G:H21	79:t:138:C:H41	1.47	0.62
79:t:1224:C:OP2	79:t:1252:G:N2	2.31	0.62
6:SF:136:ARG:O	6:SF:203:ASN:ND2	2.32	0.62
14:SS:39:ARG:HH11	15:ST:38:LYS:HB2	1.65	0.62
22:Sg:236:ILE:HG22	22:Sg:252:THR:HA	1.80	0.62
49:O:181:HIS:NE2	79:t:286:G:O6	2.32	0.62
79:t:182:C:OP1	79:t:250:G:N2	2.31	0.62
1:S2:1593:C:O2	15:ST:12:GLN:NE2	2.33	0.62
76:p:28:LYS:NZ	79:t:4306:U:H1'	2.12	0.62
1:S2:695:C:N4	1:S2:736:C:OP2	2.33	0.62
13:SR:28:PHE:HA	13:SR:55:THR:HG21	1.82	0.62
30:SY:21:LYS:HB2	30:SY:75:ILE:HB	1.82	0.62
41:G:283:PRO:O	41:G:284:HIS:ND1	2.31	0.62
44:J:18:ILE:HG12	44:J:27:VAL:HG22	1.80	0.62
44:J:61:TRP:HZ2	54:T:152:PHE:CD2	2.18	0.62
1:S2:55:U:OP1	1:S2:451:G:N1	2.30	0.62
1:S2:752:G:N2	1:S2:793:G:N3	2.47	0.62
1:S2:986:G:H5'	28:SO:138:ASP:OD2	1.99	0.62
37:C:55:SER:OG	79:t:351:U:P	2.57	0.62
42:H:169:LEU:H	42:H:169:LEU:CD2	2.12	0.62
61:a:14:LEU:HD21	61:a:81:MET:HG2	1.82	0.62
66:f:44:ARG:NH1	79:t:1298:C:OP2	2.32	0.62
1:S2:1352:G:H4'	6:SF:61:PHE:HA	1.82	0.61
17:SV:43:THR:OG1	17:SV:45:ARG:NH1	2.32	0.61
52:R:37:ARG:NH1	79:t:2067:G:N7	2.48	0.61
55:U:110:LYS:HB2	55:U:110:LYS:NZ	2.15	0.61
61:a:76:ASN:OD1	61:a:79:HIS:ND1	2.32	0.61
79:t:727:C:H42	79:t:914:G:H1	1.46	0.61
79:t:1952:C:N4	79:t:1982:G:OP1	2.33	0.61
11:SP:92:SER:HB2	11:SP:107:ILE:HD12	1.82	0.61
36:B:246:ARG:NH1	79:t:4487:C:OP1	2.33	0.61
50:P:87:MET:SD	79:t:1893:G:N2	2.73	0.61
60:Z:54:GLU:H	60:Z:54:GLU:CD	2.06	0.61
67:g:45:LYS:HZ3	67:g:109:ARG:CZ	2.06	0.61
79:t:963:G:H22	79:t:1262:A:H2	1.48	0.61
79:t:2484:C:O2'	79:t:2485:G:N2	2.33	0.61
2:SA:3:GLY:HA2	17:SV:79:VAL:HG22	1.81	0.61
2:SA:77:ILE:HG22	2:SA:99:ILE:HB	1.82	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:L:110:GLN:HG3	79:t:4213:A:H1'	1.81	0.61
57:W:31:ASN:ND2	57:W:115:SER:OG	2.33	0.61
79:t:1059:C:O2	79:t:1218:G:N2	2.30	0.61
5:SE:87:MET:HE2	5:SE:123:LEU:HB2	1.81	0.61
43:I:161:VAL:HG21	43:I:167:VAL:CG2	2.29	0.61
44:J:10:VAL:HB	44:J:55:LEU:HB3	1.82	0.61
10:SL:115:PRO:O	10:SL:118:ARG:NH2	2.31	0.61
49:O:155:VAL:O	49:O:162:ARG:NH2	2.33	0.61
28:SO:102:GLY:HA2	28:SO:136:PRO:HD3	1.82	0.61
49:O:49:ARG:NH2	79:t:150:G:OP2	2.32	0.61
52:R:184:ARG:NH1	62:b:55:LYS:O	2.33	0.61
57:W:85:ARG:HH21	57:W:100:ASP:HA	1.65	0.61
79:t:189:G:H1	79:t:244:G:H22	1.48	0.61
1:S2:1495:G:N2	21:Sd:21:CYS:SG	2.73	0.61
67:g:109:ARG:HD2	67:g:110:ILE:HD12	1.78	0.61
79:t:1414:C:H42	79:t:1435:A:H61	1.45	0.61
16:SU:32:LEU:HD21	16:SU:85:HIS:HB2	1.83	0.61
49:O:42:PRO:HG3	49:O:61:ILE:HG13	1.81	0.61
54:T:160:ARG:HD3	54:T:163:HIS:CG	2.32	0.61
79:t:1416:A:N6	79:t:1433:C:O2'	2.34	0.61
5:SE:183:VAL:HG21	5:SE:220:THR:HG21	1.83	0.61
42:H:95:ILE:HD12	42:H:96:ARG:HG2	1.83	0.61
72:l:38:CYS:SG	72:l:39:SER:N	2.70	0.61
5:SE:238:LEU:HD11	5:SE:242:LYS:HG3	1.83	0.61
53:S:99:MET:HG2	53:S:103:ARG:HE	1.65	0.61
61:a:15:ALA:HB3	61:a:79:HIS:HD2	1.66	0.61
4:SD:42:THR:H	4:SD:46:THR:HG22	1.66	0.60
16:SU:18:HIS:HD2	16:SU:94:PRO:HA	1.65	0.60
28:SO:75:MET:SD	28:SO:79:GLN:NE2	2.74	0.60
40:F:28:THR:O	79:t:4242:A:N6	2.33	0.60
43:I:165:GLU:O	43:I:166:LEU:C	2.43	0.60
45:K:14:ASN:ND2	79:t:1845:G:OP2	2.34	0.60
50:P:185:VAL:O	50:P:185:VAL:HG22	2.01	0.60
54:T:161:ARG:O	54:T:162:GLN:HB2	2.00	0.60
67:g:56:ASN:O	67:g:65:ASN:O	2.19	0.60
76:p:28:LYS:HZ1	79:t:4306:U:C1'	2.12	0.60
79:t:38:A:H2'	79:t:41:C:H41	1.66	0.60
79:t:66:A:HO2'	79:t:320:C:HO2'	1.49	0.60
79:t:451:G:H1	79:t:691:G:H1	1.47	0.60
79:t:1997:C:H2'	79:t:1998:A:H8	1.66	0.60
2:SA:104:THR:OG1	2:SA:107:THR:OG1	2.18	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:Sd:10:HIS:HB3	21:Sd:12:ARG:HH12	1.66	0.60
37:C:53:ALA:HB2	79:t:342:G:N2	2.16	0.60
48:N:5:ARG:HB2	48:N:11:ARG:HH12	1.65	0.60
66:f:128:ARG:NH2	79:t:2285:G:OP1	2.33	0.60
1:S2:325:C:C2	58:X:119:LYS:CE	2.84	0.60
24:SG:70:HIS:HA	24:SG:98:ARG:HH12	1.66	0.60
29:SW:23:ARG:NH1	29:SW:66:THR:O	2.35	0.60
40:F:197:LYS:HB3	40:F:202:GLN:HG2	1.82	0.60
1:S2:326:C:O2	1:S2:327:G:N2	2.34	0.60
19:Sa:87:ARG:NH1	19:Sa:94:ASP:OD1	2.35	0.60
43:I:234:ARG:CZ	70:j:46:GLU:O	2.46	0.60
55:U:108:ARG:HA	55:U:111:GLU:HG3	1.84	0.60
59:Y:117:TYR:O	59:Y:152:LYS:NZ	2.33	0.60
7:SH:5:SER:N	7:SH:20:GLU:O	2.35	0.60
20:Sc:28:THR:O	20:Sc:45:ASN:CA	2.50	0.60
35:A:30:ARG:O	35:A:163:ARG:NH2	2.34	0.60
35:A:104:VAL:O	35:A:139:HIS:NE2	2.31	0.60
36:B:300:LYS:HB3	36:B:313:SER:HB2	1.82	0.60
64:d:51:ASN:HD22	64:d:77:ASN:HD21	1.48	0.60
79:t:2626:A:H62	79:t:2665:G:H8	1.48	0.60
79:t:2841:G:N2	79:t:3595:A:O2'	2.33	0.60
11:SP:110:GLU:OE2	14:SS:113:ARG:HG2	1.99	0.60
37:C:315:LYS:HE2	42:H:169:LEU:CD2	2.32	0.60
44:J:5:LEU:C	44:J:5:LEU:HD23	2.27	0.60
50:P:179:LYS:C	50:P:182:GLU:HG2	2.26	0.60
21:Sd:38:MET:HE3	21:Sd:43:PHE:HD1	1.63	0.60
37:C:198:ASN:HD22	60:Z:10:ASP:HB3	1.66	0.60
52:R:29:VAL:HG22	52:R:51:LEU:HB3	1.84	0.60
55:U:112:ASN:HD21	55:U:128:LEU:HD22	1.66	0.60
1:S2:1546:G:H21	1:S2:1670:C:H1'	1.67	0.60
11:SP:17:TYR:OH	11:SP:18:ARG:NH2	2.35	0.60
79:t:2838:G:N2	79:t:3808:C:O2	2.35	0.60
1:S2:1552:G:H5''	4:SD:5:ILE:HG22	1.84	0.60
8:SI:48:VAL:HG11	8:SI:54:LYS:HE3	1.84	0.60
43:I:164:ILE:HG22	49:O:22:LEU:CD1	2.23	0.60
65:e:64:ILE:HG22	65:e:106:VAL:HB	1.84	0.60
13:SR:106:LEU:HA	13:SR:109:LEU:HB3	1.83	0.59
37:C:20:LYS:NZ	37:C:254:GLU:OE2	2.33	0.59
76:p:3:ASN:ND2	76:p:95:GLY:O	2.34	0.59
12:SQ:51:LEU:HB2	12:SQ:84:ILE:HD11	1.84	0.59
76:p:27:LYS:H	76:p:27:LYS:CD	2.15	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:t:3909:G:N2	79:t:4133:C:OP2	2.34	0.59
21:Sd:21:CYS:HB2	21:Sd:39:CYS:SG	2.42	0.59
37:C:55:SER:CB	79:t:351:U:P	2.90	0.59
58:X:49:ILE:O	58:X:52:THR:HG22	2.02	0.59
60:Z:54:GLU:OE1	60:Z:54:GLU:N	2.24	0.59
60:Z:73:VAL:HG13	60:Z:80:ILE:HG22	1.84	0.59
79:t:2373:G:N2	79:t:2798:U:OP2	2.35	0.59
15:ST:11:GLN:OE1	15:ST:62:ARG:NH2	2.36	0.59
39:E:27:G:OP1	46:L:146:ARG:NH2	2.35	0.59
35:A:207:VAL:HG23	35:A:208:GLU:HG3	1.84	0.59
37:C:6:PRO:HB3	79:t:661:G:H4'	1.83	0.59
38:D:39:G:O2'	38:D:103:A:N6	2.35	0.59
40:F:4:VAL:HG13	40:F:5:LYS:HG2	1.84	0.59
22:Sg:249:CYS:SG	22:Sg:250:ALA:N	2.75	0.59
35:A:117:GLU:HG2	35:A:124:GLY:H	1.68	0.59
53:S:59:SER:HA	79:t:2613:C:H5'	1.83	0.59
1:S2:1452:A:O2'	1:S2:1475:G:N2	2.35	0.59
2:SA:27:GLY:O	2:SA:45:GLY:O	2.21	0.59
20:Sc:28:THR:O	20:Sc:45:ASN:HA	2.01	0.59
22:Sg:289:LEU:HD12	22:Sg:298:LEU:HD11	1.85	0.59
36:B:170:LEU:O	36:B:328:ASN:ND2	2.36	0.59
51:Q:15:CYS:SG	51:Q:16:LYS:N	2.75	0.59
53:S:107:ARG:NH2	79:t:2645:U:OP1	2.36	0.59
79:t:83:C:O2'	79:t:100:C:N4	2.35	0.59
1:S2:325:C:C2	58:X:119:LYS:CD	2.85	0.59
1:S2:748:C:O2'	1:S2:794:A:N6	2.35	0.59
1:S2:1361:G:O2'	1:S2:1380:C:N4	2.35	0.59
1:S2:1636:G:O2'	6:SF:164:ARG:NH1	2.36	0.59
2:SA:163:CYS:SG	2:SA:164:ASN:N	2.74	0.59
12:SQ:97:GLN:HE22	22:Sg:60:ARG:HH21	1.51	0.59
71:k:11:ARG:NH1	79:t:1516:A:O2'	2.36	0.59
79:t:1320:A:H62	79:t:2325:C:H5	1.50	0.59
4:SD:136:VAL:HG23	4:SD:186:VAL:HG22	1.85	0.59
16:SU:80:PHE:HB3	21:Sd:52:PHE:HB3	1.83	0.59
22:Sg:195:LEU:HA	22:Sg:211:GLY:HA3	1.85	0.59
47:M:17:ASP:O	47:M:21:ARG:NH2	2.36	0.59
11:SP:110:GLU:CG	14:SS:117:ILE:HG21	2.32	0.59
43:I:161:VAL:HG21	43:I:167:VAL:HG21	1.84	0.59
49:O:125:SER:HB2	79:t:3908:C:H1'	1.83	0.59
62:b:132:ARG:NH2	79:t:1450:C:OP1	2.33	0.59
1:S2:29:G:OP1	18:SX:124:LYS:NZ	2.37	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:SF:76:MET:O	6:SF:159:ARG:NH2	2.36	0.58
17:SV:16:LYS:HD3	17:SV:21:ASN:HD21	1.68	0.58
41:G:246:ARG:HH12	79:t:4898:C:H1'	1.68	0.58
63:c:120:ARG:O	79:t:1223:G:N2	2.36	0.58
79:t:2674:A:H4'	79:t:2675:A:H5'	1.85	0.58
22:Sg:106:LYS:HA	22:Sg:126:ASP:HB2	1.84	0.58
67:g:106:TYR:HB2	67:g:107:PRO:HD2	1.78	0.58
80:v:11:C:H42	80:v:24:G:H1	1.51	0.58
1:S2:1550:G:H3'	1:S2:1579:A:H61	1.68	0.58
49:O:143:ARG:CD	69:i:99:GLU:OE1	2.49	0.58
79:t:490:G:N2	79:t:652:C:O2	2.37	0.58
74:n:96:CYS:SG	74:n:97:ARG:N	2.76	0.58
18:SX:5:ARG:CZ	18:SX:5:ARG:HB3	2.33	0.58
35:A:122:ASP:O	35:A:123:ARG:HB2	2.04	0.58
38:D:37:A:OP2	69:i:89:ARG:NH1	2.35	0.58
44:J:173:ARG:NH2	79:t:4437:G:OP2	2.37	0.58
79:t:132:G:O6	79:t:136:G:N2	2.37	0.58
79:t:1056:G:H22	79:t:1221:A:H2	1.51	0.58
79:t:1741:G:H1	79:t:1755:U:H3	1.49	0.58
79:t:4373:G:H1	79:t:4393:U:H3	1.52	0.58
60:Z:54:GLU:HA	60:Z:69:LYS:HA	1.85	0.58
66:f:5:ARG:NH1	79:t:449:C:O2'	2.36	0.58
3:SB:149:GLN:HE21	3:SB:151:ARG:HG3	1.68	0.58
41:G:105:ARG:HH21	79:t:464:A:H61	1.52	0.58
61:a:5:MET:O	61:a:28:ASN:ND2	2.36	0.58
76:p:104:ILE:O	76:p:104:ILE:HG22	2.02	0.58
78:r:65:LYS:HD3	78:r:70:GLN:HE22	1.69	0.58
79:t:1389:G:H1	79:t:1394:C:H42	1.51	0.58
79:t:2001:U:H2'	79:t:2002:G:H8	1.68	0.58
1:S2:732:U:OP2	1:S2:733:C:N4	2.37	0.58
36:B:223:THR:O	36:B:343:ARG:NH1	2.35	0.58
44:J:115:ARG:HB3	44:J:123:ILE:HG22	1.85	0.58
58:X:49:ILE:CD1	58:X:52:THR:HG22	1.96	0.58
69:i:98:HIS:CE1	79:t:137:G:OP1	2.57	0.58
79:t:4539:U:H3	79:t:4688:G:H1	1.50	0.58
11:SP:18:ARG:NH1	11:SP:36:LEU:O	2.37	0.58
16:SU:97:ILE:HB	16:SU:100:GLN:HE21	1.69	0.58
1:S2:1352:G:H5'	6:SF:60:ARG:HA	1.86	0.58
10:SL:35:ARG:NH1	10:SL:53:GLY:O	2.37	0.58
22:Sg:199:THR:HG21	22:Sg:240:CYS:HA	1.86	0.58
53:S:103:ARG:NH1	53:S:124:TYR:OH	2.36	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:333:G:O6	24:SG:186:GLN:NE2	2.37	0.57
1:S2:621:C:C5'	18:SX:107:ARG:NH2	2.64	0.57
8:SI:34:ALA:HB2	8:SI:56:ARG:HH11	1.68	0.57
19:Sa:87:ARG:NH1	19:Sa:91:ALA:O	2.36	0.57
20:Sc:31:ARG:HG2	20:Sc:31:ARG:O	2.04	0.57
35:A:174:ARG:NH2	79:t:3655:G:OP1	2.37	0.57
38:D:153:C:H2'	38:D:154:G:H8	1.69	0.57
67:g:109:ARG:CD	67:g:109:ARG:H	2.17	0.57
77:q:15:GLY:O	77:q:23:ARG:NH1	2.36	0.57
79:t:4077:G:O6	79:t:4078:G:N2	2.37	0.57
54:T:11:LYS:HD2	54:T:29:ARG:HD2	1.86	0.57
79:t:2438:G:N2	79:t:2441:C:OP2	2.37	0.57
79:t:2849:A:OP2	79:t:2858:A:N6	2.37	0.57
1:S2:155:G:H4'	24:SG:15:LEU:HD13	1.86	0.57
21:Sd:21:CYS:HB3	21:Sd:26:ASN:H	1.69	0.57
36:B:396:ARG:HD3	36:B:397:ILE:HG23	1.86	0.57
41:G:59:ARG:HB3	79:t:1220:C:H5''	1.86	0.57
43:I:234:ARG:NH2	70:j:46:GLU:C	2.36	0.57
49:O:172:ARG:NH1	79:t:62:A:OP1	2.38	0.57
53:S:143:HIS:O	53:S:147:ALA:N	2.37	0.57
60:Z:2:LYS:NZ	60:Z:4:ASN:O	2.37	0.57
79:t:3660:G:O2'	79:t:3789:U:OP2	2.22	0.57
2:SA:189:ILE:HG22	2:SA:191:ARG:H	1.70	0.57
10:SL:73:LEU:HD12	10:SL:140:PHE:HE2	1.69	0.57
28:SO:30:VAL:HG12	28:SO:94:HIS:HB2	1.85	0.57
38:D:52:A:H4'	73:m:19:GLN:HA	1.87	0.57
43:I:165:GLU:C	43:I:167:VAL:H	2.12	0.57
45:K:158:LYS:NZ	79:t:4375:C:O2	2.33	0.57
71:k:8:PHE:HD1	71:k:11:ARG:HE	1.51	0.57
72:l:23:VAL:HG22	72:l:36:VAL:HG22	1.86	0.57
78:r:32:LEU:O	78:r:113:ARG:NE	2.32	0.57
79:t:2790:G:N1	79:t:2793:C:OP2	2.34	0.57
1:S2:649:U:C5'	18:SX:108:LYS:HD2	2.33	0.57
1:S2:1199:A:OP1	19:Sa:2:THR:N	2.37	0.57
8:SI:67:TRP:HD1	8:SI:70:GLU:H	1.50	0.57
43:I:35:ARG:NH1	79:t:4097:A:O2'	2.38	0.57
58:X:49:ILE:HD12	58:X:49:ILE:O	2.04	0.57
73:m:27:ILE:O	73:m:33:ASN:ND2	2.37	0.57
4:SD:23:GLU:OE1	21:Sd:46:TYR:OH	2.20	0.57
4:SD:25:LEU:HD13	4:SD:50:ILE:HD11	1.86	0.57
30:SY:15:ASN:HD21	30:SY:18:LEU:HD12	1.68	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:J:23:ARG:NH1	79:t:4726:A:OP1	2.37	0.57
60:Z:54:GLU:HG2	60:Z:67:ILE:HD11	1.86	0.57
65:e:28:ASN:HA	65:e:83:ARG:HA	1.87	0.57
69:i:27:GLU:O	69:i:31:LEU:N	2.36	0.57
79:t:4713:G:N2	79:t:4907:G:O6	2.38	0.57
44:J:6:SER:CB	44:J:67:LEU:HD13	2.31	0.57
47:M:77:SER:HB2	47:M:102:ARG:HD2	1.86	0.57
49:O:96:ARG:NH2	79:t:2439:A:O2'	2.37	0.57
55:U:27:LEU:HB3	55:U:31:MET:HE2	1.85	0.57
40:F:120:GLU:O	40:F:248:ARG:NH2	2.38	0.57
53:S:134:ASN:HD22	79:t:2875:G:H5''	1.69	0.57
69:i:95:LEU:HD12	69:i:95:LEU:N	2.19	0.57
7:SH:25:GLN:HA	7:SH:28:LEU:HD12	1.87	0.57
18:SX:105:PHE:HD1	18:SX:121:LYS:HD3	1.70	0.57
23:SC:103:LYS:HE2	23:SC:216:MET:HE2	1.87	0.57
35:A:54:ARG:NH2	79:t:3651:U:OP1	2.37	0.57
54:T:165:PRO:HG2	54:T:168:THR:CB	2.10	0.57
62:b:116:LYS:HB2	79:t:1381:A:H62	1.70	0.57
79:t:3612:U:OP2	79:t:3617:A:N6	2.37	0.57
1:S2:539:C:N4	1:S2:542:U:OP2	2.38	0.57
1:S2:1313:A:H61	26:SM:35:ILE:HG12	1.70	0.57
51:Q:127:ARG:NH1	79:t:2399:A:OP2	2.38	0.57
79:t:2827:G:N2	79:t:3810:G:OP2	2.35	0.57
1:S2:1300:U:O2'	21:Sd:5:GLN:NE2	2.38	0.56
1:S2:1566:G:OP2	15:ST:102:ARG:NH1	2.37	0.56
6:SF:127:ARG:H	6:SF:135:ARG:HD3	1.71	0.56
29:SW:30:CYS:SG	29:SW:31:SER:N	2.78	0.56
49:O:114:ARG:NH1	49:O:151:ILE:O	2.38	0.56
60:Z:2:LYS:HD2	60:Z:7:VAL:HG13	1.87	0.56
67:g:27:LEU:HA	67:g:85:ARG:HA	1.85	0.56
79:t:949:C:N4	79:t:2076:G:O6	2.37	0.56
79:t:1831:A:N3	79:t:2262:G:O2'	2.38	0.56
1:S2:985:G:C4'	28:SO:138:ASP:OD2	2.29	0.56
1:S2:1481:G:N2	21:Sd:56:ASP:OD2	2.37	0.56
1:S2:1864:U:OP2	19:Sa:5:ARG:NH2	2.38	0.56
57:W:45:ILE:HG21	57:W:53:PRO:HB3	1.87	0.56
76:p:37:GLY:O	80:v:75:C:N4	2.37	0.56
79:t:4163:G:O2'	79:t:4165:A:N6	2.38	0.56
1:S2:93:U:OP1	5:SE:2:ALA:N	2.38	0.56
1:S2:429:C:OP1	5:SE:10:LYS:NZ	2.34	0.56
1:S2:1543:U:OP2	15:ST:62:ARG:NH1	2.36	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:SE:51:ARG:NH2	5:SE:109:PHE:O	2.38	0.56
5:SE:80:ILE:HG13	5:SE:81:THR:HG23	1.87	0.56
17:SV:17:CYS:SG	17:SV:18:SER:N	2.78	0.56
18:SX:5:ARG:NH1	18:SX:5:ARG:HB3	2.20	0.56
18:SX:5:ARG:O	18:SX:9:THR:HG22	2.02	0.56
37:C:192:GLY:O	37:C:195:LYS:NZ	2.37	0.56
37:C:250:CYS:SG	37:C:252:TRP:NE1	2.78	0.56
38:D:122:G:N1	38:D:129:C:O2'	2.36	0.56
49:O:61:ILE:HG23	49:O:133:ILE:HG22	1.86	0.56
51:Q:23:ARG:NH2	51:Q:125:MET:SD	2.77	0.56
52:R:15:ARG:NH2	52:R:53:MET:O	2.38	0.56
56:V:101:ARG:HG2	56:V:115:PHE:HB3	1.86	0.56
65:e:44:ARG:NH2	79:t:2812:A:OP2	2.38	0.56
71:k:52:LYS:NZ	79:t:369:G:OP2	2.32	0.56
82:u:27:G:H1	82:u:43:C:H5	1.54	0.56
36:B:60:VAL:HG11	36:B:67:VAL:HG12	1.87	0.56
50:P:183:LYS:HD2	50:P:183:LYS:C	2.31	0.56
52:R:155:ALA:O	52:R:161:SER:HB2	2.06	0.56
38:D:62:A:OP1	69:i:52:LYS:NZ	2.38	0.56
55:U:102:ARG:HD2	79:t:1783:A:H4'	1.86	0.56
78:r:71:ARG:NH2	79:t:660:C:O2'	2.37	0.56
1:S2:166:A2M:H2'	1:S2:167:G:C8	2.41	0.56
20:Sc:30:VAL:CG2	20:Sc:32:VAL:CG1	2.80	0.56
40:F:77:ALA:O	40:F:108:ARG:NH1	2.38	0.56
46:L:95:ARG:HG2	46:L:175:LEU:HD22	1.88	0.56
54:T:160:ARG:CD	54:T:163:HIS:HD2	1.97	0.56
56:V:45:GLU:OE1	56:V:46:ARG:CZ	2.53	0.56
57:W:15:ARG:NH1	57:W:16:ILE:O	2.39	0.56
58:X:8:PHE:HE2	58:X:51:TRP:HZ2	1.54	0.56
79:t:4410:G:H5''	79:t:4411:A:H5''	1.88	0.56
1:S2:1596:U:OP2	31:SZ:85:ARG:NH1	2.37	0.56
1:S2:1597:C:OP2	31:SZ:85:ARG:NH2	2.38	0.56
38:D:87:G:N1	60:Z:114:ASP:OD2	2.32	0.56
76:p:22:LYS:HE2	76:p:73:VAL:HG23	1.87	0.56
1:S2:38:A:O3'	25:SJ:5:ARG:NH1	2.38	0.56
19:Sa:22:ARG:NH1	19:Sa:27:ALA:O	2.39	0.56
23:SC:106:VAL:HG11	23:SC:151:ILE:HD11	1.87	0.56
24:SG:159:ARG:HH21	24:SG:171:THR:HG23	1.71	0.56
37:C:326:LEU:HD23	79:t:963:G:H4'	1.86	0.56
52:R:29:VAL:HG22	52:R:51:LEU:HD22	1.86	0.56
53:S:105:LEU:HD23	53:S:138:LEU:HD12	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:g:58:VAL:HG23	67:g:60:PRO:HD2	1.88	0.56
1:S2:1677:U:OP1	6:SF:148:ASN:ND2	2.39	0.56
5:SE:92:ILE:HD12	30:SY:17:LEU:HD21	1.88	0.56
7:SH:69:LEU:HD13	7:SH:96:ALA:HB2	1.88	0.56
14:SS:84:LEU:O	14:SS:87:GLN:NE2	2.38	0.56
41:G:273:SER:OG	79:t:4839:U:O2'	2.24	0.56
66:f:22:ARG:NH2	79:t:2326:A:OP1	2.34	0.56
79:t:474:C:H42	79:t:668:C:H42	1.53	0.56
79:t:2522:A:O2'	79:t:2525:G:O2'	2.23	0.56
37:C:165:LYS:NZ	79:t:219:C:O2	2.39	0.56
37:C:235:LEU:HD23	37:C:240:LEU:HD11	1.86	0.56
37:C:239:LYS:O	37:C:248:ARG:NH1	2.36	0.56
69:i:88:THR:HG22	69:i:91:MET:HG2	1.88	0.56
73:m:25:GLN:OE1	73:m:28:ARG:NH2	2.35	0.56
1:S2:681:U:O3'	18:SX:8:ARG:NE	2.38	0.55
9:SK:76:ILE:HG22	9:SK:80:ARG:HH21	1.71	0.55
30:SY:16:ARG:O	30:SY:19:GLN:NE2	2.39	0.55
42:H:146:ASN:ND2	79:t:930:A:OP1	2.35	0.55
60:Z:126:ARG:NH1	79:t:193:C:OP1	2.39	0.55
1:S2:1533:A:OP1	6:SF:164:ARG:NH1	2.39	0.55
37:C:83:GLY:N	83:y:10:LEU:CB	2.67	0.55
37:C:221:PHE:HB3	37:C:229:LEU:HD11	1.87	0.55
54:T:165:PRO:O	54:T:167:PHE:C	2.49	0.55
79:t:3839:G:N2	79:t:3871:G:O2'	2.36	0.55
1:S2:124:U:OP1	24:SG:201:LYS:NZ	2.39	0.55
1:S2:1006:C:H5'	64:d:11:LEU:H	1.72	0.55
24:SG:137:ARG:HD2	24:SG:178:ARG:HD3	1.87	0.55
43:I:104:PRO:HG2	43:I:194:VAL:HG23	1.89	0.55
46:L:18:ARG:HB3	46:L:133:VAL:HG23	1.88	0.55
47:M:76:PHE:N	47:M:76:PHE:CD2	2.73	0.55
54:T:173:ASN:HA	79:t:4724:A:H2	1.63	0.55
62:b:21:ARG:NH1	79:t:1301:C:OP2	2.39	0.55
1:S2:439:A:OP2	8:SI:23:LYS:NZ	2.40	0.55
1:S2:871:U:O2	53:S:163:ARG:NH2	2.35	0.55
1:S2:1100:A:O2'	13:SR:132:ARG:NH2	2.38	0.55
25:SJ:111:GLN:NE2	25:SJ:123:ILE:O	2.39	0.55
43:I:230:TYR:CE2	43:I:234:ARG:HD2	2.42	0.55
49:O:12:ARG:NH2	79:t:273:A:N7	2.54	0.55
56:V:42:PHE:CE2	56:V:46:ARG:HG2	2.41	0.55
59:Y:149:VAL:HG13	59:Y:152:LYS:HE3	1.87	0.55
69:i:88:THR:CG2	69:i:91:MET:HG2	2.37	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:737:G:H2'	1:S2:738:C:H4'	1.88	0.55
4:SD:14:ASP:HA	4:SD:17:PHE:HB3	1.88	0.55
22:Sg:5:MET:HE2	22:Sg:270:LEU:HD21	1.86	0.55
56:V:105:ASN:ND2	56:V:111:GLU:OE1	2.39	0.55
57:W:43:LYS:HD2	57:W:62:MET:HE2	1.89	0.55
78:r:107:ARG:NH2	79:t:2242:A:OP1	2.40	0.55
79:t:2773:C:N4	83:y:11:LEU:CB	2.70	0.55
1:S2:1544:C:O2'	12:SQ:80:GLN:NE2	2.40	0.55
5:SE:35:PRO:HD2	5:SE:83:PRO:HG2	1.89	0.55
6:SF:40:ALA:HB3	6:SF:67:PRO:HA	1.89	0.55
9:SK:95:ARG:NH2	9:SK:98:ARG:O	2.40	0.55
60:Z:70:VAL:HG12	60:Z:82:ILE:HG12	1.89	0.55
67:g:56:ASN:OD1	67:g:64:PRO:CG	2.52	0.55
1:S2:1079:C:O2'	1:S2:1182:A:N1	2.40	0.55
1:S2:1206:G:N2	1:S2:1835:A:OP1	2.39	0.55
1:S2:1219:B8Q:O2'	20:Sc:26:GLN:OE1	2.25	0.55
3:SB:36:PRO:HB2	3:SB:38:MET:HG2	1.88	0.55
14:SS:89:ASP:OD1	14:SS:94:LYS:N	2.34	0.55
26:SM:75:ASN:OD1	26:SM:75:ASN:N	2.40	0.55
39:E:6:C:H4'	40:F:52:ILE:HD13	1.89	0.55
45:K:96:VAL:HG22	45:K:125:THR:HG22	1.88	0.55
63:c:51:LYS:NZ	79:t:1384:C:OP1	2.34	0.55
67:g:22:ARG:NH2	79:t:2051:U:OP1	2.40	0.55
71:k:34:CYS:SG	71:k:35:GLY:N	2.80	0.55
79:t:69:A:N1	79:t:318:A:O2'	2.36	0.55
79:t:2067:G:N2	79:t:2250:C:O2	2.40	0.55
1:S2:820:U:OP1	25:SJ:83:ARG:NH2	2.39	0.55
1:S2:867:G:H1	10:SL:150:GLY:H	1.53	0.55
1:S2:1130:G:N2	1:S2:1130:G:OP2	2.40	0.55
1:S2:1275:G:OP1	1:S2:1506:A:N6	2.39	0.55
2:SA:94:THR:OG1	2:SA:186:ARG:NH2	2.40	0.55
23:SC:211:LYS:HG2	23:SC:215:MET:HE2	1.88	0.55
36:B:165:HIS:HB3	36:B:180:LEU:HD12	1.88	0.55
36:B:225:GLY:HA3	79:t:4935:A:H5''	1.89	0.55
69:i:91:MET:CA	69:i:94:ARG:HG3	2.37	0.55
1:S2:526:A:O2'	25:SJ:125:HIS:ND1	2.40	0.55
1:S2:1309:C:OP1	34:Sf:118:ARG:NE	2.39	0.55
4:SD:205:PRO:HA	13:SR:42:PRO:HG2	1.88	0.55
20:Sc:29:GLN:CB	20:Sc:44:ARG:O	2.54	0.55
24:SG:64:LYS:HZ1	24:SG:81:HIS:HB3	1.72	0.55
24:SG:77:LEU:HD12	24:SG:95:LYS:HB2	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:F:60:ILE:HG22	40:F:80:ALA:HB2	1.88	0.55
41:G:262:LYS:NZ	41:G:268:GLN:OE1	2.40	0.55
43:I:73:ARG:NH1	79:t:4046:G:OP1	2.40	0.55
43:I:81:ASN:HD22	43:I:236:HIS:CD2	2.22	0.55
50:P:90:HIS:O	50:P:96:GLN:NE2	2.40	0.55
53:S:143:HIS:NE2	79:t:3569:C:OP1	2.40	0.55
54:T:164:LYS:CG	54:T:165:PRO:HD2	2.37	0.55
71:k:56:ARG:NH2	79:t:369:G:N7	2.55	0.55
11:SP:75:VAL:HG12	11:SP:93:MET:HB3	1.88	0.55
28:SO:57:THR:HG22	28:SO:59:GLY:H	1.72	0.55
40:F:238:GLU:HG3	40:F:242:LYS:HG3	1.89	0.55
46:L:144:LYS:O	46:L:148:THR:OG1	2.25	0.55
49:O:84:PRO:HA	49:O:87:HIS:CD2	2.42	0.55
76:p:99:ARG:O	76:p:102:GLN:CG	2.53	0.55
1:S2:1554:C:H5''	1:S2:1555:U:H3'	1.89	0.54
20:Sc:29:GLN:CA	20:Sc:44:ARG:O	2.55	0.54
39:E:38:U:N3	39:E:41:G:OP2	2.40	0.54
52:R:29:VAL:CB	52:R:51:LEU:HD13	2.37	0.54
53:S:104:ARG:HB3	53:S:107:ARG:HH11	1.72	0.54
77:q:17:ARG:NH2	79:t:1559:G:OP1	2.38	0.54
79:t:1062:C:H1'	79:t:1216:G:H22	1.71	0.54
1:S2:322:C:O2'	1:S2:324:C:N4	2.40	0.54
7:SH:138:GLU:HG3	27:SN:19:ARG:HD3	1.87	0.54
38:D:29:G:H5''	47:M:27:ASN:HB3	1.90	0.54
41:G:246:ARG:NH2	79:t:4898:C:O2	2.39	0.54
58:X:19:ARG:NH2	79:t:4592:G:O5'	2.39	0.54
37:C:56:GLU:HG3	37:C:57:LEU:N	2.21	0.54
67:g:21:GLN:NE2	67:g:23:GLU:OE2	2.40	0.54
73:m:45:ARG:HH21	79:t:2775:G:H5'	1.72	0.54
22:Sg:106:LYS:HE2	22:Sg:130:LYS:HG3	1.89	0.54
36:B:13:SER:HB2	79:t:4584:A:H4'	1.89	0.54
40:F:17:GLN:O	79:t:4227:U:N3	2.32	0.54
42:H:191:ILE:HA	42:H:194:ILE:HG22	1.89	0.54
48:N:27:ILE:HA	48:N:38:VAL:HG12	1.89	0.54
52:R:29:VAL:HG12	52:R:33:ARG:HE	1.72	0.54
58:X:52:THR:HG23	58:X:55:TYR:H	1.72	0.54
62:b:42:ARG:NH1	79:t:4338:A:O2'	2.40	0.54
76:p:12:CYS:SG	76:p:19:GLN:NE2	2.81	0.54
1:S2:835:C:OP1	1:S2:836:G:N2	2.41	0.54
7:SH:70:LYS:HD2	7:SH:73:GLN:HG3	1.90	0.54
20:Sc:29:GLN:HA	20:Sc:44:ARG:O	2.08	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:J:63:ASN:HD22	44:J:64:ARG:H	1.54	0.54
54:T:165:PRO:CG	54:T:168:THR:CB	2.80	0.54
58:X:51:TRP:CD1	58:X:51:TRP:C	2.85	0.54
65:e:79:ASN:ND2	79:t:4615:C:OP1	2.40	0.54
2:SA:27:GLY:HA2	2:SA:46:ILE:HD13	1.90	0.54
20:Sc:14:VAL:HG11	20:Sc:30:VAL:CG1	2.38	0.54
41:G:227:HIS:O	79:t:447:G:N2	2.41	0.54
47:M:78:LEU:O	47:M:81:LEU:N	2.41	0.54
55:U:47:THR:O	79:t:4244:A:N6	2.40	0.54
59:Y:139:ARG:NH1	79:t:2512:C:OP1	2.41	0.54
61:a:40:HIS:HA	61:a:76:ASN:HA	1.89	0.54
63:c:44:ARG:HA	63:c:47:LYS:HB2	1.89	0.54
22:Sg:298:LEU:HB3	22:Sg:310:TRP:HB2	1.90	0.54
23:SC:235:ASN:O	23:SC:239:ALA:N	2.36	0.54
29:SW:26:LEU:HD11	29:SW:60:LYS:HD3	1.90	0.54
35:A:129:ALA:HB3	35:A:132:ASN:HD22	1.73	0.54
38:D:13:G:O2'	51:Q:121:LYS:O	2.24	0.54
1:S2:191:A:N6	1:S2:209:A:O2'	2.41	0.54
6:SF:138:ALA:O	6:SF:204:ARG:NH2	2.41	0.54
14:SS:22:GLY:HA2	14:SS:56:ALA:HB3	1.90	0.54
25:SJ:136:ARG:HA	25:SJ:141:VAL:HA	1.89	0.54
37:C:71:ARG:NH1	83:y:13:LEU:CB	2.71	0.54
44:J:135:SER:HB3	44:J:145:ILE:HB	1.89	0.54
73:m:44:TRP:O	73:m:48:LYS:NZ	2.41	0.54
79:t:198:C:H42	79:t:209:A:H61	1.55	0.54
1:S2:17:C:O2'	1:S2:1194:A:N1	2.41	0.54
1:S2:1610:G:O2'	14:SS:110:ASP:OD2	2.26	0.54
17:SV:33:GLN:HE21	23:SC:261:PHE:HB3	1.73	0.54
44:J:4:ILE:HA	44:J:61:TRP:CZ3	2.43	0.54
48:N:46:ARG:NH2	79:t:925:C:O5'	2.41	0.54
79:t:1706:G:N2	79:t:1857:U:OP1	2.39	0.54
1:S2:649:U:C5'	18:SX:108:LYS:CE	2.72	0.54
1:S2:1040:G:H5''	77:q:25:MET:HE2	1.90	0.54
1:S2:1547:C:O2'	16:SU:62:ARG:NH2	2.41	0.54
1:S2:1692:U:H1'	19:Sa:86:ASN:HD21	1.72	0.54
8:SI:6:ASP:OD2	8:SI:8:TRP:NE1	2.41	0.54
24:SG:98:ARG:NH1	24:SG:99:GLY:O	2.41	0.54
35:A:2:GLY:N	79:t:4147:G:OP1	2.41	0.54
38:D:71:A:OP2	60:Z:50:ARG:NH1	2.41	0.54
53:S:62:ARG:NH2	79:t:4608:U:OP2	2.41	0.54
3:SB:137:LEU:HD23	3:SB:215:VAL:HG22	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:SP:72:LYS:HE2	11:SP:93:MET:HG3	1.90	0.53
34:Sf:98:VAL:HB	34:Sf:100:LEU:HD23	1.91	0.53
41:G:223:ARG:NH2	41:G:225:PRO:O	2.42	0.53
79:t:2576:G:H1	79:t:2727:C:H5	1.56	0.53
47:M:11:LYS:NZ	62:b:52:TYR:OH	2.38	0.53
47:M:25:TRP:HE1	49:O:199:GLN:HE21	1.56	0.53
54:T:160:ARG:CG	54:T:163:HIS:CD2	2.91	0.53
60:Z:91:ASN:HA	79:t:383:A:H1'	1.90	0.53
70:j:88:GLU:O	70:j:92:ASN:ND2	2.41	0.53
80:v:55:U:H2'	80:v:56:C:H2'	1.90	0.53
3:SB:175:GLU:HG3	3:SB:193:ILE:HG12	1.91	0.53
7:SH:53:VAL:HG12	7:SH:175:GLY:HA3	1.90	0.53
7:SH:75:ILE:HG22	7:SH:78:ARG:HD2	1.91	0.53
18:SX:107:ARG:HD3	18:SX:112:VAL:HG12	1.90	0.53
22:Sg:287:THR:N	22:Sg:301:GLY:O	2.41	0.53
30:SY:110:ARG:NH2	30:SY:125:VAL:O	2.41	0.53
42:H:115:ARG:HD3	52:R:3:VAL:HG21	1.89	0.53
51:Q:4:TYR:HE1	51:Q:18:ARG:HD2	1.74	0.53
56:V:31:ASP:OD2	56:V:114:TYR:OH	2.26	0.53
67:g:54:LYS:CD	79:t:437:G:P	2.92	0.53
70:j:44:ILE:HA	70:j:47:VAL:HG12	1.89	0.53
79:t:459:G:H1	79:t:683:U:H3	1.55	0.53
79:t:1956:G:N2	79:t:1964:A:OP1	2.41	0.53
1:S2:1352:G:H8	6:SF:63:LYS:HG3	1.72	0.53
7:SH:116:ARG:HD3	7:SH:121:THR:HB	1.90	0.53
13:SR:98:VAL:HG23	13:SR:119:VAL:HG12	1.91	0.53
22:Sg:252:THR:HG21	22:Sg:257:LYS:HG3	1.90	0.53
52:R:29:VAL:HG22	52:R:51:LEU:CG	2.38	0.53
53:S:105:LEU:HD22	53:S:135:LYS:HG3	1.90	0.53
54:T:112:ASP:OD1	54:T:116:ARG:NH1	2.42	0.53
59:Y:129:ARG:NH1	59:Y:131:ASP:OD2	2.42	0.53
79:t:217:C:O2	79:t:233:G:N2	2.42	0.53
79:t:1742:G:H2'	79:t:1743:G:H8	1.73	0.53
1:S2:596:U:HO2'	1:S2:645:C:HO2'	1.55	0.53
37:C:55:SER:OG	79:t:351:U:OP1	2.25	0.53
38:D:58:G:O6	71:k:63:ARG:NH1	2.41	0.53
50:P:12:ARG:NH2	79:t:4723:G:OP2	2.36	0.53
58:X:8:PHE:HE2	58:X:51:TRP:CZ2	2.26	0.53
79:t:1409:G:N1	79:t:1440:C:OP2	2.32	0.53
1:S2:559:G:OP2	25:SJ:177:ASN:ND2	2.40	0.53
1:S2:984:C:O2'	28:SO:138:ASP:O	2.26	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:SE:56:LEU:HB2	5:SE:60:GLU:HG3	1.89	0.53
10:SL:101:ARG:NH2	18:SX:5:ARG:HH11	1.94	0.53
36:B:154:LYS:HE3	36:B:191:ALA:HA	1.91	0.53
37:C:53:ALA:HB2	79:t:342:G:H22	1.74	0.53
37:C:108:TRP:O	49:O:204:ARG:NH1	2.41	0.53
67:g:10:ILE:HA	67:g:100:ARG:HA	1.88	0.53
79:t:4065:G:O6	79:t:4083:C:N4	2.41	0.53
79:t:4731:G:N2	79:t:4732:U:O4	2.41	0.53
1:S2:531:A:O2'	1:S2:554:A:N6	2.42	0.53
3:SB:113:MET:HE3	3:SB:209:ASP:HB3	1.89	0.53
28:SO:44:VAL:HG13	28:SO:53:ILE:HB	1.89	0.53
29:SW:90:GLN:HA	29:SW:94:LEU:HD23	1.91	0.53
36:B:276:HIS:O	36:B:277:ARG:NH1	2.36	0.53
43:I:234:ARG:NH2	70:j:46:GLU:HA	2.24	0.53
54:T:68:PHE:HE2	79:t:722:G:H1'	1.73	0.53
1:S2:1665:G:H22	15:ST:87:VAL:HG22	1.73	0.53
25:SJ:26:ASP:O	25:SJ:30:LYS:NZ	2.41	0.53
41:G:188:ARG:NH1	41:G:214:ASP:OD1	2.41	0.53
79:t:3625:G:O2'	79:t:3664:U:OP1	2.22	0.53
1:S2:924:G:OP1	27:SN:3:ARG:NE	2.39	0.53
1:S2:1166:G:OP2	18:SX:25:LYS:NZ	2.42	0.53
11:SP:94:VAL:HG13	11:SP:107:ILE:HD11	1.91	0.53
20:Sc:14:VAL:HG11	20:Sc:30:VAL:HG11	1.91	0.53
23:SC:64:THR:HG23	23:SC:67:GLY:H	1.74	0.53
36:B:123:HIS:NE2	79:t:5019:A:OP1	2.42	0.53
36:B:264:PHE:N	50:P:64:THR:O	2.41	0.53
67:g:91:ASN:ND2	79:t:433:G:O2'	2.42	0.53
74:n:100:TYR:OH	79:t:4387:G:OP1	2.27	0.53
1:S2:1351:G:H8	6:SF:56:TYR:HB3	1.74	0.53
14:SS:25:LYS:HA	14:SS:55:ARG:HA	1.91	0.53
23:SC:176:LYS:O	23:SC:200[B]:ARG:NH1	2.42	0.53
37:C:242:PRO:HB2	79:t:2276:G:H4'	1.90	0.53
45:K:110:ARG:NH1	79:t:4403:A:OP2	2.42	0.53
46:L:89:VAL:HG21	46:L:114:ASP:HB3	1.90	0.53
82:u:1:G:N2	82:u:73:A:N7	2.47	0.53
1:S2:334:C:OP2	24:SG:190:ARG:NH2	2.42	0.52
1:S2:359:U:OP2	18:SX:18:ARG:NH1	2.42	0.52
7:SH:146:VAL:HA	7:SH:152:ARG:HA	1.90	0.52
12:SQ:37:ARG:HB3	15:ST:7:LYS:HG3	1.91	0.52
16:SU:26:SER:HB2	16:SU:32:LEU:HD23	1.91	0.52
22:Sg:166:VAL:HG12	22:Sg:176:VAL:HG22	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:N:44:GLN:NE2	79:t:922:A:O2'	2.42	0.52
76:p:44:LYS:NZ	79:t:91:G:OP1	2.35	0.52
77:q:19:GLY:O	77:q:23:ARG:NE	2.42	0.52
1:S2:74:G:H21	1:S2:75:G:H22	1.57	0.52
1:S2:94:G:O2'	1:S2:508:A:O2'	2.27	0.52
1:S2:1546:G:N2	1:S2:1670:C:O2	2.42	0.52
35:A:179:ILE:HG21	35:A:185:ALA:HB2	1.89	0.52
43:I:157:ILE:HD12	43:I:170:LEU:HD22	1.91	0.52
44:J:63:ASN:HD22	44:J:64:ARG:N	2.04	0.52
60:Z:55:VAL:HG11	60:Z:104:VAL:HG13	1.89	0.52
71:k:12:ARG:NH1	79:t:2780:U:O2'	2.42	0.52
79:t:455:G:H22	79:t:687:A:H2	1.56	0.52
1:S2:297:A:H2'	1:S2:298:G:H8	1.75	0.52
1:S2:1398:G:H1'	22:Sg:63:SER:HB3	1.90	0.52
28:SO:27:VAL:HG13	28:SO:90:ILE:HD12	1.90	0.52
30:SY:63:HIS:ND1	30:SY:68:LYS:O	2.38	0.52
32:Sb:40:CYS:SG	32:Sb:41:TYR:N	2.82	0.52
40:F:12:TYR:OH	79:t:4227:U:OP1	2.27	0.52
47:M:78:LEU:HA	47:M:81:LEU:HD12	1.91	0.52
76:p:39:ARG:NH1	79:t:289:A:OP2	2.42	0.52
79:t:1463:C:O2	79:t:1464:G:N2	2.42	0.52
1:S2:70:G:N7	24:SG:170:ARG:NH2	2.53	0.52
47:M:25:TRP:HZ3	79:t:1343:G:H5''	1.73	0.52
50:P:189:ILE:HD12	50:P:192:TYR:CD2	2.44	0.52
54:T:28:TYR:HE2	54:T:52:LYS:HG3	1.74	0.52
79:t:2590:A:H5'	79:t:2667:G:H4'	1.91	0.52
4:SD:101:GLN:HG3	4:SD:126:ILE:HD11	1.91	0.52
9:SK:52:LEU:HD12	9:SK:57:TYR:HB2	1.90	0.52
20:Sc:18:LEU:N	20:Sc:18:LEU:CD2	2.73	0.52
40:F:50:ARG:NH2	40:F:72:ASP:OD2	2.42	0.52
42:H:169:LEU:HD23	42:H:170:THR:H	1.73	0.52
47:M:27:ASN:O	47:M:31:ARG:N	2.42	0.52
47:M:63:THR:HG21	62:b:66:ASN:CG	2.33	0.52
79:t:40:G:N3	79:t:3885:U:N3	2.57	0.52
1:S2:1259:A:N6	1:S2:1519:U:O4'	2.43	0.52
22:Sg:76:GLN:NE2	22:Sg:91:ASP:OD1	2.42	0.52
26:SM:106:CYS:SG	26:SM:107:SER:N	2.82	0.52
41:G:155:GLY:HA2	79:t:4900:C:H5''	1.91	0.52
50:P:177:LEU:O	50:P:181:ALA:N	2.31	0.52
79:t:4433:U:HO2'	79:t:4647:U:HO2'	1.58	0.52
79:t:4480:A:OP1	79:t:4482:G:O2'	2.24	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:1549:U:OP1	21:Sd:34:TYR:OH	2.28	0.52
1:S2:1846:G:O6	75:o:8:LYS:NZ	2.43	0.52
7:SH:33:ASN:ND2	7:SH:82:GLU:OE2	2.42	0.52
20:Sc:14:VAL:CG1	20:Sc:30:VAL:CB	2.85	0.52
22:Sg:107:ASP:O	22:Sg:125:ARG:N	2.41	0.52
24:SG:139:SER:HA	24:SG:142:ARG:HB3	1.91	0.52
42:H:169:LEU:CD2	42:H:169:LEU:N	2.73	0.52
66:f:29:VAL:HG23	79:t:1315:C:H5'	1.91	0.52
70:j:74:LYS:NZ	79:t:3699:A:OP1	2.42	0.52
79:t:358:G:N2	79:t:370:A:OP2	2.35	0.52
79:t:3917:G:H1	79:t:4037:U:H3	1.56	0.52
79:t:4562:G:H1'	79:t:4563:U:H5	1.75	0.52
1:S2:27:A2M:HM'1	1:S2:483:C:H1'	1.91	0.52
1:S2:1288:U:HO2'	1:S2:1315:U:HO2'	1.44	0.52
5:SE:131:VAL:HA	5:SE:137:PRO:HA	1.91	0.52
23:SC:84:PHE:HB3	23:SC:86:LEU:HD23	1.91	0.52
39:E:26:C:O2'	46:L:147:ARG:NH1	2.34	0.52
50:P:89:PRO:HD3	79:t:1895:C:H4'	1.92	0.52
69:i:85:PRO:HB2	69:i:87:LYS:HE2	1.92	0.52
79:t:352:C:H2'	79:t:353:A:H8	1.75	0.52
79:t:659:G:N2	79:t:661:G:OP2	2.43	0.52
1:S2:1075:C:OP1	27:SN:107:LYS:NZ	2.43	0.52
1:S2:1570:G:H2'	1:S2:1571:G:H8	1.75	0.52
1:S2:1585:U:H5	15:ST:67:ARG:HD3	1.73	0.52
18:SX:19:ASP:HA	18:SX:22:TRP:HD1	1.75	0.52
24:SG:194:LEU:HD13	24:SG:197:GLN:HE21	1.74	0.52
36:B:315:ASN:ND2	36:B:325:GLU:OE2	2.43	0.52
37:C:10:VAL:HA	37:C:153:VAL:HG23	1.92	0.52
37:C:55:SER:HB3	79:t:351:U:P	2.50	0.52
79:t:1297:C:OP1	79:t:3852:G:N2	2.42	0.52
79:t:1427:G:N7	79:t:1429:C:N4	2.57	0.52
80:v:8:U:H3	80:v:14:C:H41	1.57	0.52
1:S2:167:G:O2'	24:SG:131:ARG:NE	2.43	0.52
1:S2:1048:G:N1	1:S2:1069:U:OP2	2.36	0.52
2:SA:38:ILE:HD11	2:SA:47:TYR:HB3	1.90	0.52
47:M:64:VAL:CG2	79:t:71:C:H5'	2.40	0.52
57:W:69:LYS:HB2	57:W:72:LEU:HD13	1.92	0.52
64:d:20:LEU:HD22	64:d:102:SER:HB3	1.91	0.52
69:i:95:LEU:N	69:i:95:LEU:CD1	2.73	0.52
72:l:33:LYS:NZ	79:t:2671:U:OP1	2.39	0.52
1:S2:1300:U:O2'	11:SP:51:ARG:NH2	2.43	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:Sg:40:ILE:HD11	22:Sg:66:VAL:HG21	1.91	0.51
50:P:189:ILE:HG23	50:P:190:ASP:N	2.25	0.51
52:R:29:VAL:HG23	52:R:51:LEU:HD22	1.91	0.51
76:p:27:LYS:CD	76:p:27:LYS:N	2.73	0.51
1:S2:1480:A:H5'	12:SQ:131:LYS:HE3	1.91	0.51
22:Sg:256:ILE:HB	22:Sg:270:LEU:HB2	1.93	0.51
22:Sg:297:THR:HG22	22:Sg:311:GLN:HG3	1.92	0.51
36:B:282:LYS:NZ	79:t:4636:C:O2'	2.43	0.51
55:U:112:ASN:O	55:U:115:LYS:N	2.35	0.51
1:S2:448:A:H61	8:SI:29:LEU:HD12	1.75	0.51
1:S2:692:G:N7	1:S2:734:C:N4	2.59	0.51
1:S2:954:U:O2	28:SO:55:ARG:NH2	2.40	0.51
3:SB:163:GLN:HG3	3:SB:204:ILE:HD13	1.92	0.51
5:SE:18:TRP:NE1	5:SE:41:CYS:O	2.41	0.51
22:Sg:73:SER:OG	22:Sg:114:SER:O	2.28	0.51
25:SJ:78:LEU:HA	25:SJ:81:LEU:HD23	1.92	0.51
54:T:85:ASP:HB2	54:T:123:SER:HB2	1.92	0.51
54:T:165:PRO:O	54:T:167:PHE:CA	2.58	0.51
68:h:6:THR:HG22	79:t:2379:G:H21	1.75	0.51
69:i:106:LYS:NZ	79:t:112:C:OP2	2.38	0.51
79:t:1997:C:H2'	79:t:1998:A:C8	2.44	0.51
79:t:2552:A:H62	79:t:2740:U:H3	1.58	0.51
82:u:9:A:O4'	82:u:46:G:N2	2.44	0.51
1:S2:596:U:O2'	1:S2:645:C:O2'	2.25	0.51
1:S2:899:U:N3	1:S2:902:G:OP2	2.43	0.51
1:S2:1245:G:O2'	1:S2:1492:U:OP1	2.25	0.51
1:S2:1720:U:O4	1:S2:1813:A:N6	2.41	0.51
4:SD:123:LEU:HD22	4:SD:152:PHE:HB3	1.91	0.51
11:SP:38:SER:OG	11:SP:41:GLN:OE1	2.28	0.51
37:C:323:ARG:HA	37:C:326:LEU:HB2	1.93	0.51
44:J:63:ASN:ND2	44:J:64:ARG:H	2.07	0.51
52:R:15:ARG:NH1	79:t:1673:G:OP1	2.43	0.51
58:X:70:LYS:HD3	58:X:71:ARG:HG2	1.91	0.51
63:c:95:ARG:NH1	79:t:1247:C:OP1	2.40	0.51
79:t:191:C:H42	79:t:242:C:H42	1.57	0.51
79:t:4438:C:O2'	79:t:4440:G:OP2	2.25	0.51
79:t:4853:C:N4	79:t:4854:G:N3	2.58	0.51
1:S2:882:U:H3	1:S2:904:A:H62	1.57	0.51
1:S2:1419:C:O2	1:S2:1420:G:O2'	2.24	0.51
1:S2:1650:A:H5''	12:SQ:139:ALA:HB2	1.91	0.51
2:SA:122:LEU:HB3	2:SA:144:THR:HG22	1.91	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Sa:44:ILE:HD11	28:SO:97:LEU:HD23	1.91	0.51
51:Q:115:GLU:OE1	51:Q:151:THR:OG1	2.26	0.51
52:R:67:ILE:HD11	52:R:92:VAL:HG21	1.93	0.51
67:g:9:ALA:HA	67:g:30:ILE:HA	1.92	0.51
68:h:89:ASP:O	68:h:93:ARG:N	2.40	0.51
79:t:3592:A:O2'	79:t:4620:G:O2'	2.27	0.51
79:t:3753:C:N4	79:t:3780:G:N7	2.58	0.51
79:t:4857:G:N2	79:t:4879:C:O2	2.37	0.51
1:S2:955:A:N6	1:S2:971:G:O2'	2.44	0.51
51:Q:69:ARG:NH2	79:t:4938:C:N3	2.58	0.51
51:Q:84:PRO:HB2	51:Q:87:SER:HB3	1.93	0.51
79:t:4383:C:H42	79:t:4437:G:H22	1.57	0.51
2:SA:31:ASP:N	2:SA:150:THR:O	2.44	0.51
2:SA:139:TYR:CE2	6:SF:61:PHE:HB2	2.46	0.51
22:Sg:8:ARG:NH1	22:Sg:311:GLN:OE1	2.41	0.51
22:Sg:46:THR:OG1	22:Sg:51:ASN:O	2.29	0.51
37:C:143:ARG:NH1	79:t:2279:A:N7	2.59	0.51
38:D:109:C:N3	71:k:20:ARG:NH2	2.59	0.51
63:c:99:ILE:O	63:c:109:ARG:NH1	2.41	0.51
67:g:109:ARG:CD	67:g:109:ARG:N	2.73	0.51
76:p:65:LYS:HE3	76:p:87:ARG:HH21	1.75	0.51
1:S2:649:U:P	18:SX:108:LYS:CD	2.87	0.51
1:S2:1138:C:H5'	1:S2:1138:C:H6	1.75	0.51
13:SR:27:ASP:O	13:SR:31:ASN:ND2	2.44	0.51
47:M:28:GLN:HG3	47:M:29:PRO:HD3	1.92	0.51
55:U:8:ARG:NH1	79:t:4295:C:O2'	2.40	0.51
60:Z:87:ARG:NH1	79:t:380:A:O2'	2.44	0.51
67:g:58:VAL:HG22	67:g:64:PRO:HA	1.91	0.51
78:r:68:SER:OG	79:t:663:C:OP1	2.29	0.51
79:t:4933:G:O2'	79:t:4935:A:N6	2.43	0.51
80:v:5:C:N4	80:v:6:G:O6	2.43	0.51
1:S2:869:A:O3'	1:S2:915:G:N2	2.44	0.51
6:SF:130:ARG:N	6:SF:130:ARG:CD	2.73	0.51
11:SP:106:GLU:CD	11:SP:107:ILE:O	2.54	0.51
15:ST:51:ASN:HB2	15:ST:54:TYR:HD2	1.76	0.51
22:Sg:139:LYS:HG3	22:Sg:140:TYR:HD1	1.76	0.51
22:Sg:165:ILE:HD11	22:Sg:179:LEU:HD22	1.92	0.51
41:G:110:ARG:NH2	79:t:955:C:O4'	2.43	0.51
43:I:59:ARG:HH21	79:t:2450:G:H5'	1.75	0.51
43:I:162:ASP:CB	43:I:163:PRO:HD3	2.38	0.51
67:g:56:ASN:OD1	67:g:64:PRO:HG2	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:i:80:PRO:O	69:i:84:ARG:HG3	2.11	0.51
79:t:4199:C:OP1	79:t:4289:C:O2'	2.25	0.51
79:t:4735:C:O2'	79:t:4736:C:O2	2.24	0.51
5:SE:137:PRO:HG2	5:SE:150:PRO:HD2	1.92	0.51
9:SK:59:LYS:O	9:SK:70:TYR:N	2.40	0.51
37:C:13:GLU:OE1	37:C:161:TYR:OH	2.28	0.51
37:C:316:LYS:NZ	79:t:1266:G:OP2	2.38	0.51
54:T:13:VAL:HG22	54:T:63:TYR:HB3	1.93	0.51
58:X:6:CYS:SG	58:X:9:SER:OG	2.64	0.51
65:e:87:ARG:HH12	65:e:122:VAL:HG11	1.75	0.51
79:t:2881:G:O6	79:t:3569:C:N4	2.43	0.51
79:t:4562:G:O2'	79:t:4571:G:O6	2.29	0.51
1:S2:406:U:O2'	1:S2:408:A:OP1	2.29	0.50
1:S2:495:U:OP1	5:SE:49:ARG:NH1	2.37	0.50
1:S2:1275:G:O2'	1:S2:1321:G:N2	2.40	0.50
1:S2:1563:G:OP1	15:ST:121:ARG:NH2	2.44	0.50
7:SH:162:GLN:NE2	7:SH:165:ASN:OD1	2.44	0.50
20:Sc:14:VAL:HG12	20:Sc:30:VAL:CB	2.40	0.50
36:B:242:ARG:NH2	79:t:2835:C:O2	2.45	0.50
37:C:144:ILE:HD13	37:C:150:LEU:HD21	1.93	0.50
42:H:159:TYR:CD1	42:H:168:ALA:HA	2.46	0.50
44:J:17:ASP:N	44:J:17:ASP:OD1	2.43	0.50
53:S:76:MET:SD	53:S:88:ARG:NH2	2.81	0.50
79:t:4485:A:H5''	79:t:4486:G:H5'	1.93	0.50
1:S2:1220:A:N3	1:S2:1677:U:O2'	2.38	0.50
3:SB:82:ARG:HH22	3:SB:191:ASP:HB2	1.75	0.50
6:SF:134:VAL:HG12	6:SF:135:ARG:HG2	1.94	0.50
10:SL:120:VAL:HG22	10:SL:145:VAL:HG21	1.93	0.50
13:SR:10:LYS:O	13:SR:14:ARG:NH1	2.44	0.50
36:B:372:SER:HB3	36:B:377:GLY:HA3	1.93	0.50
45:K:37:GLY:HA3	45:K:86:HIS:HA	1.93	0.50
47:M:50:PRO:HB3	47:M:149:GLN:HB2	1.91	0.50
47:M:63:THR:HG22	62:b:66:ASN:ND2	2.24	0.50
51:Q:112:LEU:HD22	51:Q:150:LEU:HB3	1.93	0.50
67:g:54:LYS:CD	79:t:437:G:OP1	2.57	0.50
79:t:4727:G:H22	79:t:4825:G:H1	1.58	0.50
1:S2:386:C:OP2	8:SI:10:LYS:NZ	2.42	0.50
1:S2:430:C:H2'	1:S2:431:G:H8	1.75	0.50
1:S2:1357:A:H62	25:SJ:65:GLU:C	2.19	0.50
1:S2:1386:A:OP2	4:SD:160:SER:OG	2.23	0.50
3:SB:171:ILE:HG12	3:SB:174:ARG:HH21	1.76	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:SH:154:ILE:HB	7:SH:185:VAL:HG12	1.93	0.50
35:A:203:ALA:O	79:t:1613:A:O2'	2.29	0.50
42:H:64:MET:HA	42:H:67:THR:HG22	1.93	0.50
43:I:81:ASN:ND2	43:I:236:HIS:HD2	2.01	0.50
50:P:183:LYS:HD2	50:P:184:ASN:HD22	1.77	0.50
69:i:66:LYS:NZ	69:i:82:ASP:OD2	2.45	0.50
1:S2:1751:C:N4	1:S2:1782:G:OP2	2.44	0.50
8:SI:177:SER:OG	8:SI:182:CYS:SG	2.62	0.50
21:Sd:46:TYR:O	21:Sd:47:ALA:C	2.53	0.50
42:H:169:LEU:H	42:H:169:LEU:HD22	1.76	0.50
54:T:111:ARG:NH2	79:t:2043:C:O2'	2.45	0.50
62:b:117:LEU:HD12	62:b:118:PRO:HD2	1.93	0.50
1:S2:1578:U:C6	4:SD:5:ILE:HA	2.47	0.50
1:S2:1658:G:OP2	1:S2:1660:C:N4	2.44	0.50
2:SA:75:SER:HA	2:SA:97:THR:HG23	1.94	0.50
28:SO:140:THR:HG23	28:SO:141:ARG:N	2.01	0.50
36:B:2:SER:O	36:B:3:HIS:ND1	2.45	0.50
37:C:339:THR:HA	37:C:342:ARG:HG2	1.94	0.50
38:D:71:A:OP1	60:Z:27:ARG:NH2	2.44	0.50
39:E:6:C:O2'	40:F:72:ASP:OD2	2.24	0.50
41:G:88:VAL:HG23	79:t:2237:C:H42	1.75	0.50
43:I:234:ARG:NH2	70:j:46:GLU:HB2	2.27	0.50
48:N:12:VAL:O	48:N:58:THR:OG1	2.24	0.50
55:U:7:LYS:O	79:t:4296:U:O2'	2.24	0.50
1:S2:165:G:OP2	1:S2:165:G:N2	2.38	0.50
4:SD:105:LEU:HA	4:SD:108:LYS:HB2	1.94	0.50
7:SH:145:ARG:NH1	29:SW:51:GLU:OE2	2.44	0.50
25:SJ:84:ILE:HD12	25:SJ:150:ARG:HA	1.93	0.50
32:Sb:23:ARG:NH1	32:Sb:27:SER:OG	2.45	0.50
36:B:99:LEU:HB2	79:t:4544:C:H4'	1.94	0.50
37:C:159:GLU:HA	37:C:217:ILE:HB	1.94	0.50
52:R:81:VAL:HB	52:R:138:LEU:HA	1.93	0.50
67:g:4:ARG:NH1	79:t:4715:U:OP1	2.44	0.50
79:t:1977:C:N4	79:t:1981:G:OP2	2.41	0.50
79:t:2772:G:H5''	79:t:2773:C:H5''	1.94	0.50
5:SE:123:LEU:HD22	5:SE:228:ILE:HG22	1.94	0.50
6:SF:204:ARG:HH12	20:Sc:63:ARG:HD2	1.77	0.50
48:N:12:VAL:HB	48:N:60:PHE:HB2	1.94	0.50
52:R:15:ARG:NE	52:R:53:MET:H	2.05	0.50
54:T:161:ARG:C	54:T:162:GLN:NE2	2.69	0.50
60:Z:82:ILE:HD12	60:Z:99:ILE:HD11	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
77:q:21:SER:OG	79:t:3664:U:O3'	2.29	0.50
1:S2:625:G:O2'	1:S2:629:A:N1	2.43	0.50
1:S2:929:G:N2	1:S2:1013:U:O2	2.38	0.50
22:Sg:120:ILE:O	22:Sg:132:TRP:N	2.45	0.50
37:C:55:SER:HB3	37:C:58:ALA:HB2	1.92	0.50
40:F:20:PHE:O	40:F:24:ARG:NE	2.44	0.50
40:F:22:ARG:O	40:F:26:GLY:N	2.44	0.50
41:G:206:VAL:O	41:G:256:GLN:NE2	2.44	0.50
56:V:104:ALA:HA	56:V:110:TYR:HA	1.93	0.50
72:l:17:ARG:NH2	79:t:2751:C:O2'	2.45	0.50
79:t:189:G:H22	79:t:244:G:H22	1.60	0.50
79:t:452:C:H42	79:t:690:C:H42	1.59	0.50
79:t:1952:C:OP2	79:t:1984:G:N1	2.43	0.50
1:S2:72:C:N3	1:S2:74:G:N2	2.60	0.50
1:S2:1145:A:O2'	1:S2:1200:A:OP1	2.30	0.50
1:S2:1495:G:N1	21:Sd:24:CYS:SG	2.83	0.50
1:S2:1720:U:O2'	79:t:3767:U:O2'	2.30	0.50
1:S2:1814:G:H21	79:t:3777:G:H21	1.59	0.50
1:S2:1866:A:OP1	19:Sa:95:ARG:NH1	2.44	0.50
24:SG:116:LYS:NZ	24:SG:125:THR:OG1	2.44	0.50
31:SZ:65:TYR:OH	31:SZ:76:ARG:NH1	2.45	0.50
42:H:115:ARG:HB3	52:R:3:VAL:HG21	1.93	0.50
49:O:124:ASP:OD1	79:t:3908:C:O2'	2.30	0.50
56:V:24:ASP:OD1	56:V:68:SER:OG	2.30	0.50
56:V:55:ASN:OD1	56:V:55:ASN:N	2.42	0.50
62:b:100:ILE:HA	62:b:123:ILE:HG13	1.93	0.50
79:t:2553:G:N1	79:t:2742:U:O4	2.45	0.50
1:S2:325:C:C4	58:X:119:LYS:CE	2.95	0.49
1:S2:325:C:C4	58:X:119:LYS:CD	2.95	0.49
1:S2:1356:G:H22	25:SJ:68:PRO:HG3	1.77	0.49
8:SI:191:GLU:O	10:SL:19:ASN:ND2	2.44	0.49
15:ST:23:LYS:HD3	15:ST:51:ASN:HD22	1.76	0.49
36:B:265:SER:OG	79:t:4421:U:O3'	2.29	0.49
45:K:76:MET:HE1	45:K:138:ILE:HD13	1.92	0.49
79:t:196:G:N2	79:t:206:U:OP1	2.45	0.49
79:t:1460:C:H2'	79:t:1461:G:H8	1.77	0.49
83:y:21:ALA:O	83:y:22:GLN:CB	2.59	0.49
1:S2:65:C:H4'	24:SG:172:LYS:HE2	1.93	0.49
1:S2:1299:A:OP1	11:SP:59:ARG:NH1	2.42	0.49
37:C:108:TRP:HB2	49:O:204:ARG:HH12	1.77	0.49
39:E:70:G:H2'	39:E:71:G:H8	1.77	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:J:4:ILE:C	44:J:60:TRP:O	2.53	0.49
76:p:25:GLN:NE2	76:p:26:TYR:O	2.39	0.49
79:t:108:A:N1	79:t:327:U:O2'	2.43	0.49
79:t:2030:G:H2'	79:t:2031:G:H8	1.76	0.49
1:S2:1423:C:N4	12:SQ:3:SER:OG	2.44	0.49
36:B:119:TYR:OH	36:B:129:ALA:N	2.46	0.49
45:K:156:LYS:HD2	45:K:165:ILE:HD11	1.94	0.49
47:M:64:VAL:HG22	79:t:71:C:H5'	1.94	0.49
54:T:83:ARG:HB3	54:T:125:GLN:HB2	1.93	0.49
54:T:162:GLN:NE2	54:T:162:GLN:N	2.60	0.49
79:t:2026:G:N2	79:t:2027:G:O6	2.45	0.49
1:S2:89:C:H2'	1:S2:90:G:H8	1.78	0.49
2:SA:184:ARG:HH21	2:SA:189:ILE:HG21	1.78	0.49
14:SS:23:ARG:HG3	31:SZ:48:VAL:HG21	1.93	0.49
18:SX:118:VAL:O	18:SX:119:ARG:NH1	2.38	0.49
25:SJ:162:ARG:NH2	25:SJ:168:GLY:O	2.45	0.49
35:A:123:ARG:NH1	79:t:4053:U:OP1	2.45	0.49
37:C:263:LEU:HD12	37:C:273:LEU:HD22	1.94	0.49
46:L:120:ASP:O	46:L:124:GLY:N	2.45	0.49
59:Y:95:THR:HG22	59:Y:139:ARG:HG3	1.93	0.49
62:b:114:LYS:HE2	79:t:1380:A:C8	2.48	0.49
76:p:28:LYS:HD3	76:p:28:LYS:C	2.37	0.49
76:p:61:LYS:NZ	79:t:4300:G:N7	2.57	0.49
79:t:741:U:O4	79:t:900:U:N3	2.45	0.49
79:t:3879:A:C2	83:y:20:ARG:HA	2.47	0.49
1:S2:86:C:O2'	1:S2:171:A:N1	2.41	0.49
1:S2:104:A:OP1	8:SI:12:ARG:NE	2.44	0.49
1:S2:682:U:H5'	18:SX:8:ARG:NH1	2.27	0.49
7:SH:144:ILE:HG23	29:SW:52:ILE:HB	1.94	0.49
7:SH:144:ILE:HD11	7:SH:152:ARG:HH11	1.77	0.49
26:SM:121:LYS:HA	26:SM:124:ILE:HG22	1.94	0.49
40:F:260:GLU:HG3	40:F:261:VAL:HG13	1.94	0.49
49:O:22:LEU:HA	49:O:25:VAL:HG12	1.94	0.49
69:i:17:LEU:O	69:i:21:LEU:N	2.44	0.49
70:j:34:THR:OG1	79:t:270:C:OP2	2.30	0.49
76:p:6:LYS:HE2	76:p:94:GLY:HA3	1.94	0.49
22:Sg:165:ILE:HB	22:Sg:177:TRP:HB2	1.94	0.49
26:SM:62:VAL:HA	26:SM:65:VAL:HG12	1.95	0.49
35:A:206:PRO:HG3	35:A:213:GLY:HA3	1.95	0.49
37:C:155:GLU:OE2	37:C:157:LYS:NZ	2.45	0.49
44:J:63:ASN:C	44:J:65:LYS:N	2.71	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:O:84:PRO:HA	49:O:87:HIS:HD2	1.78	0.49
60:Z:26:ARG:HG3	60:Z:78:TYR:HE1	1.78	0.49
63:c:14:ARG:NH2	79:t:1858:G:OP2	2.45	0.49
65:e:88:LEU:HG	65:e:106:VAL:HG22	1.94	0.49
1:S2:453:C:O2'	24:SG:92:ARG:O	2.31	0.49
1:S2:614:C:OP2	1:S2:626:G:O2'	2.30	0.49
1:S2:1495:G:N2	21:Sd:21:CYS:HG	2.10	0.49
31:SZ:47:LEU:CD1	31:SZ:47:LEU:CD2	2.81	0.49
37:C:315:LYS:HE2	42:H:169:LEU:HD21	1.95	0.49
79:t:112:C:H2'	79:t:113:A:H8	1.75	0.49
79:t:2795:G:N2	79:t:3593:C:O2	2.45	0.49
79:t:4292:G:H2'	79:t:4293:G:H8	1.77	0.49
79:t:4428:C:H2'	79:t:4429:A:H8	1.77	0.49
1:S2:531:A:N7	1:S2:532:C:N4	2.61	0.49
1:S2:838:G:O2'	1:S2:840:C:OP2	2.30	0.49
1:S2:1567:G:H1	14:SS:83:PHE:HB2	1.78	0.49
1:S2:1568:C:OP2	15:ST:98:SER:OG	2.31	0.49
13:SR:20:TYR:HD1	13:SR:23:ARG:HD3	1.78	0.49
30:SY:120:THR:O	30:SY:124:ASN:N	2.46	0.49
35:A:143:THR:HG23	35:A:145:LYS:HB2	1.95	0.49
35:A:159:SER:O	35:A:162:ASN:ND2	2.45	0.49
42:H:151:ASN:HA	42:H:191:ILE:HD11	1.94	0.49
44:J:37:ASP:OD1	44:J:37:ASP:N	2.45	0.49
51:Q:67:VAL:HG22	51:Q:82:ARG:HH21	1.76	0.49
52:R:17:GLU:C	52:R:52:PHE:CD1	2.90	0.49
55:U:108:ARG:HA	55:U:111:GLU:HG2	1.94	0.49
57:W:112:MET:HE1	57:W:117:ILE:HG13	1.95	0.49
57:W:115:SER:O	57:W:135:ASN:ND2	2.45	0.49
68:h:20:THR:HA	68:h:35:THR:HG22	1.94	0.49
73:m:2:SER:N	79:t:2385:G:O6	2.46	0.49
76:p:106:PHE:N	76:p:106:PHE:CD1	2.81	0.49
79:t:353:A:N3	79:t:357:A:O2'	2.46	0.49
79:t:425:G:H8	79:t:3859:G:H2'	1.78	0.49
79:t:727:C:N4	79:t:914:G:H1	2.11	0.49
79:t:3917:G:N2	79:t:4037:U:O2	2.32	0.49
13:SR:7:LYS:O	13:SR:11:LYS:N	2.43	0.49
22:Sg:20:GLN:HG2	22:Sg:68:ASP:HA	1.95	0.49
37:C:295:SER:OG	37:C:297:GLU:OE1	2.30	0.49
67:g:17:GLY:HA2	79:t:2049:C:H4'	1.94	0.49
79:t:132:G:N2	79:t:135:G:O6	2.46	0.49
79:t:1152:G:H2'	79:t:1153:G:H8	1.78	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
82:u:58:A:O2'	82:u:61:C:N4	2.46	0.49
1:S2:197:U:H1'	1:S2:201:C:H42	1.78	0.49
1:S2:379:C:O2	8:SI:31:ARG:NE	2.46	0.49
17:SV:35:ASN:ND2	23:SC:267:GLN:OE1	2.46	0.49
34:Sf:91:ASN:HD22	34:Sf:92:LYS:H	1.61	0.49
36:B:56:ILE:HG22	36:B:74:GLU:H	1.78	0.49
43:I:162:ASP:N	43:I:163:PRO:CD	2.76	0.49
45:K:57:TYR:HD1	45:K:130:HIS:HA	1.76	0.49
46:L:98:ASN:HD22	79:t:4212:G:H5''	1.77	0.49
49:O:20:ARG:HA	49:O:23:LEU:HB3	1.95	0.49
70:j:27:SER:N	79:t:157:G:OP2	2.44	0.49
73:m:28:ARG:HA	73:m:33:ASN:HD21	1.78	0.49
1:S2:325:C:H5	1:S2:328:U:H3	1.61	0.48
1:S2:888:U:OP2	1:S2:900:C:N4	2.46	0.48
3:SB:47:THR:OG1	3:SB:65:ARG:NH1	2.46	0.48
3:SB:89:GLU:HB3	3:SB:223:PHE:HE1	1.78	0.48
3:SB:138:PHE:HD2	3:SB:214:LYS:HB3	1.78	0.48
4:SD:105:LEU:HD22	4:SD:122:VAL:HG11	1.95	0.48
5:SE:73:ASP:OD2	5:SE:145:ARG:NH2	2.40	0.48
23:SC:103:LYS:NZ	23:SC:132:ASP:O	2.45	0.48
32:Sb:56:CYS:SG	32:Sb:57:VAL:N	2.86	0.48
37:C:155:GLU:HA	37:C:254:GLU:HG3	1.95	0.48
59:Y:60:TYR:CE2	69:i:84:ARG:NH2	2.81	0.48
70:j:31:GLY:HA2	79:t:302:G:H21	1.78	0.48
73:m:10:LYS:HD3	79:t:2760:G:H5''	1.94	0.48
79:t:2499:C:H5	79:t:2514:G:H1	1.61	0.48
79:t:4063:G:OP2	79:t:4063:G:N2	2.34	0.48
79:t:4722:G:H2'	79:t:4723:G:C8	2.47	0.48
1:S2:524:U:H5''	1:S2:525:A:H4'	1.96	0.48
1:S2:1174:U:OP1	75:o:21:ARG:NH1	2.46	0.48
5:SE:198:ARG:HA	5:SE:208:VAL:HG12	1.96	0.48
18:SX:7:LEU:HD23	18:SX:7:LEU:H	1.77	0.48
38:D:74:U:O2'	38:D:76:C:OP2	2.29	0.48
54:T:101:THR:HG23	54:T:104:GLY:H	1.78	0.48
56:V:103:VAL:O	56:V:111:GLU:N	2.45	0.48
79:t:1080:C:N4	79:t:1081:G:O6	2.46	0.48
1:S2:1152:U:H1'	29:SW:16:ASN:HD21	1.77	0.48
50:P:133:ARG:NH1	79:t:2036:G:OP2	2.43	0.48
57:W:61:VAL:N	57:W:79:ALA:O	2.42	0.48
78:r:37:SER:HB3	78:r:40:TYR:HB2	1.93	0.48
79:t:470:G:N3	79:t:672:G:N1	2.60	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:328:U:O2'	1:S2:329:G:O4'	2.31	0.48
1:S2:652:U:H2'	1:S2:653:A:H8	1.79	0.48
1:S2:1226:G:N1	1:S2:1639:G:OP2	2.39	0.48
4:SD:119:CYS:SG	4:SD:120:TYR:N	2.86	0.48
7:SH:166:VAL:HG12	7:SH:169:LYS:HD2	1.95	0.48
17:SV:78:ILE:HG23	17:SV:80:SER:H	1.78	0.48
21:Sd:41:GLN:H	21:Sd:41:GLN:CD	2.18	0.48
31:SZ:99:LEU:HD11	31:SZ:102:LYS:HB2	1.94	0.48
42:H:94:ARG:HB2	42:H:114:LEU:HD23	1.94	0.48
54:T:160:ARG:HG2	54:T:163:HIS:CG	2.48	0.48
54:T:174:THR:O	54:T:175:PHE:CB	2.60	0.48
55:U:41:ASP:HA	55:U:61:THR:HA	1.96	0.48
79:t:2558:G:N2	79:t:2561:A:OP2	2.39	0.48
3:SB:175:GLU:OE1	3:SB:187:LYS:NZ	2.43	0.48
16:SU:22:ILE:HG22	16:SU:114:VAL:HG22	1.95	0.48
22:Sg:129:ILE:O	22:Sg:141:THR:OG1	2.32	0.48
38:D:94:G:OP2	71:k:72:ARG:NH2	2.45	0.48
43:I:154:LEU:HD21	43:I:222:ILE:HG21	1.95	0.48
78:r:51:VAL:HG12	78:r:62:VAL:HG22	1.96	0.48
79:t:1309:A:OP2	79:t:4407:U:O2'	2.29	0.48
79:t:4601:G:H1	79:t:4622:G:H22	1.62	0.48
1:S2:752:G:OP2	1:S2:792:C:O2'	2.24	0.48
24:SG:68:LEU:H	24:SG:100:CYS:H	1.61	0.48
31:SZ:84:ALA:O	31:SZ:88:LEU:N	2.40	0.48
36:B:174:ARG:HH12	79:t:4932:C:H4'	1.78	0.48
43:I:79:ALA:HB3	49:O:18:VAL:HG21	1.95	0.48
43:I:175:ARG:HG2	43:I:227:ASN:HD22	1.78	0.48
68:h:107:LEU:HA	68:h:110:GLN:HE21	1.78	0.48
72:l:24:LYS:HD2	72:l:69:LEU:HD22	1.94	0.48
79:t:344:C:OP1	79:t:2273:G:O2'	2.31	0.48
1:S2:688:U:OP1	7:SH:121:THR:OG1	2.31	0.48
1:S2:730:C:H2'	1:S2:731:G:H4'	1.95	0.48
1:S2:1422:G:O2'	1:S2:1424:G:OP2	2.28	0.48
5:SE:95:THR:HB	30:SY:16:ARG:HD2	1.95	0.48
20:Sc:27:CYS:HA	20:Sc:47:LYS:HA	1.95	0.48
30:SY:18:LEU:O	30:SY:85:ASN:ND2	2.44	0.48
45:K:185:VAL:HA	45:K:190:LEU:HB2	1.95	0.48
53:S:20:LYS:NZ	79:t:2801:G:N7	2.52	0.48
64:d:31:TYR:OH	64:d:59:GLU:OE2	2.28	0.48
67:g:33:VAL:HG23	67:g:38:GLU:HG3	1.96	0.48
73:m:40:LYS:HZ3	79:t:360:A:H5'	1.79	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:1498:A:OP2	4:SD:27:ARG:NH2	2.38	0.48
14:SS:108:ARG:HH21	46:L:113:ILE:HD13	1.78	0.48
25:SJ:114:VAL:HG21	25:SJ:135:ILE:HD13	1.96	0.48
29:SW:116:ALA:O	29:SW:120:HIS:N	2.46	0.48
30:SY:6:THR:HB	30:SY:28:LEU:HB3	1.95	0.48
35:A:236:GLY:N	79:t:3658:A:O2'	2.47	0.48
47:M:163:LYS:HE3	47:M:165:LYS:HB3	1.96	0.48
64:d:48:LEU:HD13	64:d:57:LYS:HG3	1.96	0.48
79:t:220:G:HO2'	79:t:239:U:HO2'	1.59	0.48
1:S2:943:U:O2'	28:SO:135:ILE:O	2.31	0.48
1:S2:1156:U:O4	23:SC:194:ARG:NH1	2.46	0.48
3:SB:121:ILE:HG22	3:SB:161:VAL:HG13	1.95	0.48
4:SD:220:THR:OG1	4:SD:221:THR:N	2.44	0.48
5:SE:114:ILE:HG12	5:SE:118:GLU:HB3	1.96	0.48
7:SH:159:ASP:OD1	7:SH:159:ASP:N	2.45	0.48
16:SU:19:ARG:HB3	16:SU:119:ALA:HA	1.95	0.48
31:SZ:69:THR:HG22	31:SZ:71:ALA:H	1.79	0.48
36:B:384:GLU:OE2	58:X:14:TYR:OH	2.30	0.48
49:O:16:SER:OG	70:j:48:CYS:SG	2.63	0.48
51:Q:141:SER:OG	51:Q:142:SER:N	2.47	0.48
76:p:65:LYS:NZ	79:t:4300:G:OP1	2.43	0.48
78:r:66:ARG:NE	78:r:75:THR:O	2.46	0.48
79:t:207:C:H2'	79:t:208:G:H8	1.78	0.48
79:t:2532:A:H2	79:t:2744:A:H62	1.61	0.48
79:t:3636:G:N2	79:t:3656:C:O2'	2.47	0.48
79:t:4494:U:OP2	79:t:4516:G:N1	2.34	0.48
1:S2:871:U:H5'	27:SN:76:LYS:HE3	1.96	0.48
22:Sg:124:SER:OG	22:Sg:128:THR:O	2.32	0.48
23:SC:91:SER:HB2	23:SC:156:ILE:HG23	1.96	0.48
24:SG:79:LYS:HG3	24:SG:86:PRO:HG3	1.96	0.48
36:B:125:SER:OG	79:t:4925:A:OP2	2.31	0.48
37:C:323:ARG:NH2	79:t:1263:C:O2'	2.45	0.48
49:O:39:ALA:HB2	49:O:63:ARG:HE	1.78	0.48
49:O:93:LYS:O	79:t:294:A:O2'	2.30	0.48
50:P:116:LYS:N	79:t:4718:C:OP2	2.43	0.48
53:S:5:ARG:NH2	79:t:2364:U:OP1	2.47	0.48
53:S:23:TRP:CD1	53:S:50:ILE:HG12	2.49	0.48
55:U:110:LYS:HB2	55:U:110:LYS:HZ3	1.77	0.48
58:X:49:ILE:HB	58:X:51:TRP:CZ3	2.49	0.48
58:X:49:ILE:HD13	58:X:52:THR:HB	1.89	0.48
61:a:136:PHE:O	79:t:4091:G:O2'	2.31	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:d:28:VAL:HG23	64:d:34:THR:HG22	1.95	0.48
68:h:20:THR:HG22	68:h:34:TYR:HA	1.96	0.48
79:t:32:G:H1'	79:t:51:A:H61	1.79	0.48
79:t:1853:G:O2'	79:t:4181:A:N3	2.41	0.48
1:S2:572:U:OP1	30:SY:59:GLY:N	2.47	0.47
1:S2:1825:A:O2'	81:w:19:C:O2'	2.32	0.47
7:SH:42:GLU:HG2	7:SH:43:LEU:HD12	1.96	0.47
20:Sc:62:GLU:HG2	28:SO:121:ARG:HG3	1.95	0.47
25:SJ:162:ARG:HH22	25:SJ:169:ARG:HB3	1.78	0.47
29:SW:44:HIS:NE2	29:SW:112:ASP:OD2	2.45	0.47
32:Sb:19:HIS:HD2	32:Sb:21:LYS:H	1.62	0.47
36:B:220:ILE:HG12	36:B:278:THR:HG22	1.96	0.47
55:U:8:ARG:NH2	55:U:52:MET:SD	2.73	0.47
79:t:4727:G:N2	79:t:4825:G:H22	2.12	0.47
1:S2:67:C:N4	24:SG:168:LYS:O	2.46	0.47
1:S2:323:C:H2'	1:S2:327:G:H22	1.78	0.47
1:S2:1550:G:N2	1:S2:1559:C:O2	2.45	0.47
3:SB:138:PHE:O	3:SB:213:ARG:N	2.46	0.47
4:SD:167:TYR:OH	4:SD:202:LYS:O	2.32	0.47
14:SS:124:ARG:HH21	14:SS:129:LEU:HB3	1.79	0.47
18:SX:91:LEU:HD12	18:SX:94:ILE:HD11	1.96	0.47
41:G:64:SER:HA	79:t:1055:C:H41	1.79	0.47
42:H:154:ILE:O	42:H:169:LEU:HD11	2.14	0.47
63:c:25:ARG:HH21	79:t:1825:G:H5''	1.79	0.47
79:t:183:G:O2'	79:t:1349:G:N3	2.44	0.47
1:S2:1314:U:O2'	9:SK:2:LEU:O	2.29	0.47
35:A:201:GLY:N	79:t:3660:G:OP1	2.47	0.47
42:H:245:ARG:HH22	79:t:930:A:P	2.38	0.47
44:J:58:ASP:OD1	44:J:58:ASP:N	2.47	0.47
47:M:28:GLN:HA	47:M:31:ARG:HG2	1.97	0.47
69:i:91:MET:HA	69:i:94:ARG:CG	2.43	0.47
79:t:1924:A:N6	79:t:2020:G:O2'	2.47	0.47
79:t:4566:G:O2'	79:t:4568:G:N7	2.41	0.47
1:S2:788:G:O6	24:SG:233:ARG:NH2	2.41	0.47
1:S2:960:U:OP2	28:SO:38:ASN:ND2	2.47	0.47
1:S2:1251:A:N6	12:SQ:146:ARG:OXT	2.48	0.47
1:S2:1541:G:OP1	15:ST:56:ARG:NE	2.45	0.47
37:C:24:LEU:HD12	37:C:25:PRO:HD2	1.96	0.47
38:D:126:C:N4	79:t:2471:C:O2'	2.46	0.47
43:I:162:ASP:N	43:I:162:ASP:OD2	2.34	0.47
47:M:61:CYS:HB3	47:M:62:PRO:HD2	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:SD:164:VAL:HG23	4:SD:168:VAL:HG21	1.97	0.47
6:SF:20:PHE:O	6:SF:22:LYS:NZ	2.44	0.47
6:SF:170:ALA:HB3	31:SZ:106:GLN:HE21	1.79	0.47
11:SP:96:VAL:HG23	11:SP:120:SER:HB2	1.96	0.47
22:Sg:254:PRO:HB2	22:Sg:283:PRO:HB2	1.97	0.47
30:SY:21:LYS:N	30:SY:75:ILE:O	2.46	0.47
42:H:167:ILE:HD13	42:H:174:LEU:HD23	1.96	0.47
44:J:63:ASN:OD1	44:J:65:LYS:CE	2.62	0.47
46:L:150:CYS:SG	46:L:151:ILE:N	2.83	0.47
50:P:167:HIS:HA	50:P:170:LYS:HG2	1.97	0.47
68:h:25:THR:HG22	79:t:2500:G:H5'	1.97	0.47
71:k:13:ASN:OD1	71:k:13:ASN:N	2.41	0.47
74:n:100:TYR:O	79:t:4434:G:O2'	2.32	0.47
78:r:91:SER:HA	78:r:94:ARG:HG2	1.96	0.47
1:S2:1314:U:H4'	9:SK:3:MET:HG2	1.97	0.47
24:SG:119:LYS:HE3	24:SG:121:ILE:HG12	1.96	0.47
25:SJ:52:LYS:O	25:SJ:56:ALA:N	2.45	0.47
40:F:52:ILE:N	40:F:63:GLN:O	2.47	0.47
55:U:9:ARG:HB3	55:U:55:LYS:HE3	1.97	0.47
58:X:51:TRP:CG	58:X:52:THR:H	2.31	0.47
67:g:109:ARG:HD2	67:g:109:ARG:N	2.29	0.47
79:t:435:G:H2'	79:t:436:G:H8	1.80	0.47
79:t:1196:G:OP2	79:t:1196:G:N2	2.45	0.47
79:t:3879:A:C8	83:y:22:GLN:CB	2.96	0.47
79:t:4712:G:H22	79:t:4909:G:N2	2.13	0.47
1:S2:346:C:O2'	5:SE:30:ARG:NH1	2.48	0.47
1:S2:509:OMG:H2'	1:S2:510:G:C8	2.46	0.47
1:S2:644:OMG:H2'	1:S2:645:C:O4'	2.15	0.47
1:S2:844:U:H2'	1:S2:845:G:H8	1.79	0.47
1:S2:990:A:OP1	3:SB:116:LYS:NZ	2.40	0.47
1:S2:1024:A:OP2	27:SN:124:ARG:NH2	2.37	0.47
4:SD:59:LEU:HD22	4:SD:66:ILE:HD11	1.97	0.47
6:SF:93:VAL:HA	6:SF:96:ALA:HB3	1.97	0.47
18:SX:107:ARG:HG3	18:SX:112:VAL:HG12	1.97	0.47
20:Sc:21:THR:HG23	20:Sc:27:CYS:HB2	1.97	0.47
22:Sg:73:SER:HB2	22:Sg:117:ASN:HD21	1.79	0.47
49:O:105:ARG:NH1	79:t:2438:G:N7	2.63	0.47
52:R:182:ALA:HB2	52:R:187:LYS:HE3	1.96	0.47
54:T:164:LYS:HE3	54:T:164:LYS:HB3	1.74	0.47
55:U:3:ASN:OD1	55:U:9:ARG:NH2	2.48	0.47
57:W:84:GLN:NE2	57:W:86:LYS:O	2.48	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:Y:79:PHE:HE1	69:i:32:ARG:HD3	1.80	0.47
66:f:38:PRO:HB2	66:f:43:ASN:HD21	1.79	0.47
67:g:6:TRP:CD2	67:g:102:ARG:HG3	2.50	0.47
69:i:90:ALA:O	69:i:94:ARG:HG2	2.15	0.47
77:q:70:THR:OG1	77:q:71:TYR:N	2.48	0.47
79:t:1337:A:N1	79:t:1368:G:O2'	2.39	0.47
79:t:4486:G:OP1	79:t:4521:A:N6	2.42	0.47
1:S2:682:U:H5'	18:SX:8:ARG:HE	1.80	0.47
1:S2:1256:G:OP2	21:Sd:40:ARG:HD3	2.15	0.47
14:SS:24:ARG:HB2	14:SS:29:ALA:HB2	1.96	0.47
18:SX:107:ARG:CG	18:SX:112:VAL:HG12	2.44	0.47
20:Sc:12:ALA:HB1	20:Sc:32:VAL:HB	1.95	0.47
20:Sc:32:VAL:HG21	20:Sc:58:LEU:HD11	1.97	0.47
21:Sd:38:MET:HE3	21:Sd:43:PHE:CD1	2.46	0.47
22:Sg:202:PRO:HG2	22:Sg:243:PRO:HA	1.97	0.47
37:C:137:VAL:HG11	37:C:150:LEU:HD11	1.97	0.47
45:K:204:GLY:HA3	45:K:208:LYS:HE3	1.96	0.47
51:Q:7:ASP:N	51:Q:7:ASP:OD1	2.46	0.47
54:T:161:ARG:HH21	54:T:161:ARG:HG3	1.80	0.47
63:c:5:LYS:NZ	79:t:1854:A:OP2	2.35	0.47
79:t:445:C:O2	79:t:1279:G:N2	2.44	0.47
79:t:1069:C:N4	79:t:1193:C:H42	2.13	0.47
79:t:4666:C:H2'	79:t:4667:A:H8	1.79	0.47
3:SB:35:ALA:HB2	3:SB:44:ILE:HD11	1.97	0.47
6:SF:47:LYS:HE3	12:SQ:116:ASP:HB3	1.95	0.47
18:SX:67:ARG:NH1	18:SX:114:ASP:OD2	2.44	0.47
25:SJ:131:ARG:HA	25:SJ:143:ASN:HB2	1.97	0.47
47:M:108:GLU:HG2	70:j:18:THR:HG22	1.96	0.47
49:O:4:TYR:OH	79:t:149:U:OP2	2.29	0.47
51:Q:60:PHE:O	51:Q:78:TRP:NE1	2.48	0.47
66:f:128:ARG:HH22	79:t:2285:G:H3'	1.80	0.47
74:n:94:MET:HG2	74:n:105:PRO:HA	1.97	0.47
78:r:39:ARG:NH1	78:r:105:ASP:OD2	2.48	0.47
79:t:2618:U:O2'	79:t:2673:G:N1	2.32	0.47
79:t:4235:A:N6	79:t:4296:U:O4	2.48	0.47
79:t:4722:G:H2'	79:t:4723:G:H8	1.79	0.47
1:S2:1046:U:O2'	28:SO:140:THR:HG23	2.15	0.47
26:SM:95:ASP:HB3	26:SM:98:GLY:H	1.80	0.47
36:B:219:VAL:HG11	36:B:337:VAL:HG13	1.97	0.47
41:G:50:LEU:HD12	41:G:51:VAL:HG23	1.96	0.47
47:M:76:PHE:H	47:M:76:PHE:HD2	1.62	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:T:142:VAL:HG12	54:T:146:HIS:HE1	1.80	0.47
61:a:51:ARG:HB2	61:a:65:ARG:HB3	1.97	0.47
79:t:2374:A:O2'	79:t:2786:A:OP2	2.32	0.47
1:S2:193:C:O2'	1:S2:195:C:N4	2.34	0.46
1:S2:985:G:H4'	28:SO:138:ASP:CG	2.30	0.46
1:S2:1138:C:H42	6:SF:60:ARG:HH12	1.61	0.46
14:SS:63:GLU:OE1	14:SS:66:ARG:NH2	2.48	0.46
29:SW:55:ASP:OD2	29:SW:57:ARG:NH1	2.42	0.46
30:SY:89:HIS:CD2	30:SY:90:ARG:HG3	2.51	0.46
35:A:97:ASN:H	35:A:100:ASN:HD22	1.63	0.46
42:H:169:LEU:HD23	42:H:169:LEU:N	2.31	0.46
45:K:147:HIS:O	45:K:151:ALA:N	2.35	0.46
79:t:133:C:N4	79:t:135:G:N3	2.63	0.46
79:t:690:C:N4	79:t:691:G:O6	2.48	0.46
79:t:748:G:O6	79:t:892:C:N4	2.49	0.46
79:t:1908:U:OP1	79:t:1930:U:O2'	2.33	0.46
1:S2:652:U:H2'	1:S2:653:A:C8	2.50	0.46
1:S2:1265:A:H2	1:S2:1517:G:H22	1.63	0.46
2:SA:30:LEU:HA	2:SA:150:THR:HB	1.97	0.46
2:SA:106:GLY:O	2:SA:113:GLN:NE2	2.45	0.46
4:SD:69:LEU:HA	4:SD:72:VAL:HG22	1.96	0.46
6:SF:130:ARG:H	6:SF:130:ARG:CD	2.27	0.46
20:Sc:26:GLN:O	20:Sc:47:LYS:CB	2.61	0.46
29:SW:96:SER:OG	29:SW:98:GLN:NE2	2.49	0.46
37:C:195:LYS:NZ	79:t:2313:C:OP2	2.47	0.46
43:I:100:HIS:CE1	43:I:103:ARG:HH21	2.34	0.46
47:M:61:CYS:CB	47:M:62:PRO:HD2	2.44	0.46
67:g:109:ARG:HD2	67:g:110:ILE:N	2.22	0.46
69:i:96:ASN:O	69:i:100:GLU:HG3	2.15	0.46
5:SE:212:ASP:OD1	5:SE:216:ASN:N	2.44	0.46
15:ST:118:ASP:OD1	15:ST:118:ASP:N	2.48	0.46
36:B:181:MET:HG2	36:B:182:GLU:H	1.79	0.46
37:C:325:MET:O	37:C:329:ASN:N	2.49	0.46
40:F:4:VAL:N	79:t:1760:C:O2'	2.45	0.46
41:G:232:ILE:O	41:G:237:LYS:NZ	2.48	0.46
44:J:63:ASN:ND2	44:J:63:ASN:C	2.73	0.46
46:L:90:ARG:NH2	46:L:108:GLY:O	2.48	0.46
47:M:77:SER:CB	47:M:102:ARG:O	2.63	0.46
52:R:49:LYS:O	52:R:53:MET:SD	2.74	0.46
54:T:81:TRP:HB3	54:T:127:MET:HE3	1.96	0.46
54:T:161:ARG:HG3	54:T:161:ARG:NH2	2.29	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:i:88:THR:HG22	69:i:91:MET:CG	2.44	0.46
79:t:465:A:H62	79:t:677:G:H21	1.61	0.46
79:t:708:U:H3	79:t:938:G:H1	1.63	0.46
79:t:1410:A:OP2	79:t:1439:G:N2	2.38	0.46
80:v:62:C:H2'	80:v:63:G:C8	2.50	0.46
1:S2:137:U:OP1	58:X:101:ARG:NE	2.44	0.46
1:S2:325:C:N4	1:S2:329:G:O2'	2.49	0.46
1:S2:1544:C:N4	1:S2:1589:A:OP2	2.48	0.46
6:SF:57:ALA:HB3	23:SC:157:LEU:HD11	1.97	0.46
14:SS:36:VAL:HG13	14:SS:40:TYR:HD2	1.79	0.46
26:SM:64:LEU:HD11	34:Sf:106:TYR:HB2	1.97	0.46
35:A:189:TYR:HB2	35:A:196:TRP:HB2	1.98	0.46
36:B:11:HIS:HE1	57:W:48:ARG:HH22	1.63	0.46
37:C:190:ARG:HA	37:C:202:ILE:HD11	1.97	0.46
43:I:81:ASN:ND2	43:I:236:HIS:NE2	2.62	0.46
43:I:164:ILE:CG2	49:O:22:LEU:HD12	2.25	0.46
44:J:62:GLY:O	44:J:67:LEU:CD2	2.53	0.46
55:U:13:TYR:OH	79:t:1772:U:OP2	2.33	0.46
64:d:43:ALA:HA	64:d:97:ILE:HG22	1.96	0.46
69:i:48:ARG:HA	69:i:51:ARG:HG2	1.98	0.46
79:t:67:C:N4	79:t:319:U:O2'	2.48	0.46
79:t:2637:G:N2	79:t:2637:G:OP2	2.49	0.46
79:t:3850:G:O2'	79:t:3852:G:OP2	2.33	0.46
80:v:63:G:H2'	80:v:64:A:C8	2.51	0.46
1:S2:212:C:N4	1:S2:213:G:O6	2.49	0.46
1:S2:373:G:OP1	10:SL:137:THR:OG1	2.25	0.46
1:S2:377:G:H5''	8:SI:98:LYS:HB3	1.96	0.46
9:SK:51:SER:O	9:SK:55:ARG:NE	2.45	0.46
22:Sg:82:SER:OG	22:Sg:83:TRP:N	2.48	0.46
36:B:378:ARG:NH1	79:t:4961:U:OP2	2.47	0.46
38:D:102:G:OP2	38:D:104:A:O2'	2.29	0.46
40:F:184:ASP:HB3	40:F:187:SER:HB3	1.97	0.46
52:R:11:ARG:NH2	79:t:1672:C:OP2	2.38	0.46
55:U:105:PHE:HA	55:U:108:ARG:HG2	1.97	0.46
56:V:88:LYS:HE2	56:V:97:ARG:HH21	1.80	0.46
62:b:73:VAL:HG13	62:b:77:LYS:HB2	1.96	0.46
63:c:36:ASP:OD1	63:c:36:ASP:N	2.49	0.46
65:e:97:ASP:N	65:e:97:ASP:OD1	2.48	0.46
79:t:413:A:N3	79:t:1315:C:O2'	2.46	0.46
1:S2:560:A:C6	25:SJ:165:TYR:HA	2.51	0.46
1:S2:649:U:C5'	18:SX:108:LYS:CD	2.91	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:1060:A:O2'	1:S2:1062:A:N7	2.44	0.46
1:S2:1858:G:H2'	1:S2:1859:A:H8	1.79	0.46
2:SA:74:VAL:HG12	2:SA:121:LEU:HB3	1.97	0.46
12:SQ:19:ALA:HB2	12:SQ:75:GLY:HA3	1.97	0.46
23:SC:166:ARG:NH1	23:SC:254:ASP:OD2	2.49	0.46
23:SC:203:GLY:H	23:SC:221:ASP:HB3	1.81	0.46
41:G:138:ARG:NH1	41:G:169:ALA:O	2.49	0.46
62:b:103:VAL:HB	62:b:108:TYR:HB2	1.98	0.46
5:SE:90:ILE:HG13	5:SE:99:PHE:HB2	1.96	0.46
20:Sc:29:GLN:HA	20:Sc:45:ASN:CA	2.19	0.46
21:Sd:38:MET:HE1	21:Sd:43:PHE:CD1	2.51	0.46
44:J:4:ILE:CD1	54:T:144:GLN:CD	2.89	0.46
62:b:87:ARG:O	62:b:120:GLN:NE2	2.37	0.46
62:b:116:LYS:HE2	79:t:1402:G:C6	2.50	0.46
69:i:88:THR:HG22	69:i:91:MET:HB2	1.98	0.46
71:k:36:LYS:HA	71:k:45:ARG:HH21	1.81	0.46
79:t:1951:A:H2'	79:t:1997:C:H42	1.81	0.46
8:SI:81:VAL:HG22	8:SI:102:VAL:HG23	1.96	0.46
8:SI:178:ARG:HD3	8:SI:181:GLN:HG2	1.98	0.46
35:A:55:GLY:HA3	35:A:174:ARG:HH11	1.80	0.46
40:F:144:CYS:SG	40:F:145:TYR:N	2.89	0.46
79:t:671:C:H2'	79:t:672:G:C8	2.51	0.46
79:t:723:A:H61	79:t:921:C:H42	1.63	0.46
79:t:2348:U:OP1	79:t:2806:G:N1	2.37	0.46
79:t:2737:G:O2'	79:t:2744:A:N3	2.45	0.46
1:S2:916:A:C4	27:SN:73:ARG:HD3	2.51	0.46
1:S2:986:G:O4'	28:SO:138:ASP:CG	2.58	0.46
1:S2:1122:A:N3	3:SB:146:ARG:NH1	2.64	0.46
1:S2:1222:G:H5''	6:SF:78:MET:HE1	1.98	0.46
1:S2:1480:A:H2'	1:S2:1481:G:H8	1.80	0.46
21:Sd:46:TYR:CB	21:Sd:49:ASP:HB2	2.38	0.46
23:SC:107:LEU:HD22	23:SC:209:VAL:HG23	1.97	0.46
37:C:55:SER:HG	79:t:351:U:P	2.39	0.46
37:C:116:ASN:OD1	37:C:116:ASN:N	2.48	0.46
42:H:60:GLU:HA	42:H:63:GLN:HG2	1.98	0.46
42:H:226:HIS:CD2	42:H:234:GLY:HA3	2.50	0.46
43:I:209:SER:HA	43:I:212:LYS:HB2	1.98	0.46
51:Q:64:ASN:ND2	51:Q:80:GLN:OE1	2.49	0.46
52:R:122:THR:H	52:R:125:GLN:HE21	1.64	0.46
56:V:60:VAL:HG23	56:V:61:VAL:HG12	1.97	0.46
69:i:95:LEU:CD1	69:i:95:LEU:H	2.29	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
71:k:46:LYS:NZ	79:t:24:G:N7	2.49	0.46
79:t:2070:U:H4'	79:t:2071:C:H3'	1.97	0.46
1:S2:97:U:O2	1:S2:434:G:N2	2.49	0.46
1:S2:1276:A:O2'	9:SK:50:GLN:O	2.34	0.46
1:S2:1830:UR3:H4'	1:S2:1851:MA6:H103	1.99	0.46
33:Se:34:ARG:HD3	33:Se:37:GLN:HE21	1.81	0.46
43:I:165:GLU:HG2	43:I:166:LEU:N	2.31	0.46
62:b:2:PRO:HG2	79:t:1491:C:H5''	1.97	0.46
63:c:32:LEU:HD13	63:c:40:LEU:HD11	1.98	0.46
64:d:21:VAL:HG21	64:d:104:ILE:HD11	1.98	0.46
79:t:1152:G:H2'	79:t:1153:G:C8	2.51	0.46
79:t:1460:C:H2'	79:t:1461:G:C8	2.51	0.46
79:t:1972:A:H2'	79:t:1973:U:H2'	1.97	0.46
79:t:2462:G:N2	79:t:2474:U:O2	2.33	0.46
1:S2:1644:C:H4'	12:SQ:140:ARG:HB2	1.98	0.45
27:SN:87:ASP:OD1	27:SN:87:ASP:N	2.49	0.45
37:C:245:HIS:NE2	79:t:2317:C:O2	2.46	0.45
43:I:163:PRO:CB	43:I:166:LEU:HG	2.41	0.45
79:t:216:G:H1	79:t:233:G:H1	1.64	0.45
79:t:4064:G:N1	79:t:4083:C:N3	2.64	0.45
1:S2:1357:A:N3	25:SJ:70:ARG:HD3	2.30	0.45
1:S2:1507:G:N2	34:Sf:85:TYR:O	2.49	0.45
4:SD:8:LYS:HE3	16:SU:59:LYS:HD3	1.98	0.45
11:SP:92:SER:O	11:SP:107:ILE:HG13	2.15	0.45
36:B:245:HIS:HB3	79:t:4487:C:H5''	1.97	0.45
41:G:149:ILE:HD12	41:G:271:LEU:HD21	1.98	0.45
42:H:68:GLU:O	42:H:72:ALA:N	2.43	0.45
47:M:128:PRO:HD3	47:M:136:LYS:HG2	1.97	0.45
49:O:195:ARG:NH2	79:t:98:A:O3'	2.49	0.45
62:b:26:ARG:NH2	79:t:1638:U:OP2	2.49	0.45
71:k:12:ARG:NH2	79:t:1599:G:O3'	2.49	0.45
79:t:1058:G:H1	79:t:1218:G:H1	1.64	0.45
79:t:4566:G:N2	79:t:4569:A:OP2	2.49	0.45
79:t:4727:G:H22	79:t:4825:G:H22	1.63	0.45
1:S2:317:C:OP2	24:SG:183:ARG:NH2	2.49	0.45
1:S2:1017:U:H5	27:SN:14:SER:HB2	1.80	0.45
1:S2:1298:G:N2	1:S2:1514:G:O2'	2.49	0.45
5:SE:20:LEU:HD21	5:SE:46:ILE:HG21	1.97	0.45
12:SQ:112:LEU:HD22	12:SQ:119:LEU:HD22	1.97	0.45
20:Sc:37:ASP:OD2	20:Sc:39:SER:OG	2.31	0.45
24:SG:217:MET:HA	24:SG:220:ALA:HB3	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:SJ:83:ARG:HE	25:SJ:150:ARG:HD3	1.80	0.45
36:B:3:HIS:ND1	79:t:4478:G:OP2	2.49	0.45
36:B:339:GLY:N	79:t:4587:C:OP1	2.46	0.45
48:N:92:ALA:HA	48:N:95:ILE:HG13	1.99	0.45
54:T:164:LYS:CB	54:T:165:PRO:HD3	2.15	0.45
67:g:3:GLY:O	79:t:4903:G:N1	2.42	0.45
79:t:162:A:H61	79:t:265:C:H42	1.65	0.45
79:t:1380:A:HO2'	79:t:1449:C:HO2'	1.59	0.45
82:u:14:A:N6	82:u:22:G:N3	2.64	0.45
1:S2:409:C:H2'	1:S2:410:G:H8	1.81	0.45
11:SP:98:ASN:OD1	11:SP:101:THR:N	2.38	0.45
20:Sc:14:VAL:HG12	20:Sc:32:VAL:HG12	1.98	0.45
22:Sg:84:ASP:OD1	22:Sg:84:ASP:N	2.46	0.45
23:SC:144:SER:HB3	23:SC:150:ALA:HB2	1.97	0.45
24:SG:55:GLY:HA3	24:SG:109:LEU:HA	1.98	0.45
29:SW:96:SER:OG	29:SW:97:ARG:N	2.49	0.45
37:C:218:ILE:HD12	37:C:229:LEU:HD22	1.98	0.45
53:S:128:LYS:NZ	79:t:2647:G:OP1	2.50	0.45
76:p:99:ARG:O	76:p:102:GLN:OE1	2.34	0.45
79:t:713:G:N2	79:t:934:C:O2	2.49	0.45
79:t:900:U:N3	79:t:901:U:O4	2.49	0.45
1:S2:1568:C:O2'	1:S2:1569:A:O4'	2.35	0.45
1:S2:1751:C:H6	58:X:76:VAL:HG12	1.82	0.45
23:SC:183:LYS:HD3	23:SC:194:ARG:HH21	1.81	0.45
24:SG:49:VAL:HG22	24:SG:115:LYS:HB3	1.97	0.45
29:SW:111:MET:HE1	29:SW:119:LYS:HE2	1.99	0.45
46:L:30:GLY:O	46:L:34:THR:OG1	2.26	0.45
48:N:29:ASP:O	48:N:37:LEU:N	2.49	0.45
54:T:160:ARG:CD	54:T:163:HIS:CG	2.94	0.45
61:a:70:SER:OG	61:a:111:ARG:O	2.31	0.45
69:i:88:THR:HG22	69:i:91:MET:CB	2.47	0.45
79:t:2314:C:H2'	79:t:2315:G:H8	1.82	0.45
1:S2:1005:G:C4	64:d:8:LYS:HB2	2.51	0.45
6:SF:188:TYR:HA	6:SF:191:LYS:HG2	1.99	0.45
8:SI:84:ASN:HD22	8:SI:90:LEU:HB2	1.80	0.45
31:SZ:47:LEU:CD1	31:SZ:47:LEU:CB	2.81	0.45
50:P:120:VAL:HG12	50:P:122:ALA:H	1.81	0.45
79:t:25:A:N3	79:t:333:C:O2'	2.46	0.45
79:t:950:G:O6	79:t:2075:A:N6	2.49	0.45
79:t:3754:A:H2	79:t:3761:U:H3	1.65	0.45
79:t:3872:A:N6	79:t:4408:U:O2'	2.49	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:t:4723:G:H1'	79:t:4727:G:H5'	1.98	0.45
1:S2:847:A:O3'	5:SE:106:LYS:NZ	2.50	0.45
2:SA:65:ILE:HG23	2:SA:74:VAL:HG11	1.98	0.45
2:SA:177:MET:SD	2:SA:180:ARG:NH2	2.75	0.45
22:Sg:212:LYS:HA	22:Sg:235:ILE:HG13	1.98	0.45
35:A:126:LEU:HD13	35:A:150:LEU:HD11	1.99	0.45
36:B:89:ILE:HG13	36:B:201:LEU:HD21	1.99	0.45
44:J:63:ASN:HB3	44:J:66:GLU:OE1	2.16	0.45
49:O:12:ARG:HG2	79:t:273:A:H2'	1.98	0.45
50:P:14:HIS:HE1	50:P:120:VAL:H	1.65	0.45
74:n:119:ASN:ND2	79:t:1927:G:OP1	2.50	0.45
80:v:63:G:H2'	80:v:64:A:H8	1.81	0.45
1:S2:1447:G:H2'	1:S2:1448:A:C8	2.52	0.45
2:SA:159:ILE:HD11	17:SV:34:MET:HE1	1.99	0.45
3:SB:107:ARG:NH1	28:SO:131:ASP:OD2	2.50	0.45
3:SB:123:ALA:HB2	3:SB:165:ARG:HG3	1.98	0.45
11:SP:81:ARG:HH12	11:SP:98:ASN:HA	1.82	0.45
25:SJ:78:LEU:HD23	25:SJ:92:MET:HB2	1.98	0.45
31:SZ:47:LEU:HA	31:SZ:47:LEU:HD23	1.64	0.45
40:F:107:ARG:HG2	40:F:248:ARG:HA	1.98	0.45
40:F:206:ASP:OD1	40:F:209:ARG:NH1	2.48	0.45
46:L:20:LEU:HD13	46:L:132:VAL:HG22	1.99	0.45
47:M:58:ILE:HG23	47:M:70:VAL:HG13	1.99	0.45
52:R:4:ASP:OD1	52:R:4:ASP:N	2.49	0.45
52:R:158:THR:CB	52:R:159:PRO:CD	2.92	0.45
79:t:301:A:N3	79:t:304:G:O2'	2.37	0.45
79:t:2532:A:N3	79:t:2743:A:N6	2.65	0.45
79:t:2773:C:H42	83:y:11:LEU:CB	2.29	0.45
79:t:4479:A:H5''	79:t:4480:A:H5''	1.98	0.45
1:S2:846:G:OP2	5:SE:108:ARG:NH2	2.49	0.45
1:S2:913:A:N6	7:SH:99:ARG:O	2.50	0.45
4:SD:5:ILE:HD11	4:SD:10:LYS:HD3	1.98	0.45
4:SD:6:SER:O	4:SD:9:ARG:HG2	2.17	0.45
22:Sg:257:LYS:HG2	22:Sg:269:GLU:HG2	1.99	0.45
30:SY:55:ILE:HG13	30:SY:75:ILE:HG12	1.99	0.45
41:G:164:PHE:HA	41:G:175:VAL:HG23	1.99	0.45
41:G:190:HIS:HD2	41:G:192:LYS:HG2	1.81	0.45
52:R:18:PRO:CD	52:R:52:PHE:HE1	2.26	0.45
58:X:11:TYR:OH	79:t:4999:G:N2	2.50	0.45
77:q:36:LYS:HE3	77:q:48:LYS:HD3	1.99	0.45
79:t:675:G:H2'	79:t:676:G:C8	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:t:2462:G:H1	79:t:2474:U:H3	1.65	0.45
79:t:3879:A:C2	83:y:20:ARG:CA	2.99	0.45
1:S2:641:A:O5'	25:SJ:40:LYS:NZ	2.50	0.45
1:S2:1446:A:H1'	16:SU:55:ARG:HD2	1.99	0.45
24:SG:142:ARG:HA	58:X:83:THR:HG21	1.99	0.45
35:A:51:ASP:HB2	35:A:54:ARG:HB3	1.99	0.45
36:B:8:ALA:HB2	57:W:49:LEU:HD12	1.97	0.45
42:H:242:ARG:NH2	79:t:929:G:OP2	2.50	0.45
44:J:123:ILE:H	44:J:123:ILE:HG13	1.59	0.45
48:N:82:ILE:O	48:N:86:TRP:N	2.42	0.45
50:P:184:ASN:HD22	50:P:184:ASN:N	2.15	0.45
59:Y:86:ALA:HB1	59:Y:97:VAL:HG21	1.99	0.45
59:Y:100:VAL:HG11	59:Y:109:ILE:HD11	1.98	0.45
63:c:101:HIS:HB3	63:c:104:LEU:HB2	1.98	0.45
1:S2:76:U:O2'	24:SG:159:ARG:NH1	2.50	0.44
1:S2:616:A:OP1	18:SX:68:LYS:NZ	2.50	0.44
1:S2:1578:U:H6	4:SD:5:ILE:HA	1.82	0.44
3:SB:152:LYS:HD3	13:SR:133:GLY:HA3	1.98	0.44
24:SG:32:MET:HB3	24:SG:100:CYS:HB2	1.99	0.44
36:B:86:VAL:HG12	36:B:201:LEU:HD23	1.99	0.44
40:F:241:LYS:HA	40:F:244:HIS:HD2	1.82	0.44
52:R:29:VAL:HG22	52:R:51:LEU:CD2	2.47	0.44
53:S:99:MET:HE1	53:S:128:LYS:HA	2.00	0.44
62:b:9:ARG:HH12	79:t:2270:G:H1	1.65	0.44
67:g:19:ARG:NH2	79:t:1870:U:OP1	2.50	0.44
79:t:1223:G:N2	79:t:1224:C:N3	2.64	0.44
79:t:1375:A:N6	79:t:1453:U:OP1	2.38	0.44
8:SI:67:TRP:NE1	8:SI:70:GLU:OE1	2.41	0.44
14:SS:10:GLN:NE2	14:SS:61:GLU:OE2	2.50	0.44
18:SX:5:ARG:NH1	18:SX:5:ARG:CB	2.80	0.44
23:SC:201:GLY:O	25:SJ:58:ARG:NH1	2.50	0.44
31:SZ:97:ILE:HD12	31:SZ:109:TYR:CG	2.51	0.44
42:H:101:VAL:HG13	42:H:139:TYR:HE2	1.83	0.44
52:R:187:LYS:NZ	79:t:4259:G:OP1	2.50	0.44
54:T:154:LEU:HB3	54:T:157:ARG:HD3	1.98	0.44
58:X:50:ASN:CG	58:X:55:TYR:CZ	2.95	0.44
62:b:3:SER:OG	79:t:2323:U:O4	2.31	0.44
65:e:26:THR:HG22	65:e:85:ARG:HD3	1.98	0.44
65:e:57:MET:O	65:e:90:ARG:NH2	2.39	0.44
76:p:8:ARG:NH2	79:t:4254:A:O2'	2.50	0.44
79:t:4627:A:H1'	79:t:5005:C:H42	1.82	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
80:v:30:G:N2	80:v:41:C:O2	2.50	0.44
80:v:60:U:OP1	80:v:62:C:N4	2.50	0.44
1:S2:1104:G:OP1	3:SB:157:GLN:NE2	2.49	0.44
1:S2:1261:C:O2	21:Sd:10:HIS:NE2	2.31	0.44
1:S2:1562:C:H2'	1:S2:1563:G:H8	1.83	0.44
1:S2:1858:G:OP2	28:SO:146:ARG:NH2	2.36	0.44
13:SR:90:ALA:O	13:SR:93:GLN:NE2	2.49	0.44
25:SJ:70:ARG:O	25:SJ:74:GLY:N	2.49	0.44
36:B:245:HIS:CD2	36:B:246:ARG:HG3	2.53	0.44
37:C:27:VAL:HA	37:C:279:LEU:HD11	1.99	0.44
42:H:223:LYS:HD2	79:t:1888:A:H4'	1.99	0.44
52:R:91:ARG:HG3	62:b:76:ASP:HB3	1.99	0.44
66:f:19:LYS:NZ	79:t:2297:G:O6	2.36	0.44
79:t:749:G:N2	79:t:893:C:O2	2.50	0.44
79:t:1088:C:H2'	79:t:1089:A:H8	1.82	0.44
79:t:1149:G:N3	79:t:1150:C:O2'	2.50	0.44
1:S2:222:U:H5''	10:SL:17:PHE:CG	2.53	0.44
1:S2:682:U:P	18:SX:8:ARG:HE	2.41	0.44
1:S2:1378:A:N1	6:SF:62:ARG:HA	2.33	0.44
1:S2:1863:A:OP2	19:Sa:4:LYS:NZ	2.33	0.44
3:SB:144:LYS:HD2	3:SB:208:HIS:HB3	1.98	0.44
6:SF:167:LYS:HA	31:SZ:71:ALA:HB1	2.00	0.44
7:SH:126:HIS:O	7:SH:177:TYR:OH	2.25	0.44
7:SH:144:ILE:HD13	7:SH:154:ILE:HG13	1.98	0.44
8:SI:165:GLN:O	8:SI:169:GLY:N	2.51	0.44
17:SV:17:CYS:HB2	17:SV:24:ILE:HD11	2.00	0.44
36:B:90:VAL:HG13	36:B:104:THR:HG22	2.00	0.44
47:M:62:PRO:CG	79:t:101:A:O3'	2.65	0.44
54:T:162:GLN:HE21	54:T:162:GLN:N	2.14	0.44
62:b:94:LYS:HE2	62:b:94:LYS:HB2	1.76	0.44
79:t:1865:C:H2'	79:t:1866:G:H8	1.83	0.44
1:S2:110:U:H3	1:S2:351:G:H1	1.64	0.44
1:S2:554:A:O2'	1:S2:555:A:O4'	2.27	0.44
1:S2:677:G:H21	1:S2:1028:A:H62	1.64	0.44
1:S2:1392:U:H2'	1:S2:1393:G:C8	2.53	0.44
4:SD:76:ARG:HB2	9:SK:22:VAL:HG11	1.98	0.44
5:SE:180:LEU:HB3	5:SE:229:GLY:HA3	1.99	0.44
10:SL:101:ARG:HG2	18:SX:7:LEU:HA	1.99	0.44
46:L:24:ILE:HG21	46:L:126:TYR:HB3	1.99	0.44
47:M:55:ILE:O	47:M:76:PHE:HE2	2.00	0.44
47:M:63:THR:CG2	62:b:66:ASN:CG	2.91	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:O:49:ARG:HA	49:O:53:TYR:H	1.82	0.44
50:P:97:ALA:O	50:P:101:ARG:NE	2.51	0.44
52:R:38:ARG:NH1	79:t:2068:C:OP2	2.50	0.44
52:R:49:LYS:O	52:R:53:MET:CE	2.66	0.44
53:S:153:LYS:HE2	53:S:153:LYS:HB3	1.87	0.44
54:T:95:ARG:NH2	79:t:1933:G:H5'	2.32	0.44
64:d:32:LYS:HG2	79:t:2654:G:N7	2.33	0.44
69:i:122:LYS:HD2	69:i:122:LYS:HA	1.84	0.44
76:p:28:LYS:CE	79:t:4306:U:H1'	2.47	0.44
78:r:84:LYS:HB2	78:r:89:THR:HB	2.00	0.44
1:S2:1170:A:N6	1:S2:1189:A:OP2	2.48	0.44
30:SY:74:MET:HE2	30:SY:74:MET:HB2	1.74	0.44
36:B:292:LEU:HB2	36:B:299:ILE:CG2	2.47	0.44
42:H:70:ARG:NH1	79:t:1193:C:O2'	2.39	0.44
48:N:124:LYS:HA	48:N:127:VAL:HG12	1.98	0.44
52:R:48:LEU:HD22	52:R:51:LEU:HD12	2.00	0.44
58:X:16:GLY:O	79:t:4590:U:O2'	2.36	0.44
72:l:24:LYS:HG2	72:l:67:LYS:HB3	1.99	0.44
79:t:3915:G:H2'	79:t:3916:A:C8	2.53	0.44
1:S2:1072:U:H5''	1:S2:1073:U:H5	1.83	0.44
8:SI:57:ALA:H	8:SI:180:GLY:HA2	1.82	0.44
19:Sa:10:ARG:HG2	19:Sa:34:LYS:HB2	2.00	0.44
33:Se:18:LYS:NZ	33:Se:19:VAL:O	2.51	0.44
42:H:214:SER:OG	42:H:215:SER:N	2.51	0.44
44:J:9:THR:HB	44:J:54:ARG:HD2	1.99	0.44
44:J:41:ILE:HG21	44:J:73:ILE:HD11	1.99	0.44
49:O:62:TYR:O	49:O:132:VAL:N	2.44	0.44
49:O:64:ILE:HD11	49:O:102:ALA:HA	1.99	0.44
50:P:79:ILE:HG21	50:P:138:LEU:HD11	1.99	0.44
61:a:17:ARG:HB2	79:t:2562:C:H41	1.82	0.44
61:a:38:TYR:HB3	79:t:2635:U:H5''	1.99	0.44
65:e:113:THR:HG22	65:e:115:LYS:H	1.82	0.44
67:g:14:TYR:OH	67:g:92:LEU:O	2.36	0.44
79:t:2245:C:O2	79:t:2247:A:N6	2.50	0.44
79:t:2600:A:H2'	79:t:2601:G:H8	1.83	0.44
79:t:4368:U:H2'	79:t:4369:G:H8	1.82	0.44
79:t:4865:G:H2'	79:t:4866:G:C8	2.53	0.44
1:S2:683:OMG:N1	1:S2:1022:U:OP2	2.33	0.44
1:S2:1297:U:O2'	1:S2:1299:A:N7	2.42	0.44
1:S2:1814:G:H21	79:t:3777:G:N2	2.15	0.44
7:SH:130:LEU:HB3	7:SH:139:ILE:HD11	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:SR:25:GLY:O	13:SR:31:ASN:ND2	2.49	0.44
25:SJ:68:PRO:HA	25:SJ:71:LEU:HD12	1.98	0.44
26:SM:39:ALA:HB1	34:Sf:103:LEU:HG	2.00	0.44
36:B:78:ILE:HG22	36:B:332:MET:HB3	2.00	0.44
42:H:95:ILE:H	42:H:95:ILE:HG13	1.64	0.44
42:H:239:GLN:HE21	54:T:37:HIS:HE1	1.66	0.44
53:S:103:ARG:NH1	79:t:2645:U:OP2	2.46	0.44
54:T:9:GLU:OE2	54:T:31:ARG:NE	2.34	0.44
79:t:507:U:O2	79:t:633:U:O2'	2.36	0.44
79:t:4205:C:OP2	79:t:4226:G:N1	2.49	0.44
1:S2:1013:U:OP1	1:S2:1129:G:O2'	2.34	0.44
1:S2:1219:B8Q:O4'	20:Sc:24:GLN:OE1	2.35	0.44
1:S2:1653:U:H3	1:S2:1671:G:H1	1.65	0.44
3:SB:87:ILE:H	3:SB:101:HIS:HB2	1.83	0.44
8:SI:22:HIS:ND1	8:SI:23:LYS:O	2.51	0.44
12:SQ:3:SER:OG	12:SQ:4:LYS:N	2.51	0.44
13:SR:97:GLU:OE1	13:SR:120:THR:OG1	2.28	0.44
21:Sd:3:HIS:HE1	21:Sd:6:LEU:HD11	1.83	0.44
41:G:88:VAL:N	79:t:2238:G:O6	2.51	0.44
43:I:63:LEU:HD13	49:O:32:GLN:HB2	1.99	0.44
43:I:182:CYS:HB3	43:I:222:ILE:HG23	1.99	0.44
57:W:107:ASN:OD1	57:W:111:GLU:N	2.50	0.44
66:f:48:ARG:O	79:t:1864:G:O2'	2.35	0.44
79:t:1572:C:H4'	79:t:2836:A:H5'	1.99	0.44
79:t:4440:G:N2	79:t:4570:G:O2'	2.50	0.44
1:S2:378:U:O2	8:SI:31:ARG:NH2	2.51	0.43
1:S2:526:A:N1	1:S2:558:G:N2	2.65	0.43
1:S2:1036:A:N3	1:S2:1844:U:O2'	2.50	0.43
1:S2:1171:G:O2'	1:S2:1187:G:O6	2.34	0.43
1:S2:1348:G:H2'	1:S2:1349:G:H8	1.83	0.43
1:S2:1534:C:H41	1:S2:1600:G:H1	1.65	0.43
1:S2:1830:UR3:H3U3	81:w:17:G:H4'	2.00	0.43
3:SB:83:LYS:HE3	3:SB:106:THR:HG22	2.00	0.43
22:Sg:157:SER:HB3	22:Sg:164:ILE:H	1.83	0.43
34:Sf:109:ASP:HB2	34:Sf:113:LYS:HD2	2.00	0.43
38:D:52:A:N6	73:m:27:ILE:HD13	2.32	0.43
41:G:115:TYR:CE1	78:r:119:ARG:HD2	2.53	0.43
69:i:81:LEU:HA	69:i:84:ARG:HG3	1.99	0.43
70:j:61:LEU:HD21	70:j:91:SER:HB2	2.00	0.43
79:t:3733:U:H3'	79:t:3734:A:H8	1.83	0.43
79:t:4678:C:H2'	79:t:4679:A:C8	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:1636:G:H1'	6:SF:164:ARG:HH12	1.82	0.43
35:A:10:LYS:NZ	79:t:3658:A:OP2	2.40	0.43
36:B:86:VAL:HG13	36:B:162:VAL:HG13	2.00	0.43
36:B:246:ARG:NH2	79:t:4520:U:OP2	2.51	0.43
37:C:153:VAL:HG12	37:C:252:TRP:HB2	1.99	0.43
37:C:205:ARG:NE	79:t:2276:G:OP1	2.51	0.43
41:G:180:VAL:HG21	41:G:258:LEU:HD21	2.00	0.43
45:K:99:ILE:HB	45:K:123:GLN:HB2	1.99	0.43
65:e:39:LYS:NZ	79:t:2348:U:O2	2.45	0.43
79:t:2091:G:O6	79:t:2230:G:O2'	2.26	0.43
79:t:2569:G:HO2'	79:t:2733:G:H22	1.63	0.43
1:S2:1748:G:H2'	1:S2:1749:G:C8	2.54	0.43
2:SA:17:LYS:HG2	13:SR:91:LEU:HB3	1.99	0.43
7:SH:145:ARG:HE	7:SH:147:LYS:NZ	2.16	0.43
8:SI:153:LYS:O	8:SI:157:LYS:NZ	2.39	0.43
9:SK:71:LEU:HD13	9:SK:71:LEU:HA	1.90	0.43
31:SZ:79:ILE:H	31:SZ:79:ILE:HG13	1.63	0.43
36:B:50:LYS:HB3	36:B:345:LEU:HD21	2.00	0.43
46:L:51:SER:OG	79:t:4220:C:O3'	2.35	0.43
51:Q:57:CYS:SG	51:Q:58:VAL:N	2.90	0.43
54:T:161:ARG:C	54:T:163:HIS:H	2.25	0.43
59:Y:129:ARG:HD3	59:Y:135:LYS:HE3	1.99	0.43
79:t:1379:G:O2'	79:t:1450:C:O2'	2.34	0.43
79:t:4853:C:H41	79:t:4854:G:H21	1.66	0.43
1:S2:65:C:C2	24:SG:133:LEU:HD22	2.53	0.43
1:S2:861:A:C8	7:SH:106:ARG:HD3	2.54	0.43
1:S2:1142:G:N2	1:S2:1145:A:OP2	2.52	0.43
1:S2:1163:C:H2'	1:S2:1164:G:H8	1.83	0.43
1:S2:1617:G:N1	1:S2:1620:A:OP2	2.52	0.43
8:SI:124:LYS:HG2	8:SI:125:LYS:HG2	1.99	0.43
12:SQ:39:LEU:HD12	12:SQ:51:LEU:HG	2.01	0.43
46:L:104:ASN:HD22	46:L:133:VAL:HG12	1.84	0.43
48:N:97:ALA:HA	48:N:100:ARG:HB2	1.99	0.43
52:R:29:VAL:HG22	52:R:51:LEU:CB	2.47	0.43
70:j:62:LYS:HB3	70:j:94:LEU:HD21	2.00	0.43
79:t:123:C:H2'	79:t:124:C:H6	1.83	0.43
79:t:1185:C:N4	79:t:1186:G:O6	2.52	0.43
79:t:2401:C:O2'	79:t:3828:G:O2'	2.29	0.43
79:t:2827:G:O2'	79:t:3809:U:O4	2.37	0.43
1:S2:325:C:N3	58:X:119:LYS:CE	2.82	0.43
1:S2:328:U:O2'	1:S2:329:G:O5'	2.37	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:659:G:O4'	1:S2:662:G:N2	2.46	0.43
1:S2:1006:C:OP2	64:d:9:LYS:N	2.46	0.43
1:S2:1084:A:OP1	1:S2:1858:G:O2'	2.34	0.43
1:S2:1242:U:H4'	1:S2:1243:PSU:H5'	2.00	0.43
2:SA:176:TRP:CD2	2:SA:199:PRO:HB3	2.53	0.43
14:SS:132:ARG:HB2	14:SS:134:GLN:HE22	1.82	0.43
37:C:61:GLN:NE2	79:t:351:U:O3'	2.52	0.43
39:E:4:U:O4	39:E:5:A:N6	2.52	0.43
41:G:73:TYR:OH	79:t:969:U:O5'	2.37	0.43
41:G:136:HIS:CD2	79:t:702:A:H1'	2.54	0.43
41:G:247:LYS:HG2	79:t:4896:A:N1	2.34	0.43
47:M:149:GLN:HE21	69:i:122:LYS:HG2	1.83	0.43
51:Q:127:ARG:NH2	79:t:2401:C:OP1	2.34	0.43
52:R:42:THR:HB	79:t:1411:U:H5''	2.00	0.43
56:V:44:GLN:O	56:V:55:ASN:HA	2.19	0.43
66:f:4:LEU:HD23	66:f:4:LEU:HA	1.80	0.43
66:f:33:ARG:NH1	79:t:1286:A:OP2	2.52	0.43
79:t:1219:C:H2'	79:t:1221:A:H8	1.84	0.43
79:t:2366:G:H2'	79:t:2367:A:C8	2.53	0.43
79:t:4493:U:C5	83:y:24:ASP:CA	2.64	0.43
1:S2:399:C:O2	10:SL:106:HIS:ND1	2.36	0.43
1:S2:962:A:N6	1:S2:1055:A:O2'	2.42	0.43
6:SF:131:ALA:HA	6:SF:136:ARG:CD	2.48	0.43
6:SF:131:ALA:HA	6:SF:136:ARG:HG2	1.91	0.43
8:SI:67:TRP:CD1	8:SI:70:GLU:H	2.32	0.43
11:SP:103:ASN:ND2	11:SP:120:SER:OG	2.48	0.43
15:ST:73:GLY:O	15:ST:76:THR:OG1	2.33	0.43
22:Sg:158:PRO:HG3	22:Sg:204:GLY:HA3	2.01	0.43
25:SJ:60:LEU:HD22	25:SJ:70:ARG:HB2	2.01	0.43
35:A:118:GLU:HB3	35:A:126:LEU:HG	2.00	0.43
38:D:52:A:H62	73:m:27:ILE:HD13	1.84	0.43
40:F:64:ILE:HG13	40:F:105:LEU:HD11	2.01	0.43
41:G:233:PHE:HD2	41:G:236:GLU:HG2	1.83	0.43
44:J:80:MET:O	44:J:84:VAL:N	2.48	0.43
79:t:189:G:H1	79:t:244:G:N2	2.15	0.43
79:t:211:G:O2'	79:t:216:G:O4'	2.36	0.43
79:t:1150:C:H2'	79:t:1151:G:C8	2.54	0.43
11:SP:89:MET:O	11:SP:107:ILE:HD12	2.18	0.43
41:G:203:ILE:HB	41:G:206:VAL:HB	1.99	0.43
45:K:187:GLU:H	45:K:187:GLU:HG3	1.62	0.43
52:R:64:SER:HA	52:R:67:ILE:HG12	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:R:104:ARG:NH1	79:t:1336:G:N7	2.67	0.43
59:Y:64:SER:HB2	69:i:69:LEU:HD21	2.01	0.43
61:a:59:LYS:HE2	79:t:4111:C:H4'	2.00	0.43
79:t:1234:C:O2	79:t:1242:G:N2	2.51	0.43
79:t:1281:C:H2'	79:t:1282:G:C8	2.54	0.43
79:t:1865:C:O2'	79:t:2050:A:O2'	2.35	0.43
79:t:2728:C:H2'	79:t:2729:G:H8	1.84	0.43
79:t:4431:U:H2'	79:t:4432:G:H8	1.83	0.43
1:S2:65:C:OP2	24:SG:175:LYS:N	2.45	0.43
1:S2:325:C:N3	58:X:119:LYS:CD	2.82	0.43
1:S2:353:C:O2	10:SL:71:ARG:NH1	2.46	0.43
1:S2:649:U:OP1	18:SX:108:LYS:HD2	2.17	0.43
1:S2:1454:A:H5''	13:SR:3:ARG:HG2	2.01	0.43
43:I:161:VAL:CG1	43:I:163:PRO:HD2	2.45	0.43
48:N:137:LYS:HD2	48:N:138:ALA:HB2	2.01	0.43
50:P:90:HIS:CD2	79:t:3858:C:H41	2.37	0.43
54:T:172:PRO:O	79:t:4724:A:N1	2.52	0.43
63:c:33:LYS:HB3	63:c:33:LYS:HE2	1.79	0.43
69:i:90:ALA:O	69:i:94:ARG:CG	2.67	0.43
79:t:1388:C:H2'	79:t:1389:G:C8	2.54	0.43
79:t:4085:C:H5'	79:t:4086:U:H5	1.84	0.43
1:S2:659:G:HO2'	1:S2:662:G:HO2'	1.61	0.43
1:S2:677:G:N1	1:S2:1027:A:OP2	2.46	0.43
1:S2:1243:PSU:OP2	1:S2:1518:C:O2'	2.32	0.43
1:S2:1422:G:OP2	1:S2:1422:G:N2	2.51	0.43
7:SH:184:ASP:OD1	7:SH:184:ASP:N	2.44	0.43
24:SG:1:MET:HE3	24:SG:28:TYR:HE1	1.83	0.43
31:SZ:47:LEU:HB2	31:SZ:79:ILE:HG22	2.00	0.43
36:B:224:LYS:HD3	36:B:340:THR:HG22	2.01	0.43
37:C:14:LYS:HA	37:C:173:LYS:HD3	2.00	0.43
37:C:307:LYS:NZ	79:t:2070:U:OP2	2.39	0.43
41:G:71:ARG:NH2	79:t:969:U:O4	2.51	0.43
45:K:48:LEU:HD23	45:K:142:LEU:HA	2.00	0.43
49:O:143:ARG:HG2	69:i:99:GLU:OE1	2.19	0.43
59:Y:51:THR:OG1	59:Y:52:LEU:N	2.52	0.43
60:Z:87:ARG:NH2	79:t:398:U:O2'	2.52	0.43
71:k:22:CYS:SG	71:k:24:SER:OG	2.74	0.43
79:t:2673:G:OP2	79:t:2675:A:N6	2.52	0.43
1:S2:70:G:O6	24:SG:170:ARG:NH1	2.33	0.43
1:S2:166:A2M:H5''	24:SG:112:VAL:HG21	2.01	0.43
1:S2:1283:C:H6	1:S2:1313:A:H2	1.66	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:1286:G:H8	34:Sf:101:ALA:HA	1.83	0.43
5:SE:166:THR:HG22	5:SE:168:LYS:HD3	2.01	0.43
7:SH:90:LYS:HE3	7:SH:90:LYS:HB2	1.82	0.43
9:SK:41:PRO:HG2	9:SK:44:HIS:HD2	1.84	0.43
15:ST:124:THR:HG23	15:ST:127:GLY:H	1.84	0.43
17:SV:69:ILE:HA	17:SV:72:LEU:HG	2.01	0.43
25:SJ:122:SER:O	25:SJ:125:HIS:N	2.40	0.43
36:B:57:VAL:HG22	36:B:73:VAL:HG12	2.01	0.43
37:C:75:ARG:NH1	79:t:4353:G:OP1	2.35	0.43
53:S:104:ARG:HH12	79:t:2877:G:H5'	1.84	0.43
53:S:159:ALA:O	53:S:162:ARG:NH1	2.52	0.43
64:d:56:ARG:NH1	79:t:2653:A:O4'	2.46	0.43
66:f:31:ILE:HD11	79:t:2326:A:C4	2.54	0.43
66:f:124:ASN:HB2	66:f:127:ALA:HB2	2.01	0.43
73:m:40:LYS:NZ	79:t:359:U:O2'	2.32	0.43
75:o:7:LYS:O	75:o:11:ARG:N	2.50	0.43
78:r:41:ASN:HD22	78:r:42:GLY:H	1.66	0.43
79:t:1:C:N4	79:t:2:G:O6	2.51	0.43
79:t:317:C:H2'	79:t:318:A:C8	2.53	0.43
79:t:946:G:O2'	79:t:2242:A:N6	2.49	0.43
79:t:2773:C:N4	83:y:11:LEU:HA	2.34	0.43
1:S2:190:G:O2'	1:S2:209:A:N1	2.49	0.42
1:S2:1058:A:OP1	80:v:38:A:O2'	2.36	0.42
1:S2:1495:G:H22	21:Sd:24:CYS:H	1.67	0.42
1:S2:1593:C:H2'	1:S2:1594:A:C8	2.54	0.42
1:S2:1648:G:H5''	12:SQ:125:ARG:HB2	2.01	0.42
9:SK:4:PRO:HG2	9:SK:7:ASN:HB2	2.00	0.42
24:SG:176:ILE:HG21	24:SG:179:LEU:HD22	2.00	0.42
35:A:244:GLY:HA3	79:t:3717:A:H5''	2.01	0.42
48:N:41:PRO:HB3	48:N:70:GLN:HE21	1.84	0.42
79:t:466:C:N3	79:t:676:G:N2	2.67	0.42
80:v:17:A:H1'	80:v:18:G:H4'	2.01	0.42
1:S2:104:A:H62	1:S2:356:C:H5	1.65	0.42
1:S2:448:A:H4'	1:S2:449:A:H5''	2.01	0.42
1:S2:563:G:N7	1:S2:586:G:N2	2.67	0.42
1:S2:1284:A:O3'	1:S2:1286:G:N2	2.52	0.42
1:S2:1357:A:N3	25:SJ:70:ARG:HB3	2.34	0.42
2:SA:34:MET:HG3	2:SA:154:LEU:HD11	2.00	0.42
8:SI:107:THR:HG23	8:SI:108:PRO:HD3	2.01	0.42
11:SP:51:ARG:HH22	21:Sd:5:GLN:HE21	1.67	0.42
12:SQ:134:GLY:HA3	12:SQ:140:ARG:HA	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:SM:45:ARG:HA	26:SM:45:ARG:HD3	1.88	0.42
34:Sf:123:SER:OG	34:Sf:124:ASP:N	2.52	0.42
36:B:348:ARG:HH12	36:B:351:LEU:HD12	1.84	0.42
37:C:67:TRP:HE3	37:C:73:VAL:HG21	1.83	0.42
50:P:91:LYS:NZ	79:t:3858:C:N3	2.67	0.42
57:W:97:TYR:CE1	58:X:19:ARG:HD3	2.54	0.42
77:q:5:THR:OG1	79:t:2855:G:OP1	2.37	0.42
77:q:42:CYS:HA	79:t:2653:A:N6	2.34	0.42
78:r:63:VAL:HG12	78:r:79:ARG:HB3	2.01	0.42
79:t:1996:U:H2'	79:t:1997:C:H6	1.83	0.42
79:t:4263:U:OP2	79:t:4265:C:N4	2.52	0.42
79:t:4882:C:H2'	79:t:4883:U:C2	2.54	0.42
1:S2:571:U:H5''	30:SY:37:LYS:HG3	2.00	0.42
1:S2:812:A:H5'	5:SE:16:LYS:HD3	2.01	0.42
1:S2:1344:A:H5''	1:S2:1370:A:H4'	2.00	0.42
3:SB:103:MET:HG2	3:SB:188:LEU:HD11	2.02	0.42
3:SB:104:ASP:OD1	3:SB:104:ASP:N	2.53	0.42
4:SD:5:ILE:HB	4:SD:9:ARG:CG	2.48	0.42
5:SE:11:ARG:NH2	5:SE:21:ASP:O	2.53	0.42
11:SP:81:ARG:NH1	11:SP:97:TYR:O	2.52	0.42
19:Sa:23:CYS:SG	19:Sa:24:THR:N	2.92	0.42
36:B:228:TYR:O	79:t:2814:A:O2'	2.31	0.42
37:C:278:ASN:HD22	37:C:279:LEU:H	1.67	0.42
52:R:79:THR:HG22	52:R:99:LYS:HD2	2.00	0.42
54:T:161:ARG:HH21	54:T:161:ARG:HG2	1.83	0.42
69:i:91:MET:HA	69:i:94:ARG:HE	1.83	0.42
71:k:3:LYS:HD3	79:t:1621:U:P	2.59	0.42
79:t:3798:G:O2'	79:t:3800:G:OP2	2.26	0.42
1:S2:1528:G:O2'	1:S2:1666:C:OP1	2.35	0.42
2:SA:6:ASP:HA	2:SA:9:GLN:HG2	2.00	0.42
15:ST:5:THR:OG1	15:ST:6:VAL:N	2.53	0.42
25:SJ:76:ALA:HA	25:SJ:79:ARG:HG3	2.01	0.42
30:SY:110:ARG:HE	30:SY:114:MET:HE3	1.84	0.42
32:Sb:65:GLN:O	32:Sb:72:ARG:N	2.49	0.42
54:T:19:THR:OG1	54:T:22:CYS:O	2.34	0.42
55:U:49:GLN:HA	55:U:52:MET:HE3	2.01	0.42
60:Z:58:VAL:HG22	60:Z:59:ARG:HG2	2.01	0.42
75:o:11:ARG:HA	75:o:14:LYS:HG2	2.01	0.42
79:t:467:C:O2	79:t:676:G:N2	2.53	0.42
79:t:639:G:H2'	79:t:640:G:C8	2.53	0.42
79:t:731:G:O6	79:t:911:C:N4	2.52	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:t:4537:G:O2'	79:t:5027:U:OP1	2.28	0.42
1:S2:166:A2M:H2'	1:S2:167:G:H8	1.84	0.42
1:S2:376:A:H2'	1:S2:377:G:C8	2.55	0.42
19:Sa:53:ILE:O	19:Sa:57:SER:N	2.53	0.42
25:SJ:124:HIS:CD2	33:Se:35:ARG:HH11	2.36	0.42
26:SM:21:VAL:HG23	26:SM:123:VAL:HG13	2.01	0.42
35:A:122:ASP:O	35:A:123:ARG:CB	2.67	0.42
37:C:36:ILE:HG22	37:C:123:ALA:HB2	2.01	0.42
39:E:66:G:H5'	40:F:14:LYS:HE2	2.00	0.42
42:H:50:ILE:HG21	42:H:186:CYS:HB3	2.02	0.42
51:Q:37:LYS:HE2	51:Q:37:LYS:HB3	1.88	0.42
51:Q:66:GLY:HA2	79:t:3864:C:H5''	2.01	0.42
54:T:16:CYS:HA	54:T:59:GLY:HA2	2.02	0.42
54:T:161:ARG:CG	54:T:161:ARG:NH2	2.72	0.42
57:W:49:LEU:HD23	57:W:49:LEU:HA	1.91	0.42
65:e:39:LYS:NZ	79:t:2348:U:O2'	2.42	0.42
79:t:1897:G:N3	79:t:2048:C:O2'	2.50	0.42
1:S2:200:G:H1	1:S2:201:C:HO2'	1.60	0.42
1:S2:1006:C:P	64:d:10:SER:H	2.42	0.42
1:S2:1850:MA6:H8	1:S2:1850:MA6:OP2	2.19	0.42
8:SI:56:ARG:NH1	8:SI:180:GLY:O	2.52	0.42
15:ST:104:LEU:HD13	15:ST:121:ARG:HD2	2.00	0.42
18:SX:105:PHE:CD1	18:SX:121:LYS:HB3	2.54	0.42
22:Sg:139:LYS:HG3	22:Sg:140:TYR:CD1	2.55	0.42
26:SM:21:VAL:HG21	26:SM:122:ASP:HB3	2.01	0.42
29:SW:15:ASN:HD21	29:SW:71:LYS:HG3	1.84	0.42
35:A:96:LEU:HB2	77:q:92:GLN:HE22	1.84	0.42
36:B:174:ARG:NH2	79:t:4932:C:O2'	2.48	0.42
37:C:52:TYR:OH	79:t:2322:G:N7	2.51	0.42
43:I:89:ARG:O	43:I:93:THR:OG1	2.37	0.42
43:I:164:ILE:HD12	43:I:164:ILE:C	2.43	0.42
43:I:244:PRO:HA	43:I:247:VAL:HG12	2.01	0.42
68:h:111:ALA:O	68:h:115:LYS:NZ	2.53	0.42
69:i:89:ARG:NE	69:i:93:ARG:NH2	2.67	0.42
79:t:2068:C:H5''	79:t:2069:G:H3'	2.02	0.42
79:t:4666:C:H2'	79:t:4667:A:C8	2.54	0.42
1:S2:1410:C:H2'	1:S2:1411:G:C8	2.55	0.42
22:Sg:5:MET:HB3	22:Sg:310:TRP:HE3	1.84	0.42
30:SY:20:ARG:NH2	30:SY:74:MET:HE3	2.34	0.42
38:D:22:U:OP1	60:Z:11:ARG:NE	2.46	0.42
46:L:35:ARG:NH1	46:L:122:SER:O	2.46	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:U:52:MET:HA	55:U:53:PRO:HD3	1.90	0.42
58:X:51:TRP:O	58:X:52:THR:O	2.37	0.42
79:t:2030:G:H2'	79:t:2031:G:C8	2.54	0.42
79:t:4195:A:H62	79:t:4254:A:H62	1.67	0.42
1:S2:648:A:H5''	18:SX:106:GLY:H	1.85	0.42
1:S2:1349:G:H3'	1:S2:1350:U:C5	2.55	0.42
6:SF:70:GLU:O	6:SF:74:ASN:ND2	2.53	0.42
12:SQ:34:VAL:HG12	12:SQ:70:VAL:HB	2.01	0.42
15:ST:131:LEU:HA	15:ST:134:ILE:HG13	2.02	0.42
21:Sd:22:ARG:N	21:Sd:37:ASN:O	2.53	0.42
22:Sg:191:HIS:CD2	22:Sg:195:LEU:HD22	2.55	0.42
24:SG:74:ARG:HA	24:SG:96:SER:HA	2.01	0.42
24:SG:129:VAL:HA	24:SG:130:PRO:HD3	1.93	0.42
35:A:68:ARG:NH2	79:t:4054:G:N7	2.67	0.42
39:E:46:C:OP1	40:F:158:LYS:N	2.47	0.42
51:Q:24:VAL:HG11	51:Q:87:SER:HA	2.02	0.42
52:R:148:VAL:HG13	79:t:1329:C:H5''	2.02	0.42
53:S:99:MET:HE2	53:S:127:VAL:HG12	2.02	0.42
56:V:48:LYS:HE2	56:V:53:ALA:CB	2.43	0.42
59:Y:60:TYR:CZ	69:i:84:ARG:NH2	2.87	0.42
66:f:102:ASN:HD22	79:t:2286:A:H5''	1.85	0.42
67:g:106:TYR:O	67:g:108:SER:N	2.51	0.42
79:t:1228:C:H42	79:t:1247:C:H42	1.67	0.42
79:t:2857:G:H4'	79:t:3796:A:H5''	2.00	0.42
79:t:3879:A:C2	83:y:20:ARG:CB	3.03	0.42
1:S2:1351:G:OP2	6:SF:57:ALA:N	2.51	0.42
1:S2:1718:G:H22	1:S2:1813:A:H1'	1.84	0.42
18:SX:7:LEU:HD23	18:SX:7:LEU:N	2.34	0.42
19:Sa:47:ALA:HA	19:Sa:50:VAL:HG23	2.01	0.42
21:Sd:31:ILE:N	21:Sd:38:MET:O	2.51	0.42
21:Sd:43:PHE:CZ	21:Sd:52:PHE:HD2	2.20	0.42
28:SO:78:ALA:HA	28:SO:81:VAL:HG12	2.02	0.42
40:F:41:LYS:HB3	40:F:41:LYS:HE3	1.80	0.42
41:G:250:GLN:O	41:G:254:ASP:N	2.43	0.42
43:I:148:GLU:HA	43:I:177:MET:HE3	2.02	0.42
44:J:5:LEU:HD12	44:J:60:TRP:CH2	2.54	0.42
46:L:31:ASP:O	46:L:35:ARG:NE	2.52	0.42
47:M:80:GLU:HG2	47:M:113:ASN:HB2	2.02	0.42
47:M:96:ILE:HD13	47:M:117:LEU:HD11	2.02	0.42
54:T:172:PRO:O	79:t:4724:A:C2	2.73	0.42
79:t:158:G:N2	79:t:270:C:O2	2.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:t:1193:C:H2'	79:t:1194:G:H8	1.85	0.42
80:v:26:A:H61	80:v:44:G:H1	1.67	0.42
6:SF:39:ILE:O	6:SF:42:LYS:NZ	2.41	0.42
11:SP:51:ARG:HA	11:SP:54:HIS:HD2	1.85	0.42
11:SP:111:MET:CE	14:SS:117:ILE:CD1	2.74	0.42
14:SS:15:VAL:HG12	14:SS:16:LEU:HD12	2.02	0.42
14:SS:60:THR:HG23	14:SS:63:GLU:H	1.85	0.42
24:SG:69:THR:O	24:SG:71:GLY:N	2.53	0.42
41:G:59:ARG:NH2	79:t:964:C:OP2	2.53	0.42
41:G:240:TYR:HD2	41:G:242:ILE:HG22	1.85	0.42
49:O:12:ARG:HH22	79:t:301:A:H62	1.67	0.42
49:O:116:LEU:HD23	49:O:133:ILE:HD11	2.02	0.42
50:P:183:LYS:HD2	50:P:184:ASN:N	2.35	0.42
53:S:32:ILE:HG22	53:S:44:LEU:HD13	2.01	0.42
79:t:694:G:OP2	79:t:694:G:N2	2.50	0.42
79:t:4433:U:H2'	79:t:4434:G:H8	1.84	0.42
1:S2:38:A:O2'	25:SJ:5:ARG:NH2	2.51	0.41
1:S2:1420:G:O2'	1:S2:1421:A:O5'	2.38	0.41
1:S2:1714:U:O2	1:S2:1820:G:N2	2.53	0.41
2:SA:104:THR:HA	2:SA:105:PRO:HD3	1.89	0.41
3:SB:128:LYS:HA	3:SB:134:LEU:HA	2.02	0.41
22:Sg:206:LEU:HB2	22:Sg:218:LEU:HD12	2.02	0.41
35:A:101:VAL:HA	35:A:165:VAL:HA	2.02	0.41
42:H:163:ASN:OD1	42:H:163:ASN:N	2.51	0.41
42:H:232:ASP:HB2	42:H:236:ARG:NH2	2.32	0.41
44:J:102:ASN:HB3	44:J:115:ARG:HG3	2.02	0.41
46:L:54:ARG:HA	46:L:64:ARG:HG3	2.02	0.41
49:O:75:VAL:HG21	49:O:80:THR:HA	2.00	0.41
52:R:159:PRO:HG3	79:t:4268:U:OP2	2.20	0.41
53:S:21:LYS:HZ1	53:S:55:VAL:HG22	1.84	0.41
57:W:65:VAL:HG23	57:W:73:ARG:HG2	2.02	0.41
64:d:103:ASP:N	64:d:103:ASP:OD1	2.53	0.41
79:t:227:G:H21	79:t:234:G:H1	1.68	0.41
1:S2:642:U:H5''	25:SJ:39:ASN:HD22	1.85	0.41
1:S2:659:G:O2'	1:S2:662:G:O2'	2.28	0.41
1:S2:1866:A:C6	19:Sa:87:ARG:HD2	2.56	0.41
2:SA:81:ASN:OD1	2:SA:81:ASN:N	2.52	0.41
19:Sa:23:CYS:HB3	19:Sa:28:ARG:H	1.85	0.41
22:Sg:11:LEU:HD12	22:Sg:307:VAL:HB	2.02	0.41
23:SC:144:SER:OG	23:SC:145:LYS:N	2.52	0.41
24:SG:70:HIS:HB3	24:SG:101:ILE:HB	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:SW:89:TRP:HE3	29:SW:93:LEU:HD21	1.85	0.41
30:SY:18:LEU:HB3	30:SY:20:ARG:HE	1.84	0.41
47:M:18:TRP:NE1	79:t:1498:G:O2'	2.46	0.41
47:M:139:SER:O	47:M:141:ALA:N	2.53	0.41
51:Q:25:HIS:ND1	79:t:2340:G:O6	2.53	0.41
60:Z:54:GLU:CD	60:Z:54:GLU:N	2.73	0.41
64:d:59:GLU:HB3	68:h:96:LEU:HD11	2.02	0.41
79:t:449:C:H42	79:t:693:U:H3	1.68	0.41
79:t:735:G:H1	79:t:907:C:H42	1.67	0.41
79:t:2602:A:H2'	79:t:2603:G:H8	1.84	0.41
79:t:3681:G:O2'	79:t:3683:A:OP1	2.38	0.41
2:SA:41:ARG:HD3	2:SA:45:GLY:HA2	2.01	0.41
4:SD:28:GLU:HA	9:SK:61:GLN:HE22	1.84	0.41
13:SR:100:PRO:HD2	13:SR:122:PRO:HD2	2.00	0.41
18:SX:54:LYS:HE2	18:SX:94:ILE:HD12	2.02	0.41
23:SC:157:LEU:HD13	23:SC:157:LEU:HA	1.77	0.41
25:SJ:86:VAL:HG23	25:SJ:104:ASP:HB3	2.02	0.41
35:A:118:GLU:OE2	79:t:3633:A:O2'	2.30	0.41
42:H:99:ASN:OD1	42:H:99:ASN:N	2.53	0.41
52:R:172:ARG:NH2	79:t:88:A:OP2	2.52	0.41
54:T:96:GLU:HB2	54:T:139:ARG:HG3	2.02	0.41
63:c:36:ASP:HA	63:c:37:PRO:HD3	1.88	0.41
79:t:1533:C:H42	79:t:1558:G:H1	1.67	0.41
79:t:2602:A:H2'	79:t:2603:G:C8	2.56	0.41
1:S2:546:G:O2'	1:S2:548:C:N4	2.53	0.41
4:SD:119:CYS:HA	4:SD:122:VAL:HG12	2.03	0.41
4:SD:210:ILE:H	4:SD:210:ILE:HG13	1.70	0.41
5:SE:9:LEU:HB2	5:SE:30:ARG:HD3	2.03	0.41
5:SE:99:PHE:HA	5:SE:113:ARG:HA	2.03	0.41
12:SQ:29:ASN:OD1	12:SQ:29:ASN:N	2.54	0.41
12:SQ:51:LEU:HD12	12:SQ:84:ILE:HD11	2.00	0.41
14:SS:3:LEU:HD12	14:SS:4:VAL:HG23	2.03	0.41
25:SJ:136:ARG:HD3	25:SJ:160:SER:HA	2.03	0.41
29:SW:49:GLU:HB2	29:SW:64:ASN:HD22	1.85	0.41
37:C:30:ALA:HB2	37:C:279:LEU:HD21	2.01	0.41
41:G:118:THR:O	78:r:112:ARG:NH1	2.53	0.41
52:R:15:ARG:CZ	52:R:53:MET:C	2.94	0.41
55:U:115:LYS:HE2	55:U:115:LYS:HB3	1.87	0.41
59:Y:69:ASN:OD1	59:Y:69:ASN:N	2.52	0.41
63:c:60:ASN:OD1	63:c:61:ASN:N	2.53	0.41
70:j:68:ARG:NH1	79:t:3693:G:OP1	2.44	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:t:223:G:O6	79:t:237:G:O2'	2.37	0.41
79:t:2500:G:H5'	79:t:2619:G:H1'	2.03	0.41
79:t:3579:A:H2'	79:t:3580:G:H8	1.85	0.41
1:S2:61:A:H1'	1:S2:316:G:H1'	2.02	0.41
1:S2:327:G:N2	1:S2:328:U:O4	2.53	0.41
1:S2:1408:U:H2'	1:S2:1409:A:C8	2.55	0.41
12:SQ:1:MET:HA	12:SQ:2:PRO:HD3	1.82	0.41
17:SV:59:ILE:HD12	17:SV:59:ILE:HA	1.91	0.41
27:SN:23:PRO:HB2	27:SN:25:TRP:CD1	2.55	0.41
35:A:116:LEU:HG	35:A:126:LEU:HB2	2.01	0.41
36:B:85:VAL:HG23	36:B:165:HIS:CE1	2.55	0.41
36:B:293:ILE:HB	36:B:294:LYS:H	1.55	0.41
38:D:47:C:H1'	38:D:61:A:H2'	2.01	0.41
40:F:146:LEU:HG	40:F:163:LEU:HD23	2.03	0.41
41:G:132:PRO:HG3	79:t:1271:G:C4	2.55	0.41
43:I:234:ARG:NH2	70:j:46:GLU:CB	2.83	0.41
44:J:23:ARG:HH21	44:J:39:ASN:HD22	1.68	0.41
57:W:15:ARG:HH21	79:t:4632:C:H1'	1.85	0.41
58:X:52:THR:OG1	58:X:53:VAL:N	2.53	0.41
60:Z:55:VAL:HB	60:Z:106:ILE:HA	2.03	0.41
79:t:1658:C:N4	79:t:4340:A:H8	2.18	0.41
15:ST:43:LYS:HB3	15:ST:43:LYS:HE2	1.87	0.41
24:SG:148:SER:N	24:SG:151:ASP:OD2	2.54	0.41
29:SW:57:ARG:H	29:SW:57:ARG:HD2	1.86	0.41
40:F:65:ALA:HB2	40:F:74:ILE:HG12	2.02	0.41
40:F:68:ARG:HD3	40:F:68:ARG:HA	1.86	0.41
47:M:130:LYS:O	47:M:132:SER:N	2.44	0.41
55:U:108:ARG:CA	55:U:111:GLU:HG3	2.51	0.41
57:W:35:LYS:HB2	57:W:67:LYS:HB2	2.01	0.41
62:b:32:ARG:HD2	79:t:37:U:H4'	2.02	0.41
64:d:30:GLY:O	64:d:93:THR:OG1	2.39	0.41
69:i:91:MET:HE2	69:i:94:ARG:HH21	1.78	0.41
71:k:35:GLY:O	71:k:45:ARG:NH2	2.54	0.41
79:t:4678:C:H2'	79:t:4679:A:H8	1.86	0.41
1:S2:303:C:O2	8:SI:184:ARG:NH1	2.54	0.41
1:S2:325:C:N1	58:X:119:LYS:CE	2.84	0.41
1:S2:1006:C:C5	64:d:8:LYS:HA	2.56	0.41
5:SE:183:VAL:HB	5:SE:225:ILE:HD13	2.02	0.41
24:SG:208:GLU:O	24:SG:212:LEU:N	2.46	0.41
37:C:330:PRO:HG3	42:H:47:ARG:HH21	1.84	0.41
37:C:343:GLN:HE22	79:t:934:C:H1'	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:E:62:U:O2'	39:E:64:G:O4'	2.38	0.41
39:E:75:G:O2'	39:E:99:G:O6	2.36	0.41
43:I:120:LYS:HE2	43:I:120:LYS:HB3	1.83	0.41
43:I:162:ASP:OD1	43:I:163:PRO:HD3	2.19	0.41
46:L:167:GLN:HA	46:L:171:ASP:HA	2.03	0.41
47:M:48:PRO:HB2	69:i:120:ALA:HB2	2.02	0.41
50:P:187:LYS:H	50:P:187:LYS:HG2	1.66	0.41
60:Z:11:ARG:HG3	79:t:225:C:H5''	2.01	0.41
61:a:11:VAL:HG11	61:a:80:LEU:HD23	2.03	0.41
61:a:68:ILE:HD13	61:a:118:PHE:HB3	2.02	0.41
77:q:49:ARG:HG2	77:q:50:ARG:O	2.21	0.41
79:t:452:C:N4	79:t:690:C:H42	2.17	0.41
79:t:470:G:N2	79:t:471:C:N3	2.69	0.41
79:t:715:C:O2	79:t:932:U:O2'	2.38	0.41
79:t:1380:A:N1	79:t:1480:G:O2'	2.53	0.41
79:t:1627:C:H2'	79:t:1628:A:C8	2.56	0.41
79:t:4981:C:H41	79:t:4986:G:H21	1.68	0.41
1:S2:935:G:H2'	1:S2:936:G:C8	2.56	0.41
2:SA:28:THR:O	2:SA:29:ASN:HB3	2.19	0.41
4:SD:9:ARG:HA	4:SD:12:VAL:HG22	2.03	0.41
4:SD:132:LYS:HE3	4:SD:156:LEU:HD11	2.02	0.41
4:SD:137:VAL:HB	4:SD:185:LYS:HB3	2.03	0.41
6:SF:24:SER:O	6:SF:107:ASN:ND2	2.40	0.41
6:SF:143:PRO:HA	6:SF:146:ARG:HG2	2.01	0.41
7:SH:171:GLU:O	7:SH:174:SER:OG	2.35	0.41
10:SL:103:GLU:HG3	18:SX:11:ARG:HB2	2.02	0.41
34:Sf:113:LYS:NZ	34:Sf:114:ILE:O	2.40	0.41
37:C:61:GLN:NE2	79:t:351:U:O2'	2.43	0.41
37:C:284:MET:HE2	37:C:287:THR:HA	2.02	0.41
41:G:133:PHE:HA	41:G:136:HIS:CE1	2.55	0.41
46:L:101:ASP:HA	46:L:159:LYS:HB2	2.03	0.41
48:N:82:ILE:HD13	48:N:82:ILE:HA	1.95	0.41
48:N:130:LEU:HD13	50:P:177:LEU:HD22	2.02	0.41
60:Z:122:LYS:HG2	79:t:191:C:H4'	2.02	0.41
60:Z:126:ARG:NH2	79:t:194:A:OP1	2.53	0.41
63:c:117:ARG:HH11	79:t:1257:A:H61	1.68	0.41
64:d:8:LYS:HG3	64:d:9:LYS:HG2	2.01	0.41
66:f:90:MET:HE1	78:r:116:ALA:HB3	2.02	0.41
67:g:54:LYS:HE2	79:t:437:G:H5''	1.14	0.41
79:t:4243:A:O2'	79:t:4244:A:H8	2.04	0.41
1:S2:17:C:H2'	1:S2:18:C:C6	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:325:C:C4	1:S2:325:C:C2	3.01	0.41
1:S2:944:A:N3	28:SO:139:SER:HB3	2.36	0.41
1:S2:1006:C:O5'	64:d:7:THR:N	2.53	0.41
1:S2:1350:U:H3'	6:SF:56:TYR:HA	2.02	0.41
1:S2:1424:G:H21	15:ST:3:GLY:HA3	1.86	0.41
1:S2:1648:G:O2'	1:S2:1674:G:O6	2.32	0.41
2:SA:119:PRO:HG2	2:SA:142:LEU:HD11	2.03	0.41
2:SA:147:LEU:HA	2:SA:161:ILE:HB	2.02	0.41
4:SD:101:GLN:HA	4:SD:104:SER:HB3	2.02	0.41
6:SF:68:ILE:O	6:SF:72:LEU:N	2.49	0.41
6:SF:85:LYS:HB3	6:SF:88:MET:HG2	2.03	0.41
10:SL:30:LYS:HD3	10:SL:32:LYS:HD2	2.03	0.41
11:SP:110:GLU:HG3	14:SS:117:ILE:HG12	2.03	0.41
14:SS:4:VAL:HG12	14:SS:5:ILE:HG22	2.03	0.41
15:ST:11:GLN:HA	15:ST:14:PHE:HB3	2.03	0.41
22:Sg:215:GLN:HG3	22:Sg:231:ASP:HB2	2.03	0.41
24:SG:44:GLU:HB3	24:SG:119:LYS:HG2	2.03	0.41
25:SJ:130:ILE:HG22	25:SJ:143:ASN:HA	2.03	0.41
25:SJ:137:VAL:N	25:SJ:140:GLN:O	2.47	0.41
28:SO:136:PRO:HB2	28:SO:139:SER:HB2	2.03	0.41
35:A:183:GLY:HA2	79:t:1595:A:H5''	2.03	0.41
37:C:137:VAL:HG13	37:C:144:ILE:HG12	2.03	0.41
37:C:232:VAL:HG11	37:C:256:ALA:HA	2.02	0.41
38:D:102:G:OP1	38:D:109:C:N4	2.54	0.41
41:G:91:THR:HB	41:G:109:LEU:HD13	2.01	0.41
41:G:174:LEU:HD13	41:G:212:LEU:HD13	2.03	0.41
42:H:74:MET:HE2	42:H:74:MET:HB3	1.97	0.41
44:J:129:ARG:HB3	44:J:153:LEU:HD22	2.02	0.41
44:J:163:GLN:O	44:J:166:THR:OG1	2.36	0.41
47:M:77:SER:CB	47:M:102:ARG:HD2	2.50	0.41
49:O:15:GLN:NE2	79:t:299:A:OP2	2.36	0.41
49:O:157:LYS:NZ	79:t:56:A:OP1	2.52	0.41
61:a:10:VAL:HA	61:a:24:VAL:HA	2.03	0.41
77:q:50:ARG:HG2	77:q:51:ALA:H	1.85	0.41
79:t:189:G:H1	79:t:244:G:H1	1.69	0.41
79:t:1069:C:H2'	79:t:1070:A:H8	1.85	0.41
79:t:1244:G:H2'	79:t:1245:G:C8	2.54	0.41
79:t:1924:A:H3'	79:t:1925:A:H8	1.85	0.41
1:S2:517:OMC:HM22	1:S2:518:G:H5'	2.03	0.41
1:S2:694:G:N7	1:S2:737:G:N2	2.69	0.41
1:S2:910:G:OP2	53:S:173:ARG:NH1	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:1109:C:H2'	13:SR:124:VAL:HG23	2.03	0.41
4:SD:68:GLU:HG2	4:SD:69:LEU:HD12	2.03	0.41
15:ST:37:VAL:HG11	15:ST:52:TRP:CZ2	2.56	0.41
24:SG:49:VAL:HG23	24:SG:114:VAL:HG23	2.03	0.41
27:SN:26:LEU:HG	27:SN:28:LEU:HB3	2.03	0.41
30:SY:20:ARG:HH21	30:SY:74:MET:HE3	1.86	0.41
35:A:118:GLU:HG3	35:A:119:LYS:HG3	2.03	0.41
39:E:99:G:N7	54:T:55:LYS:NZ	2.68	0.41
40:F:51:MET:HE2	40:F:64:ILE:HD11	2.03	0.41
40:F:241:LYS:HA	40:F:244:HIS:CD2	2.56	0.41
45:K:27:PRO:HG2	45:K:124:GLY:HA2	2.03	0.41
49:O:108:ARG:HD2	49:O:108:ARG:HA	1.88	0.41
56:V:61:VAL:CG2	56:V:62:THR:N	2.83	0.41
68:h:63:VAL:H	68:h:63:VAL:HG12	1.57	0.41
70:j:50:PHE:HZ	70:j:93:VAL:HG11	1.86	0.41
71:k:18:LEU:HA	71:k:25:LYS:HA	2.03	0.41
73:m:20:ASN:ND2	73:m:42:ARG:O	2.54	0.41
76:p:47:GLY:HA2	79:t:282:G:H5'	2.02	0.41
76:p:66:ILE:H	76:p:66:ILE:HG13	1.62	0.41
79:t:463:C:H2'	79:t:464:A:O4'	2.21	0.41
79:t:4355:G:N2	79:t:4358:A:OP2	2.54	0.41
82:u:17:C:H5'	82:u:18:G:H4'	2.03	0.41
1:S2:92:A:H4'	5:SE:3:ARG:HH21	1.86	0.40
1:S2:220:U:H2'	1:S2:221:A:C8	2.56	0.40
1:S2:1005:G:N3	64:d:7:THR:OG1	2.36	0.40
1:S2:1340:U:H3'	1:S2:1341:C:H2'	2.03	0.40
2:SA:28:THR:O	2:SA:29:ASN:CB	2.69	0.40
2:SA:104:THR:O	2:SA:107:THR:OG1	2.39	0.40
7:SH:158:LEU:HD23	7:SH:158:LEU:HA	1.81	0.40
14:SS:101:ASN:O	14:SS:105:ASN:N	2.54	0.40
16:SU:20:ILE:HD11	16:SU:91:LEU:HB2	2.03	0.40
21:Sd:46:TYR:O	21:Sd:49:ASP:CA	2.69	0.40
23:SC:77:SER:O	23:SC:79:GLU:N	2.54	0.40
24:SG:146:ASN:O	58:X:86:SER:OG	2.31	0.40
25:SJ:70:ARG:HE	25:SJ:94:LEU:HG	1.86	0.40
36:B:224:LYS:HB2	36:B:224:LYS:HE3	1.89	0.40
37:C:242:PRO:O	79:t:2276:G:O2'	2.32	0.40
41:G:208:ILE:HA	41:G:209:PRO:HD3	1.91	0.40
50:P:18:ARG:NH1	79:t:2035:U:OP1	2.55	0.40
53:S:130:ASN:ND2	79:t:1553:G:O2'	2.54	0.40
54:T:8:ARG:HH21	79:t:926:G:H1	1.68	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:Z:59:ARG:HA	60:Z:59:ARG:HD3	1.84	0.40
62:b:42:ARG:NH1	79:t:4339:G:O6	2.54	0.40
68:h:67:LEU:HD12	68:h:71:LYS:HD2	2.03	0.40
73:m:23:ILE:H	73:m:23:ILE:HG13	1.51	0.40
79:t:227:G:N2	79:t:234:G:H1	2.20	0.40
79:t:1550:C:H2'	79:t:1551:U:H6	1.85	0.40
79:t:3748:G:O2'	79:t:3786:G:O6	2.29	0.40
79:t:4063:G:H2'	79:t:4064:G:C8	2.55	0.40
1:S2:376:A:H2'	1:S2:377:G:H8	1.86	0.40
1:S2:562:U:H2'	1:S2:563:G:C8	2.56	0.40
1:S2:578:C:H6	1:S2:578:C:H2'	1.72	0.40
1:S2:866:U:O3'	1:S2:867:G:H4'	2.20	0.40
1:S2:902:G:O2'	1:S2:903:A:O4'	2.39	0.40
1:S2:1156:U:H5''	29:SW:71:LYS:NZ	2.35	0.40
1:S2:1566:G:O2'	1:S2:1568:C:N4	2.43	0.40
5:SE:115:THR:HA	5:SE:116:PRO:HD3	1.88	0.40
22:Sg:63:SER:OG	22:Sg:84:ASP:OD2	2.37	0.40
29:SW:94:LEU:HD21	29:SW:102:ILE:HG23	2.02	0.40
35:A:152:SER:OG	79:t:3632:G:N7	2.49	0.40
37:C:8:ILE:HD11	37:C:24:LEU:HD13	2.01	0.40
37:C:279:LEU:HA	37:C:280:PRO:HD3	1.88	0.40
39:E:49:A:OP1	40:F:224:SER:N	2.54	0.40
42:H:166:ARG:HB3	42:H:209:TRP:CD2	2.56	0.40
44:J:31:ARG:NH1	44:J:87:GLY:HA3	2.36	0.40
52:R:156:PRO:HG2	62:b:48:TYR:HA	2.03	0.40
55:U:88:ARG:HG3	79:t:4261:U:H4'	2.02	0.40
57:W:59:ASP:OD1	57:W:59:ASP:N	2.54	0.40
57:W:100:ASP:N	57:W:100:ASP:OD1	2.53	0.40
79:t:479:C:H5	79:t:658:G:H5'	1.86	0.40
79:t:2461:C:H2'	79:t:2462:G:C8	2.56	0.40
79:t:4995:U:H2'	79:t:4996:A:C8	2.56	0.40
82:u:56:C:H3'	82:u:57:G:C8	2.56	0.40
1:S2:441:C:H5	1:S2:448:A:H1'	1.86	0.40
1:S2:1279:C:H2'	1:S2:1280:G:C8	2.57	0.40
1:S2:1375:G:H2'	1:S2:1376:A:H8	1.86	0.40
1:S2:1445:U:O2'	16:SU:55:ARG:O	2.32	0.40
7:SH:169:LYS:HA	7:SH:172:THR:HG22	2.03	0.40
11:SP:44:ARG:NH1	11:SP:82:ASP:O	2.54	0.40
17:SV:40:ASP:OD1	17:SV:40:ASP:N	2.53	0.40
22:Sg:24:THR:OG1	22:Sg:27:PHE:O	2.33	0.40
35:A:158:ILE:HD12	35:A:162:ASN:HD22	1.86	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:B:10:ARG:HH21	36:B:14:LEU:HD21	1.87	0.40
36:B:95:THR:HG22	79:t:4868:A:H4'	2.04	0.40
42:H:184:ILE:HG21	42:H:193:GLU:HG3	2.03	0.40
43:I:161:VAL:HG21	43:I:167:VAL:HG23	2.03	0.40
49:O:65:ARG:HD2	49:O:127:TYR:CD2	2.56	0.40
65:e:23:ARG:HB2	65:e:121:ASN:HA	2.02	0.40
65:e:32:ARG:HG2	65:e:48:GLU:HB3	2.03	0.40
79:t:123:C:H2'	79:t:124:C:C6	2.57	0.40
79:t:1923:A:N3	79:t:4394:C:O2'	2.45	0.40
79:t:2376:G:OP2	79:t:2785:A:N6	2.50	0.40
1:S2:554:A:H8	1:S2:555:A:H1'	1.86	0.40
1:S2:845:G:H2'	1:S2:846:G:C8	2.55	0.40
1:S2:845:G:H2'	1:S2:846:G:H8	1.86	0.40
1:S2:1693:G:OP2	19:Sa:89:ARG:NH1	2.50	0.40
3:SB:121:ILE:HD11	3:SB:207:LEU:HD21	2.02	0.40
6:SF:126:THR:HG21	20:Sc:27:CYS:SG	2.61	0.40
18:SX:105:PHE:CD1	18:SX:121:LYS:HD3	2.54	0.40
28:SO:103:ASN:ND2	28:SO:140:THR:HG21	2.36	0.40
36:B:292:LEU:HB2	36:B:299:ILE:HG21	2.04	0.40
37:C:144:ILE:H	37:C:144:ILE:HG13	1.76	0.40
41:G:264:ILE:HA	41:G:265:PRO:HD3	1.87	0.40
44:J:95:VAL:HG22	74:n:82:LEU:HD13	2.03	0.40
45:K:193:ASP:N	45:K:193:ASP:OD1	2.53	0.40
46:L:46:GLN:HE21	46:L:74:VAL:HG22	1.86	0.40
52:R:32:TYR:O	52:R:36:ALA:N	2.54	0.40
54:T:160:ARG:CG	54:T:163:HIS:CG	3.04	0.40
55:U:89:ILE:HD13	79:t:4262:U:H4'	2.03	0.40
79:t:3893:G:OP2	79:t:4145:G:N2	2.54	0.40
79:t:4819:G:H2'	79:t:4820:G:C8	2.57	0.40
79:t:4861:G:H2'	79:t:4862:G:C8	2.57	0.40
1:S2:678:U:OP2	1:S2:1026:C:N4	2.46	0.40
1:S2:1139:C:H41	1:S2:1149:A:H62	1.70	0.40
1:S2:1228:A:H2'	1:S2:1229:G:H8	1.87	0.40
6:SF:49:LEU:HD21	12:SQ:50:LYS:HG3	2.04	0.40
7:SH:141:GLY:HA3	7:SH:157:HIS:HB2	2.01	0.40
12:SQ:90:LYS:HB3	12:SQ:120:LEU:HB2	2.03	0.40
34:Sf:106:TYR:HE1	34:Sf:116:ARG:HG3	1.86	0.40
37:C:116:ASN:HD21	79:t:1488:G:H21	1.69	0.40
40:F:155:THR:HG22	40:F:179:ARG:HD3	2.04	0.40
41:G:187:ARG:NH1	79:t:4897:C:OP1	2.48	0.40
43:I:169:PHE:HB2	70:j:43:MET:HE1	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:N:89:THR:HG23	48:N:91:TRP:H	1.87	0.40
51:Q:85:LYS:HE2	51:Q:85:LYS:HB2	1.87	0.40
79:t:149:U:O2'	79:t:150:G:N2	2.55	0.40
79:t:1088:C:H2'	79:t:1089:A:C8	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	SA	219/221 (99%)	185 (84%)	31 (14%)	3 (1%)	9	37
3	SB	212/214 (99%)	190 (90%)	22 (10%)	0	100	100
4	SD	224/226 (99%)	187 (84%)	37 (16%)	0	100	100
5	SE	253/259 (98%)	222 (88%)	31 (12%)	0	100	100
6	SF	183/189 (97%)	164 (90%)	19 (10%)	0	100	100
7	SH	180/189 (95%)	152 (84%)	28 (16%)	0	100	100
8	SI	202/204 (99%)	178 (88%)	24 (12%)	0	100	100
9	SK	96/98 (98%)	77 (80%)	19 (20%)	0	100	100
10	SL	147/153 (96%)	133 (90%)	14 (10%)	0	100	100
11	SP	125/127 (98%)	110 (88%)	14 (11%)	1 (1%)	16	48
12	SQ	144/146 (99%)	123 (85%)	20 (14%)	1 (1%)	18	50
13	SR	132/134 (98%)	105 (80%)	27 (20%)	0	100	100
14	SS	143/145 (99%)	128 (90%)	15 (10%)	0	100	100
15	ST	141/143 (99%)	130 (92%)	10 (7%)	1 (1%)	18	50
16	SU	102/104 (98%)	89 (87%)	13 (13%)	0	100	100
17	SV	80/82 (98%)	71 (89%)	9 (11%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	SX	139/141 (99%)	121 (87%)	18 (13%)	0	100	100
19	Sa	100/102 (98%)	85 (85%)	14 (14%)	1 (1%)	12	43
20	Sc	62/64 (97%)	52 (84%)	10 (16%)	0	100	100
21	Sd	53/55 (96%)	41 (77%)	11 (21%)	1 (2%)	6	33
22	Sg	310/312 (99%)	250 (81%)	60 (19%)	0	100	100
23	SC	215/220 (98%)	196 (91%)	18 (8%)	1 (0%)	24	56
24	SG	235/237 (99%)	205 (87%)	30 (13%)	0	100	100
25	SJ	184/185 (100%)	161 (88%)	22 (12%)	1 (0%)	24	56
26	SM	116/118 (98%)	93 (80%)	23 (20%)	0	100	100
27	SN	148/150 (99%)	136 (92%)	12 (8%)	0	100	100
28	SO	135/137 (98%)	120 (89%)	15 (11%)	0	100	100
29	SW	127/129 (98%)	113 (89%)	14 (11%)	0	100	100
30	SY	130/131 (99%)	121 (93%)	9 (7%)	0	100	100
31	SZ	71/73 (97%)	56 (79%)	13 (18%)	2 (3%)	4	27
32	Sb	80/82 (98%)	66 (82%)	14 (18%)	0	100	100
33	Se	55/57 (96%)	45 (82%)	10 (18%)	0	100	100
34	Sf	65/67 (97%)	50 (77%)	15 (23%)	0	100	100
35	A	250/252 (99%)	224 (90%)	24 (10%)	2 (1%)	16	48
36	B	395/397 (100%)	347 (88%)	45 (11%)	3 (1%)	16	48
37	C	361/363 (99%)	324 (90%)	36 (10%)	1 (0%)	36	65
40	F	292/294 (99%)	261 (89%)	30 (10%)	1 (0%)	36	65
41	G	232/247 (94%)	182 (78%)	47 (20%)	3 (1%)	9	38
42	H	223/225 (99%)	201 (90%)	21 (9%)	1 (0%)	30	60
43	I	232/234 (99%)	204 (88%)	25 (11%)	3 (1%)	9	38
44	J	189/191 (99%)	169 (89%)	20 (11%)	0	100	100
45	K	204/211 (97%)	183 (90%)	21 (10%)	0	100	100
46	L	167/169 (99%)	148 (89%)	19 (11%)	0	100	100
47	M	203/205 (99%)	172 (85%)	31 (15%)	0	100	100
48	N	137/139 (99%)	119 (87%)	18 (13%)	0	100	100
49	O	201/203 (99%)	175 (87%)	25 (12%)	1 (0%)	24	56
50	P	193/195 (99%)	185 (96%)	8 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	Q	151/153 (99%)	140 (93%)	11 (7%)	0	100	100
52	R	185/187 (99%)	163 (88%)	20 (11%)	2 (1%)	11	42
53	S	179/181 (99%)	164 (92%)	14 (8%)	1 (1%)	21	52
54	T	173/175 (99%)	158 (91%)	13 (8%)	2 (1%)	10	40
55	U	155/157 (99%)	134 (86%)	19 (12%)	2 (1%)	9	38
56	V	97/99 (98%)	91 (94%)	6 (6%)	0	100	100
57	W	127/129 (98%)	120 (94%)	7 (6%)	0	100	100
58	X	119/121 (98%)	103 (87%)	13 (11%)	3 (2%)	4	29
59	Y	115/117 (98%)	101 (88%)	14 (12%)	0	100	100
60	Z	132/134 (98%)	125 (95%)	7 (5%)	0	100	100
61	a	132/134 (98%)	118 (89%)	14 (11%)	0	100	100
62	b	145/147 (99%)	126 (87%)	19 (13%)	0	100	100
63	c	94/121 (78%)	80 (85%)	14 (15%)	0	100	100
64	d	101/103 (98%)	87 (86%)	14 (14%)	0	100	100
65	e	104/106 (98%)	91 (88%)	13 (12%)	0	100	100
66	f	127/129 (98%)	116 (91%)	10 (8%)	1 (1%)	16	48
67	g	107/109 (98%)	89 (83%)	16 (15%)	2 (2%)	6	33
68	h	112/114 (98%)	96 (86%)	16 (14%)	0	100	100
69	i	120/122 (98%)	111 (92%)	7 (6%)	2 (2%)	7	34
70	j	95/97 (98%)	87 (92%)	6 (6%)	2 (2%)	5	31
71	k	82/84 (98%)	71 (87%)	11 (13%)	0	100	100
72	l	67/69 (97%)	64 (96%)	3 (4%)	0	100	100
73	m	48/50 (96%)	47 (98%)	1 (2%)	0	100	100
74	n	48/50 (96%)	40 (83%)	8 (17%)	0	100	100
75	o	23/25 (92%)	22 (96%)	1 (4%)	0	100	100
76	p	103/105 (98%)	95 (92%)	7 (7%)	1 (1%)	12	43
77	q	89/91 (98%)	78 (88%)	11 (12%)	0	100	100
78	r	120/122 (98%)	101 (84%)	19 (16%)	0	100	100
83	y	24/26 (92%)	21 (88%)	1 (4%)	2 (8%)	0	9
All	All	11261/11476 (98%)	9888 (88%)	1326 (12%)	47 (0%)	31	60

All (47) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
23	SC	78	LEU
42	H	170	THR
43	I	166	LEU
54	T	164	LYS
54	T	166	ARG
58	X	52	THR
67	g	107	PRO
69	i	87	LYS
83	y	5	PRO
83	y	22	GLN
2	SA	29	ASN
15	ST	41	LYS
35	A	123	ARG
35	A	251	THR
36	B	293	ILE
36	B	295	ASP
67	g	57	THR
70	j	35	LYS
12	SQ	117	ARG
31	SZ	45	ASN
31	SZ	49	LEU
36	B	4	ARG
37	C	69	THR
41	G	127	SER
55	U	18	PRO
55	U	53	PRO
58	X	87	LEU
2	SA	12	GLU
11	SP	112	ILE
19	Sa	47	ALA
40	F	260	GLU
41	G	128	HIS
41	G	136	HIS
49	O	95	ALA
52	R	6	ARG
66	f	7	LEU
43	I	163	PRO
76	p	104	ILE
21	Sd	47	ALA
25	SJ	123	ILE
52	R	7	HIS
53	S	25	ASP
58	X	74	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
69	i	96	ASN
70	j	34	THR
2	SA	26	GLY
43	I	30	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	SA	183/183 (100%)	181 (99%)	2 (1%)	65	73
3	SB	195/195 (100%)	193 (99%)	2 (1%)	68	74
4	SD	189/189 (100%)	187 (99%)	2 (1%)	65	73
5	SE	222/222 (100%)	218 (98%)	4 (2%)	51	67
6	SF	159/159 (100%)	153 (96%)	6 (4%)	29	53
7	SH	166/169 (98%)	163 (98%)	3 (2%)	51	67
8	SI	177/177 (100%)	176 (99%)	1 (1%)	78	79
9	SK	89/89 (100%)	87 (98%)	2 (2%)	45	63
10	SL	137/137 (100%)	137 (100%)	0	100	100
11	SP	113/113 (100%)	111 (98%)	2 (2%)	51	67
12	SQ	121/121 (100%)	119 (98%)	2 (2%)	53	67
13	SR	121/121 (100%)	121 (100%)	0	100	100
14	SS	126/126 (100%)	125 (99%)	1 (1%)	73	76
15	ST	113/113 (100%)	112 (99%)	1 (1%)	70	75
16	SU	94/94 (100%)	94 (100%)	0	100	100
17	SV	66/66 (100%)	66 (100%)	0	100	100
18	SX	113/113 (100%)	109 (96%)	4 (4%)	32	54
19	Sa	89/89 (100%)	89 (100%)	0	100	100
20	Sc	57/57 (100%)	56 (98%)	1 (2%)	51	67
21	Sd	48/48 (100%)	46 (96%)	2 (4%)	26	51

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	Sg	271/271 (100%)	271 (100%)	0	100	100
23	SC	187/186 (100%)	186 (100%)	1 (0%)	81	80
24	SG	207/207 (100%)	207 (100%)	0	100	100
25	SJ	162/161 (101%)	160 (99%)	2 (1%)	63	72
26	SM	98/100 (98%)	97 (99%)	1 (1%)	68	74
27	SN	130/130 (100%)	129 (99%)	1 (1%)	73	76
28	SO	107/107 (100%)	107 (100%)	0	100	100
29	SW	112/112 (100%)	109 (97%)	3 (3%)	39	59
30	SY	114/113 (101%)	114 (100%)	0	100	100
31	SZ	64/64 (100%)	62 (97%)	2 (3%)	35	57
32	Sb	74/74 (100%)	74 (100%)	0	100	100
33	Se	46/46 (100%)	45 (98%)	1 (2%)	45	63
34	Sf	60/60 (100%)	60 (100%)	0	100	100
35	A	194/194 (100%)	190 (98%)	4 (2%)	47	64
36	B	345/345 (100%)	343 (99%)	2 (1%)	78	79
37	C	302/302 (100%)	296 (98%)	6 (2%)	48	64
40	F	248/248 (100%)	248 (100%)	0	100	100
41	G	209/220 (95%)	208 (100%)	1 (0%)	81	80
42	H	194/194 (100%)	190 (98%)	4 (2%)	47	64
43	I	199/199 (100%)	195 (98%)	4 (2%)	48	64
44	J	170/170 (100%)	166 (98%)	4 (2%)	43	61
45	K	178/179 (99%)	178 (100%)	0	100	100
46	L	142/142 (100%)	141 (99%)	1 (1%)	76	77
47	M	171/171 (100%)	166 (97%)	5 (3%)	37	57
48	N	118/118 (100%)	117 (99%)	1 (1%)	73	76
49	O	171/171 (100%)	170 (99%)	1 (1%)	78	79
50	P	168/168 (100%)	165 (98%)	3 (2%)	51	67
51	Q	134/134 (100%)	130 (97%)	4 (3%)	36	57
52	R	164/164 (100%)	162 (99%)	2 (1%)	63	72
53	S	160/160 (100%)	159 (99%)	1 (1%)	78	79
54	T	156/156 (100%)	152 (97%)	4 (3%)	40	60

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
55	U	138/138 (100%)	134 (97%)	4 (3%)	37	57
56	V	89/89 (100%)	86 (97%)	3 (3%)	32	55
57	W	100/100 (100%)	99 (99%)	1 (1%)	68	74
58	X	100/100 (100%)	99 (99%)	1 (1%)	68	74
59	Y	105/105 (100%)	103 (98%)	2 (2%)	50	65
60	Z	124/124 (100%)	121 (98%)	3 (2%)	43	61
61	a	117/117 (100%)	114 (97%)	3 (3%)	40	60
62	b	120/120 (100%)	117 (98%)	3 (2%)	42	61
63	c	82/101 (81%)	81 (99%)	1 (1%)	63	72
64	d	88/88 (100%)	86 (98%)	2 (2%)	44	62
65	e	97/97 (100%)	97 (100%)	0	100	100
66	f	115/115 (100%)	115 (100%)	0	100	100
67	g	88/88 (100%)	87 (99%)	1 (1%)	65	73
68	h	98/98 (100%)	98 (100%)	0	100	100
69	i	109/109 (100%)	107 (98%)	2 (2%)	51	67
70	j	83/83 (100%)	82 (99%)	1 (1%)	63	72
71	k	71/71 (100%)	71 (100%)	0	100	100
72	l	64/64 (100%)	64 (100%)	0	100	100
73	m	47/47 (100%)	46 (98%)	1 (2%)	47	64
74	n	46/46 (100%)	46 (100%)	0	100	100
75	o	24/24 (100%)	24 (100%)	0	100	100
76	p	93/93 (100%)	90 (97%)	3 (3%)	34	56
77	q	74/74 (100%)	73 (99%)	1 (1%)	59	70
78	r	106/106 (100%)	106 (100%)	0	100	100
All	All	9811/9844 (100%)	9686 (99%)	125 (1%)	59	71

All (125) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	SA	77	ILE
2	SA	97	THR
3	SB	87	ILE
3	SB	121	ILE
4	SD	5	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	SD	126	ILE
5	SE	90	ILE
5	SE	111	VAL
5	SE	228	ILE
5	SE	236	ILE
6	SF	19	LEU
6	SF	61	PHE
6	SF	62	ARG
6	SF	130	ARG
6	SF	177	LEU
6	SF	199	VAL
7	SH	75	ILE
7	SH	144	ILE
7	SH	158	LEU
8	SI	158	ILE
9	SK	15	LEU
9	SK	40	VAL
11	SP	76	VAL
11	SP	121	ILE
12	SQ	22	VAL
12	SQ	92	LEU
14	SS	103	LEU
15	ST	131	LEU
18	SX	5	ARG
18	SX	7	LEU
18	SX	94	ILE
18	SX	125	VAL
20	Sc	18	LEU
21	Sd	26	ASN
21	Sd	39	CYS
23	SC	155	ILE
25	SJ	138[A]	ARG
25	SJ	138[B]	ARG
26	SM	68	LEU
27	SN	115	LEU
29	SW	81	VAL
29	SW	93	LEU
29	SW	103	VAL
31	SZ	48	VAL
31	SZ	62	VAL
33	Se	6	LEU
35	A	20	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	A	45	VAL
35	A	101	VAL
35	A	225	ILE
36	B	85	VAL
36	B	299	ILE
37	C	55	SER
37	C	150	LEU
37	C	193	LYS
37	C	199	ARG
37	C	209	ILE
37	C	223	ASN
41	G	279	ASN
42	H	95	ILE
42	H	167	ILE
42	H	169	LEU
42	H	179	LEU
43	I	161	VAL
43	I	162	ASP
43	I	164	ILE
43	I	170	LEU
44	J	4	ILE
44	J	42	ASN
44	J	63	ASN
44	J	123	ILE
46	L	157	ILE
47	M	46	ILE
47	M	63	THR
47	M	125	ILE
47	M	143	GLU
47	M	144	LEU
48	N	45	VAL
49	O	64	ILE
50	P	104	VAL
50	P	187	LYS
50	P	188	LYS
51	Q	24	VAL
51	Q	127	ARG
51	Q	139	TYR
51	Q	146	ILE
52	R	54	SER
52	R	163	THR
53	S	115	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
54	T	158	VAL
54	T	161	ARG
54	T	162	GLN
54	T	164	LYS
55	U	109	VAL
55	U	110	LYS
55	U	111	GLU
55	U	128	LEU
56	V	46	ARG
56	V	55	ASN
56	V	61	VAL
57	W	132	ILE
58	X	83	THR
59	Y	52	LEU
59	Y	119	ILE
60	Z	54	GLU
60	Z	74	TYR
60	Z	104	VAL
61	a	10	VAL
61	a	13	VAL
61	a	89	ILE
62	b	78	LEU
62	b	100	ILE
62	b	122	VAL
63	c	116	LEU
64	d	77	ASN
64	d	94	LEU
67	g	108	SER
69	i	88	THR
69	i	96	ASN
70	j	71	LYS
73	m	23	ILE
76	p	23	VAL
76	p	27	LYS
76	p	93	LEU
77	q	29	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (180) such sidechains are listed below:

Mol	Chain	Res	Type
2	SA	9	GLN
2	SA	50	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	SB	40	ASN
3	SB	95	ASN
3	SB	160	GLN
3	SB	186	ASN
4	SD	4	GLN
4	SD	159	HIS
4	SD	165	ASN
5	SE	98	ASN
5	SE	138	HIS
5	SE	179	ASN
6	SF	83	ASN
6	SF	148	ASN
7	SH	73	GLN
7	SH	162	GLN
7	SH	165	ASN
7	SH	168	HIS
8	SI	64	ASN
8	SI	138	ASN
9	SK	61	GLN
10	SL	13	GLN
11	SP	54	HIS
11	SP	103	ASN
12	SQ	80	GLN
12	SQ	97	GLN
13	SR	83	ASN
15	ST	126	GLN
15	ST	128	GLN
16	SU	100	GLN
17	SV	2	GLN
17	SV	21	ASN
17	SV	35	ASN
19	Sa	80	HIS
21	Sd	5	GLN
21	Sd	26	ASN
22	Sg	76	GLN
22	Sg	117	ASN
22	Sg	147	HIS
22	Sg	162	ASN
22	Sg	222	ASN
23	SC	235	ASN
24	SG	81	HIS
24	SG	163	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
24	SG	186	GLN
24	SG	197	GLN
24	SG	227	GLN
26	SM	55	ASN
26	SM	72	HIS
27	SN	5	HIS
28	SO	20	GLN
28	SO	32	HIS
28	SO	79	GLN
29	SW	15	ASN
29	SW	16	ASN
29	SW	98	GLN
29	SW	113	HIS
30	SY	2	ASN
30	SY	124	ASN
31	SZ	89	GLN
31	SZ	106	GLN
34	Sf	91	ASN
35	A	97	ASN
35	A	132	ASN
35	A	162	ASN
35	A	205	ASN
35	A	216	HIS
36	B	11	HIS
36	B	121	ASN
36	B	158	GLN
36	B	204	GLN
36	B	245	HIS
36	B	271	GLN
36	B	301	ASN
36	B	328	ASN
37	C	38	ASN
37	C	61	GLN
37	C	85	HIS
37	C	223	ASN
37	C	236	ASN
37	C	278	ASN
37	C	343	GLN
40	F	122	GLN
40	F	191	ASN
40	F	195	HIS
40	F	198	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	G	47	ASN
41	G	167	GLN
41	G	190	HIS
41	G	211	HIS
41	G	256	GLN
41	G	279	ASN
42	H	24	ASN
42	H	80	ASN
42	H	239	GLN
43	I	43	GLN
43	I	64	GLN
43	I	81	ASN
43	I	206	GLN
43	I	227	ASN
43	I	236	HIS
44	J	39	ASN
44	J	42	ASN
44	J	98	HIS
44	J	108	ASN
44	J	116	ASN
44	J	140	GLN
45	K	14	ASN
45	K	163	GLN
45	K	213	HIS
47	M	104	ASN
47	M	115	GLN
48	N	44	GLN
48	N	48	GLN
48	N	70	GLN
48	N	83	ASN
49	O	87	HIS
49	O	199	GLN
50	P	14	HIS
50	P	63	ASN
50	P	90	HIS
50	P	180	GLN
50	P	184	ASN
51	Q	64	ASN
51	Q	80	GLN
51	Q	133	HIS
52	R	125	GLN
52	R	162	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
53	S	141	HIS
54	T	117	HIS
55	U	49	GLN
55	U	54	HIS
55	U	70	HIS
55	U	131	GLN
55	U	139	HIS
57	W	27	ASN
57	W	101	ASN
57	W	135	ASN
58	X	96	GLN
59	Y	111	GLN
60	Z	20	ASN
60	Z	24	HIS
60	Z	61	HIS
60	Z	72	GLN
60	Z	91	ASN
60	Z	96	HIS
61	a	78	ASN
62	b	44	ASN
62	b	60	HIS
62	b	66	ASN
63	c	19	ASN
63	c	27	GLN
63	c	58	GLN
64	d	77	ASN
65	e	93	ASN
66	f	43	ASN
66	f	102	ASN
66	f	107	ASN
67	g	55	ASN
67	g	80	ASN
67	g	91	ASN
67	g	99	HIS
68	h	73	HIS
68	h	110	GLN
69	i	20	GLN
69	i	98	HIS
70	j	26	HIS
70	j	92	ASN
71	k	16	HIS
71	k	76	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
73	m	33	ASN
74	n	109	ASN
76	p	19	GLN
76	p	102	GLN
77	q	56	HIS
77	q	92	GLN
78	r	6	GLN
78	r	41	ASN
78	r	70	GLN
78	r	83	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	S2	1687/1714 (98%)	596 (35%)	27 (1%)
38	D	156/157 (99%)	37 (23%)	0
39	E	118/121 (97%)	22 (18%)	0
79	t	3592/3607 (99%)	1029 (28%)	0
80	v	72/76 (94%)	28 (38%)	0
81	w	9/10 (90%)	3 (33%)	0
82	u	75/76 (98%)	34 (45%)	0
All	All	5709/5761 (99%)	1749 (30%)	27 (0%)

All (1749) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	S2	2	A
1	S2	3	C
1	S2	4	C
1	S2	5	U
1	S2	9	U
1	S2	10	G
1	S2	24	C
1	S2	25	A
1	S2	33	G
1	S2	38	A
1	S2	39	A
1	S2	41	G
1	S2	42	A
1	S2	43	U
1	S2	46	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	S2	49	C
1	S2	53	C
1	S2	54	A
1	S2	55	U
1	S2	56	G
1	S2	58	C
1	S2	60	A
1	S2	61	A
1	S2	62	G
1	S2	64	A
1	S2	65	C
1	S2	66	G
1	S2	67	C
1	S2	68	A
1	S2	72	C
1	S2	73	C
1	S2	74	G
1	S2	75	G
1	S2	76	U
1	S2	79	A
1	S2	80	G
1	S2	101	U
1	S2	103	A
1	S2	113	G
1	S2	115	U
1	S2	122	G
1	S2	126	G
1	S2	127	C
1	S2	129	C
1	S2	142	C
1	S2	143	U
1	S2	155	G
1	S2	157	U
1	S2	158	A
1	S2	159	A2M
1	S2	160	U
1	S2	162	C
1	S2	166	A2M
1	S2	168	C
1	S2	170	A
1	S2	173	A
1	S2	175	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	S2	182	C
1	S2	183	G
1	S2	191	A
1	S2	192	C
1	S2	193	C
1	S2	194	C
1	S2	195	C
1	S2	196	C
1	S2	197	U
1	S2	198	U
1	S2	199	C
1	S2	200	G
1	S2	203	G
1	S2	204	G
1	S2	206	G
1	S2	214	U
1	S2	215	G
1	S2	224	A
1	S2	291	G
1	S2	292	A
1	S2	293	C
1	S2	295	C
1	S2	305	U
1	S2	308	G
1	S2	310	C
1	S2	311	C
1	S2	312	G
1	S2	313	A
1	S2	316	G
1	S2	318	A
1	S2	319	C
1	S2	323	C
1	S2	324	C
1	S2	325	C
1	S2	326	C
1	S2	327	G
1	S2	328	U
1	S2	329	G
1	S2	330	G
1	S2	332	G
1	S2	333	G
1	S2	338	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	S2	340	C
1	S2	347	G
1	S2	351	G
1	S2	360	A
1	S2	362	C
1	S2	368	U
1	S2	369	C
1	S2	373	G
1	S2	376	A
1	S2	379	C
1	S2	380	G
1	S2	385	G
1	S2	386	C
1	S2	387	C
1	S2	395	G
1	S2	407	G
1	S2	408	A
1	S2	409	C
1	S2	413	G
1	S2	419	G
1	S2	429	C
1	S2	446	G
1	S2	447	A
1	S2	448	A
1	S2	449	A
1	S2	450	C
1	S2	452	G
1	S2	464	A
1	S2	465	A
1	S2	467	G
1	S2	469	A
1	S2	470	G
1	S2	471	G
1	S2	472	C
1	S2	473	A
1	S2	474	G
1	S2	481	C
1	S2	482	G
1	S2	485	A
1	S2	487	U
1	S2	488	U
1	S2	491	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	S2	492	C
1	S2	493	A
1	S2	496	C
1	S2	500	A
1	S2	502	C
1	S2	503	C
1	S2	517	OMC
1	S2	525	A
1	S2	526	A
1	S2	527	C
1	S2	529	A
1	S2	530	U
1	S2	531	A
1	S2	532	C
1	S2	533	A
1	S2	535	G
1	S2	537	C
1	S2	538	U
1	S2	540	U
1	S2	541	U
1	S2	542	U
1	S2	543	C
1	S2	546	G
1	S2	548	C
1	S2	549	C
1	S2	553	U
1	S2	554	A
1	S2	555	A
1	S2	556	U
1	S2	557	U
1	S2	558	G
1	S2	559	G
1	S2	560	A
1	S2	561	A
1	S2	564	A
1	S2	568	E3C
1	S2	574	A
1	S2	576	A
1	S2	579	C
1	S2	583	C
1	S2	584	G
1	S2	585	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	S2	588	G
1	S2	589	G
1	S2	590	A
1	S2	591	U
1	S2	594	A
1	S2	595	U
1	S2	600	G
1	S2	604	A
1	S2	607	U
1	S2	608	C
1	S2	614	C
1	S2	615	C
1	S2	617	G
1	S2	621	C
1	S2	625	G
1	S2	627	U
1	S2	628	A
1	S2	629	A
1	S2	630	U
1	S2	631	U
1	S2	642	U
1	S2	643	A
1	S2	649	U
1	S2	659	G
1	S2	660	C
1	S2	662	G
1	S2	668	A2M
1	S2	669	A
1	S2	670	A
1	S2	671	A
1	S2	672	A
1	S2	673	G
1	S2	681	U
1	S2	683	OMG
1	S2	684	G
1	S2	687	C
1	S2	689	U
1	S2	690	G
1	S2	691	G
1	S2	692	G
1	S2	693	A
1	S2	696	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	S2	697	G
1	S2	731	G
1	S2	732	U
1	S2	733	C
1	S2	734	C
1	S2	735	C
1	S2	736	C
1	S2	738	C
1	S2	739	C
1	S2	748	C
1	S2	751	G
1	S2	752	G
1	S2	753	C
1	S2	788	G
1	S2	789	G
1	S2	790	C
1	S2	791	C
1	S2	792	C
1	S2	794	A
1	S2	795	A
1	S2	797	C
1	S2	809	A
1	S2	810	A
1	S2	811	A
1	S2	815	U
1	S2	821	G
1	S2	822	PSU
1	S2	823	PSU
1	S2	824	C
1	S2	830	A
1	S2	831	G
1	S2	835	C
1	S2	837	A
1	S2	838	G
1	S2	839	C
1	S2	841	G
1	S2	842	C
1	S2	847	A
1	S2	849	A
1	S2	851	C
1	S2	852	G
1	S2	855	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	S2	858	A
1	S2	865	A
1	S2	866	U
1	S2	867	G
1	S2	868	G
1	S2	870	A
1	S2	871	U
1	S2	872	A
1	S2	873	G
1	S2	874	G
1	S2	879	C
1	S2	882	U
1	S2	886	A
1	S2	887	U
1	S2	888	U
1	S2	889	U
1	S2	890	U
1	S2	891	G
1	S2	892	U
1	S2	894	G
1	S2	896	U
1	S2	897	U
1	S2	898	U
1	S2	899	U
1	S2	900	C
1	S2	901	G
1	S2	902	G
1	S2	903	A
1	S2	906	U
1	S2	907	G
1	S2	908	A
1	S2	913	A
1	S2	914	U
1	S2	917	U
1	S2	920	A
1	S2	922	A
1	S2	924	G
1	S2	933	G
1	S2	943	U
1	S2	949	G
1	S2	953	C
1	S2	954	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	S2	964	A
1	S2	968	U
1	S2	969	U
1	S2	970	G
1	S2	971	G
1	S2	978	G
1	S2	989	C
1	S2	990	A
1	S2	992	A
1	S2	996	A
1	S2	999	G
1	S2	1001	A
1	S2	1002	U
1	S2	1005	G
1	S2	1007	C
1	S2	1016	U
1	S2	1017	U
1	S2	1021	U
1	S2	1023	A
1	S2	1026	C
1	S2	1027	A
1	S2	1030	A
1	S2	1045	U
1	S2	1049	A
1	S2	1050	A
1	S2	1058	A
1	S2	1060	A
1	S2	1061	U
1	S2	1062	A
1	S2	1071	G
1	S2	1072	U
1	S2	1073	U
1	S2	1082	A
1	S2	1083	A
1	S2	1085	C
1	S2	1087	A
1	S2	1088	U
1	S2	1089	G
1	S2	1104	G
1	S2	1109	C
1	S2	1113	A
1	S2	1114	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	S2	1115	U
1	S2	1116	C
1	S2	1117	C
1	S2	1118	C
1	S2	1119	A
1	S2	1121	G
1	S2	1126	G
1	S2	1133	A
1	S2	1138	C
1	S2	1148	A
1	S2	1149	A
1	S2	1150	A
1	S2	1154	U
1	S2	1155	U
1	S2	1157	G
1	S2	1158	G
1	S2	1166	G
1	S2	1170	A
1	S2	1189	A
1	S2	1207	G
1	S2	1208	A
1	S2	1212	G
1	S2	1215	C
1	S2	1217	A
1	S2	1221	G
1	S2	1224	G
1	S2	1242	U
1	S2	1243	PSU
1	S2	1244	U
1	S2	1245	G
1	S2	1246	A
1	S2	1250	A
1	S2	1251	A
1	S2	1253	A
1	S2	1256	G
1	S2	1257	G
1	S2	1258	A
1	S2	1259	A
1	S2	1260	A
1	S2	1262	C
1	S2	1264	C
1	S2	1265	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	S2	1269	G
1	S2	1274	G
1	S2	1275	G
1	S2	1283	C
1	S2	1284	A
1	S2	1285	G
1	S2	1286	G
1	S2	1287	A
1	S2	1294	G
1	S2	1295	A
1	S2	1296	U
1	S2	1298	G
1	S2	1300	U
1	S2	1301	A
1	S2	1302	G
1	S2	1303	C
1	S2	1308	U
1	S2	1313	A
1	S2	1315	U
1	S2	1322	G
1	S2	1323	U
1	S2	1324	G
1	S2	1330	G
1	S2	1340	U
1	S2	1341	C
1	S2	1345	G
1	S2	1348	G
1	S2	1350	U
1	S2	1353	A
1	S2	1355	C
1	S2	1356	G
1	S2	1357	A
1	S2	1371	U
1	S2	1372	U
1	S2	1375	G
1	S2	1376	A
1	S2	1378	A
1	S2	1379	A
1	S2	1393	G
1	S2	1396	A
1	S2	1397	U
1	S2	1398	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	S2	1402	A
1	S2	1403	C
1	S2	1404	U
1	S2	1412	C
1	S2	1419	C
1	S2	1420	G
1	S2	1421	A
1	S2	1433	C
1	S2	1435	C
1	S2	1436	C
1	S2	1437	C
1	S2	1438	A
1	S2	1439	A
1	S2	1442	U
1	S2	1446	A
1	S2	1447	G
1	S2	1452	A
1	S2	1454	A
1	S2	1455	A
1	S2	1458	G
1	S2	1462	U
1	S2	1463	U
1	S2	1466	G
1	S2	1470	C
1	S2	1477	U
1	S2	1478	U
1	S2	1481	G
1	S2	1482	C
1	S2	1488	C
1	S2	1489	A
1	S2	1490	G
1	S2	1494	U
1	S2	1495	G
1	S2	1496	U
1	S2	1497	G
1	S2	1498	A
1	S2	1506	A
1	S2	1507	G
1	S2	1508	A
1	S2	1509	U
1	S2	1515	G
1	S2	1518	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	S2	1519	U
1	S2	1520	G
1	S2	1521	C
1	S2	1522	A
1	S2	1523	C
1	S2	1527	C
1	S2	1530	U
1	S2	1531	A
1	S2	1533	A
1	S2	1534	C
1	S2	1535	U
1	S2	1536	G
1	S2	1543	U
1	S2	1544	C
1	S2	1548	G
1	S2	1551	U
1	S2	1552	G
1	S2	1553	C
1	S2	1556	A
1	S2	1557	C
1	S2	1558	C
1	S2	1560	U
1	S2	1568	C
1	S2	1570	G
1	S2	1573	G
1	S2	1580	A
1	S2	1581	C
1	S2	1585	U
1	S2	1586	U
1	S2	1587	G
1	S2	1588	A
1	S2	1598	G
1	S2	1599	U
1	S2	1601	A
1	S2	1603	G
1	S2	1604	G
1	S2	1605	G
1	S2	1617	G
1	S2	1621	U
1	S2	1623	A
1	S2	1634	A
1	S2	1641	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	S2	1646	C
1	S2	1647	A
1	S2	1648	G
1	S2	1654	G
1	S2	1661	A
1	S2	1662	U
1	S2	1663	A
1	S2	1665	G
1	S2	1675	A
1	S2	1676	U
1	S2	1677	U
1	S2	1679	A
1	S2	1682	C
1	S2	1683	C
1	S2	1687	C
1	S2	1689	C
1	S2	1698	C
1	S2	1699	A
1	S2	1702	G
1	S2	1703	OMC
1	S2	1707	U
1	S2	1720	U
1	S2	1721	U
1	S2	1722	G
1	S2	1726	G
1	S2	1728	U
1	S2	1742	C
1	S2	1744	G
1	S2	1745	A
1	S2	1749	G
1	S2	1750	C
1	S2	1752	C
1	S2	1780	G
1	S2	1781	A
1	S2	1782	G
1	S2	1783	C
1	S2	1784	G
1	S2	1785	C
1	S2	1786	U
1	S2	1799	G
1	S2	1800	A
1	S2	1803	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	S2	1804	U
1	S2	1805	G
1	S2	1806	M7A
1	S2	1808	U
1	S2	1811	C
1	S2	1813	A
1	S2	1814	G
1	S2	1815	A
1	S2	1816	G
1	S2	1817	G
1	S2	1822	A
1	S2	1824	A
1	S2	1826	G
1	S2	1829	G
1	S2	1830	UR3
1	S2	1831	A
1	S2	1834	A
1	S2	1835	A
1	S2	1836	G
1	S2	1838	U
1	S2	1839	U
1	S2	1849	G
1	S2	1850	MA6
1	S2	1851	MA6
1	S2	1852	C
1	S2	1855	G
1	S2	1857	G
1	S2	1861	G
1	S2	1862	G
1	S2	1863	A
1	S2	1864	U
1	S2	1865	C
1	S2	1866	A
1	S2	1867	U
1	S2	1869	A
38	D	2	G
38	D	34	U
38	D	35	C
38	D	49	G
38	D	51	U
38	D	59	A
38	D	62	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
38	D	63	U
38	D	72	A
38	D	75	G
38	D	80	A
38	D	81	C
38	D	83	C
38	D	84	A
38	D	85	U
38	D	87	G
38	D	94	G
38	D	100	U
38	D	101	C
38	D	103	A
38	D	105	C
38	D	109	C
38	D	110	U
38	D	114	G
38	D	121	G
38	D	122	G
38	D	123	U
38	D	124	U
38	D	125	C
38	D	126	C
38	D	127	U
38	D	128	C
38	D	129	C
38	D	130	C
38	D	143	G
38	D	148	A
38	D	150	C
39	E	7	G
39	E	10	C
39	E	11	A
39	E	22	A
39	E	23	A
39	E	24	C
39	E	25	G
39	E	27	G
39	E	31	G
39	E	34	C
39	E	38	U
39	E	42	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
39	E	50	A
39	E	53	U
39	E	54	A
39	E	59	G
39	E	63	C
39	E	64	G
39	E	74	A
39	E	97	G
39	E	98	G
39	E	110	G
79	t	6	C
79	t	8	U
79	t	9	C
79	t	10	A
79	t	17	A
79	t	18	C
79	t	21	G
79	t	25	A
79	t	32	G
79	t	33	A
79	t	39	A
79	t	42	A
79	t	47	A
79	t	48	G
79	t	49	U
79	t	55	G
79	t	59	A
79	t	64	A
79	t	65	A
79	t	66	A
79	t	71	C
79	t	72	C
79	t	73	A
79	t	82	U
79	t	84	A
79	t	91	G
79	t	96	U
79	t	101	A
79	t	108	A
79	t	110	C
79	t	119	G
79	t	120	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
79	t	121	A
79	t	129	C
79	t	131	C
79	t	132	G
79	t	133	C
79	t	134	G
79	t	135	G
79	t	136	G
79	t	138	C
79	t	141	G
79	t	143	G
79	t	144	A
79	t	148	G
79	t	149	U
79	t	155	A
79	t	156	C
79	t	157	G
79	t	158	G
79	t	163	C
79	t	169	C
79	t	170	C
79	t	173	G
79	t	179	G
79	t	181	U
79	t	182	C
79	t	183	G
79	t	184	U
79	t	196	G
79	t	197	U
79	t	203	U
79	t	205	A
79	t	212	C
79	t	213	C
79	t	214	C
79	t	215	A
79	t	227	G
79	t	228	U
79	t	229	G
79	t	230	U
79	t	233	G
79	t	234	G
79	t	236	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
79	t	237	G
79	t	241	G
79	t	242	C
79	t	243	G
79	t	249	C
79	t	250	G
79	t	252	C
79	t	255	G
79	t	256	C
79	t	260	C
79	t	282	G
79	t	286	G
79	t	289	A
79	t	291	U
79	t	300	A
79	t	303	C
79	t	309	G
79	t	310	U
79	t	311	A
79	t	316	C
79	t	323	A
79	t	334	C
79	t	339	C
79	t	343	A
79	t	344	C
79	t	345	C
79	t	351	U
79	t	357	A
79	t	367	G
79	t	370	A
79	t	375	U
79	t	376	G
79	t	377	A
79	t	379	A
79	t	380	A
79	t	381	G
79	t	392	A
79	t	404	A
79	t	406	G
79	t	407	G
79	t	408	C
79	t	409	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
79	t	425	G
79	t	426	U
79	t	434	U
79	t	438	G
79	t	440	C
79	t	444	G
79	t	446	A
79	t	447	G
79	t	448	U
79	t	449	C
79	t	451	G
79	t	458	G
79	t	463	C
79	t	464	A
79	t	468	C
79	t	472	G
79	t	473	G
79	t	474	C
79	t	476	G
79	t	479	C
79	t	481	G
79	t	482	G
79	t	487	G
79	t	489	C
79	t	491	G
79	t	492	C
79	t	494	G
79	t	495	C
79	t	496	C
79	t	497	C
79	t	498	G
79	t	499	G
79	t	501	G
79	t	504	U
79	t	508	U
79	t	509	C
79	t	510	C
79	t	511	C
79	t	512	G
79	t	517	C
79	t	630	G
79	t	633	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
79	t	634	C
79	t	635	G
79	t	636	G
79	t	643	A
79	t	645	C
79	t	647	U
79	t	648	C
79	t	649	C
79	t	650	C
79	t	652	C
79	t	654	G
79	t	656	C
79	t	658	G
79	t	659	G
79	t	661	G
79	t	663	C
79	t	674	C
79	t	676	G
79	t	677	G
79	t	678	C
79	t	679	G
79	t	680	C
79	t	692	G
79	t	693	U
79	t	695	C
79	t	713	G
79	t	714	A
79	t	719	U
79	t	720	G
79	t	721	G
79	t	724	A
79	t	728	C
79	t	730	G
79	t	731	G
79	t	734	G
79	t	735	G
79	t	737	A
79	t	738	A
79	t	739	G
79	t	741	U
79	t	742	G
79	t	743	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
79	t	748	G
79	t	899	G
79	t	900	U
79	t	901	U
79	t	902	A
79	t	903	C
79	t	904	A
79	t	905	G
79	t	906	C
79	t	907	C
79	t	912	C
79	t	914	G
79	t	917	G
79	t	919	A
79	t	920	G
79	t	921	C
79	t	922	A
79	t	923	C
79	t	924	U
79	t	925	C
79	t	927	C
79	t	929	G
79	t	932	U
79	t	933	C
79	t	938	G
79	t	944	G
79	t	947	A
79	t	948	G
79	t	949	C
79	t	950	G
79	t	952	G
79	t	953	A
79	t	954	C
79	t	957	G
79	t	964	C
79	t	976	U
79	t	1055	C
79	t	1056	G
79	t	1061	A
79	t	1065	C
79	t	1066	U
79	t	1083	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
79	t	1084	C
79	t	1085	U
79	t	1086	C
79	t	1087	C
79	t	1149	G
79	t	1150	C
79	t	1156	G
79	t	1157	G
79	t	1158	A
79	t	1159	C
79	t	1162	U
79	t	1164	C
79	t	1165	C
79	t	1167	A
79	t	1173	C
79	t	1174	C
79	t	1176	C
79	t	1181	G
79	t	1187	C
79	t	1190	C
79	t	1191	G
79	t	1192	U
79	t	1193	C
79	t	1196	G
79	t	1197	C
79	t	1199	C
79	t	1201	G
79	t	1220	C
79	t	1221	A
79	t	1222	C
79	t	1223	G
79	t	1224	C
79	t	1225	G
79	t	1226	C
79	t	1228	C
79	t	1234	C
79	t	1236	G
79	t	1237	A
79	t	1238	A
79	t	1241	G
79	t	1248	G
79	t	1250	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
79	t	1251	G
79	t	1252	G
79	t	1258	G
79	t	1259	C
79	t	1261	C
79	t	1263	C
79	t	1264	G
79	t	1268	U
79	t	1269	C
79	t	1271	G
79	t	1273	G
79	t	1277	A
79	t	1278	C
79	t	1279	G
79	t	1284	C
79	t	1285	U
79	t	1301	C
79	t	1305	A
79	t	1306	A
79	t	1309	A
79	t	1315	C
79	t	1337	A
79	t	1341	G
79	t	1342	G
79	t	1348	C
79	t	1349	G
79	t	1350	C
79	t	1351	A
79	t	1353	G
79	t	1360	G
79	t	1362	C
79	t	1364	U
79	t	1370	A
79	t	1380	A
79	t	1381	A
79	t	1382	G
79	t	1389	G
79	t	1390	C
79	t	1391	G
79	t	1392	C
79	t	1393	U
79	t	1394	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
79	t	1395	G
79	t	1396	C
79	t	1401	C
79	t	1403	A
79	t	1404	G
79	t	1408	G
79	t	1420	C
79	t	1421	U
79	t	1422	C
79	t	1423	U
79	t	1424	C
79	t	1425	C
79	t	1426	A
79	t	1427	G
79	t	1428	U
79	t	1429	C
79	t	1431	G
79	t	1435	A
79	t	1439	G
79	t	1457	G
79	t	1458	C
79	t	1463	C
79	t	1464	G
79	t	1465	C
79	t	1466	G
79	t	1467	C
79	t	1468	C
79	t	1470	G
79	t	1480	G
79	t	1483	C
79	t	1496	U
79	t	1499	G
79	t	1500	A
79	t	1501	C
79	t	1505	A
79	t	1507	A
79	t	1516	A
79	t	1525	G
79	t	1531	G
79	t	1543	G
79	t	1548	C
79	t	1560	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
79	t	1573	U
79	t	1578	U
79	t	1579	G
79	t	1589	C
79	t	1596	C
79	t	1606	G
79	t	1607	G
79	t	1613	A
79	t	1614	A
79	t	1615	G
79	t	1616	A
79	t	1620	A
79	t	1625	A
79	t	1631	U
79	t	1633	G
79	t	1634	U
79	t	1636	G
79	t	1643	C
79	t	1652	G
79	t	1660	C
79	t	1663	G
79	t	1673	G
79	t	1679	G
79	t	1680	C
79	t	1700	C
79	t	1701	A
79	t	1703	G
79	t	1706	G
79	t	1707	U
79	t	1711	A
79	t	1713	C
79	t	1723	G
79	t	1739	U
79	t	1742	G
79	t	1746	G
79	t	1747	A
79	t	1748	A
79	t	1749	A
79	t	1750	C
79	t	1751	G
79	t	1754	C
79	t	1758	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
79	t	1761	U
79	t	1762	A
79	t	1767	C
79	t	1769	A
79	t	1776	A
79	t	1785	G
79	t	1786	A
79	t	1788	G
79	t	1794	C
79	t	1797	G
79	t	1802	C
79	t	1803	G
79	t	1804	U
79	t	1814	G
79	t	1816	G
79	t	1823	G
79	t	1836	G
79	t	1840	C
79	t	1850	G
79	t	1854	A
79	t	1860	C
79	t	1862	C
79	t	1863	U
79	t	1870	U
79	t	1872	A
79	t	1879	C
79	t	1887	U
79	t	1890	G
79	t	1891	G
79	t	1898	A
79	t	1902	C
79	t	1903	G
79	t	1909	C
79	t	1911	U
79	t	1912	C
79	t	1913	A
79	t	1916	C
79	t	1920	A
79	t	1921	G
79	t	1922	A
79	t	1928	U
79	t	1936	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
79	t	1939	A
79	t	1940	U
79	t	1941	A
79	t	1942	G
79	t	1943	A
79	t	1952	C
79	t	1955	U
79	t	1956	G
79	t	1958	C
79	t	1959	C
79	t	1960	A
79	t	1961	U
79	t	1962	G
79	t	1963	G
79	t	1966	G
79	t	1967	U
79	t	1968	C
79	t	1969	G
79	t	1970	G
79	t	1973	U
79	t	1977	C
79	t	1978	U
79	t	1979	A
79	t	1980	A
79	t	1983	A
79	t	1984	G
79	t	1986	G
79	t	1987	U
79	t	1989	U
79	t	1991	A
79	t	1992	C
79	t	2003	C
79	t	2007	A
79	t	2011	A
79	t	2014	A
79	t	2021	A
79	t	2023	A
79	t	2025	U
79	t	2027	G
79	t	2028	A
79	t	2029	U
79	t	2033	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
79	t	2036	G
79	t	2037	G
79	t	2050	A
79	t	2051	U
79	t	2053	C
79	t	2065	C
79	t	2067	G
79	t	2070	U
79	t	2071	C
79	t	2072	G
79	t	2073	A
79	t	2077	U
79	t	2078	G
79	t	2079	G
79	t	2081	C
79	t	2082	G
79	t	2083	G
79	t	2086	G
79	t	2087	C
79	t	2088	G
79	t	2090	C
79	t	2091	G
79	t	2092	G
79	t	2093	C
79	t	2229	C
79	t	2230	G
79	t	2231	G
79	t	2232	A
79	t	2233	G
79	t	2235	C
79	t	2236	C
79	t	2237	C
79	t	2238	G
79	t	2241	G
79	t	2246	U
79	t	2247	A
79	t	2268	C
79	t	2279	A
79	t	2280	G
79	t	2282	C
79	t	2292	A
79	t	2293	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
79	t	2299	G
79	t	2301	G
79	t	2311	A
79	t	2323	U
79	t	2325	C
79	t	2326	A
79	t	2327	G
79	t	2330	C
79	t	2336	G
79	t	2340	G
79	t	2343	G
79	t	2357	G
79	t	2375	A
79	t	2381	G
79	t	2387	U
79	t	2389	C
79	t	2396	A
79	t	2400	G
79	t	2401	C
79	t	2404	U
79	t	2405	U
79	t	2412	G
79	t	2413	G
79	t	2420	C
79	t	2425	C
79	t	2426	U
79	t	2429	G
79	t	2439	A
79	t	2442	G
79	t	2446	U
79	t	2447	U
79	t	2448	C
79	t	2449	C
79	t	2450	G
79	t	2453	G
79	t	2454	G
79	t	2455	G
79	t	2461	C
79	t	2465	G
79	t	2467	C
79	t	2468	C
79	t	2469	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
79	t	2470	C
79	t	2473	U
79	t	2481	G
79	t	2482	G
79	t	2484	C
79	t	2485	G
79	t	2490	A
79	t	2492	A
79	t	2496	A
79	t	2499	C
79	t	2511	C
79	t	2523	G
79	t	2524	U
79	t	2525	G
79	t	2526	G
79	t	2532	A
79	t	2557	G
79	t	2565	G
79	t	2566	A
79	t	2568	C
79	t	2570	A
79	t	2579	A
79	t	2580	A
79	t	2581	G
79	t	2584	G
79	t	2585	G
79	t	2597	G
79	t	2600	A
79	t	2606	C
79	t	2617	G
79	t	2626	A
79	t	2632	C
79	t	2637	G
79	t	2638	A
79	t	2639	A
79	t	2648	C
79	t	2652	G
79	t	2665	G
79	t	2666	U
79	t	2667	G
79	t	2673	G
79	t	2674	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
79	t	2675	A
79	t	2676	A
79	t	2684	G
79	t	2688	C
79	t	2689	C
79	t	2690	G
79	t	2691	G
79	t	2693	G
79	t	2699	C
79	t	2703	G
79	t	2705	G
79	t	2710	C
79	t	2717	C
79	t	2719	U
79	t	2720	U
79	t	2721	G
79	t	2722	A
79	t	2723	A
79	t	2732	G
79	t	2733	G
79	t	2734	A
79	t	2737	G
79	t	2739	G
79	t	2741	G
79	t	2742	U
79	t	2744	A
79	t	2745	A
79	t	2748	U
79	t	2766	A
79	t	2767	U
79	t	2768	A
79	t	2769	U
79	t	2772	G
79	t	2773	C
79	t	2775	G
79	t	2776	C
79	t	2777	A
79	t	2778	G
79	t	2780	U
79	t	2785	A
79	t	2793	C
79	t	2798	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
79	t	2804	A
79	t	2805	U
79	t	2806	G
79	t	2814	A
79	t	2818	U
79	t	2821	G
79	t	2822	U
79	t	2834	G
79	t	2841	G
79	t	2843	A
79	t	2854	C
79	t	2858	A
79	t	2859	U
79	t	2860	A
79	t	2861	A
79	t	2863	G
79	t	2870	U
79	t	2871	C
79	t	2877	G
79	t	2881	G
79	t	3570	A
79	t	3571	G
79	t	3574	G
79	t	3576	C
79	t	3577	U
79	t	3587	U
79	t	3588	G
79	t	3590	G
79	t	3591	G
79	t	3596	G
79	t	3597	G
79	t	3601	A
79	t	3606	A
79	t	3612	U
79	t	3614	A
79	t	3615	U
79	t	3616	U
79	t	3617	A
79	t	3627	A
79	t	3633	A
79	t	3643	G
79	t	3646	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
79	t	3649	G
79	t	3650	U
79	t	3651	U
79	t	3653	A
79	t	3662	G
79	t	3667	C
79	t	3682	A
79	t	3700	U
79	t	3707	A
79	t	3718	A
79	t	3719	A
79	t	3725	G
79	t	3727	A
79	t	3728	G
79	t	3730	A
79	t	3731	A
79	t	3744	U
79	t	3745	A
79	t	3748	G
79	t	3749	U
79	t	3751	G
79	t	3754	A
79	t	3778	A
79	t	3781	C
79	t	3782	G
79	t	3784	A
79	t	3785	U
79	t	3788	A
79	t	3789	U
79	t	3790	G
79	t	3795	A
79	t	3800	G
79	t	3809	U
79	t	3810	G
79	t	3811	U
79	t	3822	U
79	t	3838	A
79	t	3848	A
79	t	3849	C
79	t	3850	G
79	t	3852	G
79	t	3860	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
79	t	3863	U
79	t	3868	G
79	t	3869	G
79	t	3872	A
79	t	3877	A
79	t	3878	G
79	t	3879	A
79	t	3886	U
79	t	3887	G
79	t	3894	A
79	t	3900	G
79	t	3909	G
79	t	3910	G
79	t	4042	C
79	t	4046	G
79	t	4063	G
79	t	4064	G
79	t	4065	G
79	t	4067	G
79	t	4069	G
79	t	4070	C
79	t	4071	C
79	t	4073	G
79	t	4074	A
79	t	4077	G
79	t	4078	G
79	t	4079	C
79	t	4080	U
79	t	4081	C
79	t	4083	C
79	t	4084	G
79	t	4086	U
79	t	4088	C
79	t	4089	U
79	t	4091	G
79	t	4096	A
79	t	4104	G
79	t	4106	C
79	t	4107	C
79	t	4108	G
79	t	4109	G
79	t	4110	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
79	t	4124	C
79	t	4126	C
79	t	4130	G
79	t	4132	A
79	t	4139	C
79	t	4141	G
79	t	4142	G
79	t	4145	G
79	t	4146	G
79	t	4150	U
79	t	4153	G
79	t	4156	U
79	t	4162	G
79	t	4165	A
79	t	4167	A
79	t	4174	A
79	t	4175	A
79	t	4176	A
79	t	4187	G
79	t	4191	U
79	t	4195	A
79	t	4211	G
79	t	4213	A
79	t	4215	A
79	t	4216	G
79	t	4217	A
79	t	4220	C
79	t	4227	U
79	t	4228	G
79	t	4230	A
79	t	4234	G
79	t	4235	A
79	t	4238	G
79	t	4243	A
79	t	4250	C
79	t	4252	U
79	t	4253	G
79	t	4259	G
79	t	4264	U
79	t	4266	A
79	t	4267	G
79	t	4268	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
79	t	4275	A
79	t	4276	C
79	t	4279	A
79	t	4287	A
79	t	4288	G
79	t	4290	G
79	t	4291	G
79	t	4292	G
79	t	4294	C
79	t	4299	C
79	t	4300	G
79	t	4310	A
79	t	4311	C
79	t	4319	G
79	t	4333	G
79	t	4334	U
79	t	4337	C
79	t	4338	A
79	t	4339	G
79	t	4340	A
79	t	4341	A
79	t	4343	A
79	t	4344	G
79	t	4349	C
79	t	4353	G
79	t	4355	G
79	t	4356	A
79	t	4360	C
79	t	4367	G
79	t	4377	A
79	t	4381	U
79	t	4384	A
79	t	4406	C
79	t	4408	U
79	t	4414	U
79	t	4425	U
79	t	4426	A
79	t	4427	U
79	t	4428	C
79	t	4437	G
79	t	4438	C
79	t	4450	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
79	t	4453	G
79	t	4455	U
79	t	4457	G
79	t	4461	G
79	t	4465	A
79	t	4474	U
79	t	4475	A
79	t	4480	A
79	t	4485	A
79	t	4486	G
79	t	4490	G
79	t	4491	G
79	t	4492	U
79	t	4493	U
79	t	4510	A
79	t	4514	U
79	t	4517	U
79	t	4522	C
79	t	4532	G
79	t	4546	A
79	t	4552	A
79	t	4559	U
79	t	4561	A
79	t	4562	G
79	t	4567	A
79	t	4568	G
79	t	4570	G
79	t	4579	G
79	t	4586	A
79	t	4593	G
79	t	4597	A
79	t	4598	U
79	t	4599	G
79	t	4601	G
79	t	4611	G
79	t	4618	A
79	t	4621	G
79	t	4624	C
79	t	4630	U
79	t	4632	C
79	t	4634	A
79	t	4649	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
79	t	4653	A
79	t	4656	G
79	t	4657	C
79	t	4662	A
79	t	4669	A
79	t	4671	U
79	t	4680	G
79	t	4681	G
79	t	4682	C
79	t	4683	G
79	t	4690	U
79	t	4692	C
79	t	4693	G
79	t	4694	G
79	t	4695	C
79	t	4696	A
79	t	4697	G
79	t	4700	C
79	t	4703	C
79	t	4704	G
79	t	4711	C
79	t	4714	U
79	t	4715	U
79	t	4716	G
79	t	4718	C
79	t	4720	U
79	t	4722	G
79	t	4725	U
79	t	4726	A
79	t	4732	U
79	t	4736	C
79	t	4737	G
79	t	4816	C
79	t	4817	G
79	t	4820	G
79	t	4821	G
79	t	4822	U
79	t	4824	C
79	t	4827	U
79	t	4828	G
79	t	4831	G
79	t	4832	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
79	t	4833	G
79	t	4834	U
79	t	4838	C
79	t	4840	U
79	t	4847	G
79	t	4848	G
79	t	4852	A
79	t	4853	C
79	t	4854	G
79	t	4855	G
79	t	4858	C
79	t	4859	G
79	t	4860	C
79	t	4864	C
79	t	4865	G
79	t	4866	G
79	t	4867	A
79	t	4868	A
79	t	4869	A
79	t	4870	G
79	t	4871	G
79	t	4872	C
79	t	4874	G
79	t	4880	C
79	t	4883	U
79	t	4885	G
79	t	4886	C
79	t	4889	G
79	t	4893	C
79	t	4895	C
79	t	4896	A
79	t	4898	C
79	t	4901	A
79	t	4902	C
79	t	4905	U
79	t	4907	G
79	t	4909	G
79	t	4915	C
79	t	4916	C
79	t	4924	A
79	t	4925	A
79	t	4933	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
79	t	4934	U
79	t	4938	C
79	t	4943	U
79	t	4946	U
79	t	4947	U
79	t	4948	C
79	t	4949	U
79	t	4950	G
79	t	4957	G
79	t	4964	U
79	t	4971	C
79	t	4975	G
79	t	4981	C
79	t	4982	C
79	t	4984	U
79	t	4985	C
79	t	4999	G
79	t	5006	A
79	t	5007	G
79	t	5008	C
79	t	5011	U
79	t	5012	C
79	t	5013	G
79	t	5014	A
79	t	5015	C
79	t	5016	A
79	t	5019	A
79	t	5020	G
79	t	5026	G
79	t	5027	U
79	t	5028	C
80	v	3	C
80	v	5	C
80	v	8	U
80	v	10	G
80	v	16	A
80	v	17	A
80	v	19	G
80	v	20	U
80	v	21	A
80	v	30	G
80	v	47	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
80	v	48	C
80	v	49	C
80	v	50	U
80	v	51	U
80	v	54	U
80	v	56	C
80	v	57	G
80	v	58	A
80	v	61	C
80	v	62	C
80	v	64	A
80	v	68	C
80	v	69	G
80	v	70	G
80	v	71	G
80	v	72	C
80	v	76	A
81	w	19	C
81	w	21	G
81	w	22	U
82	u	2	C
82	u	4	C
82	u	5	G
82	u	6	G
82	u	7	A
82	u	8	U
82	u	11	C
82	u	17	C
82	u	18	G
82	u	19	G
82	u	20	U
82	u	21	A
82	u	24	G
82	u	37	U
82	u	44	G
82	u	46	G
82	u	47	U
82	u	48	C
82	u	49	C
82	u	50	U
82	u	51	U
82	u	52	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
82	u	55	U
82	u	56	C
82	u	57	G
82	u	59	U
82	u	61	C
82	u	63	G
82	u	64	A
82	u	70	G
82	u	72	C
82	u	73	A
82	u	74	C
82	u	76	A

All (27) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	S2	53	C
1	S2	79	A
1	S2	196	C
1	S2	205	G
1	S2	292	A
1	S2	304	C
1	S2	317	C
1	S2	417	C
1	S2	445	A
1	S2	536	A
1	S2	559	G
1	S2	814	5MU
1	S2	866	U
1	S2	872	A
1	S2	1138	C
1	S2	1261	C
1	S2	1375	G
1	S2	1378	A
1	S2	1567	G
1	S2	1572	C
1	S2	1600	G
1	S2	1661	A
1	S2	1681	U
1	S2	1749	G
1	S2	1802	C
1	S2	1813	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	S2	1828	C

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

34 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
1	OMU	S2	116	1	19,22,23	3.35	6 (31%)	25,31,34	2.16	8 (32%)
1	5MU	S2	814	1	19,22,23	7.70	8 (42%)	27,32,35	3.48	12 (44%)
1	UR3	S2	1830	1	19,22,23	2.75	6 (31%)	26,32,35	2.77	6 (23%)
1	OMC	S2	517	1	19,22,23	3.56	8 (42%)	25,31,34	0.83	0
1	4AC	S2	1337	1	21,24,25	3.45	9 (42%)	28,34,37	1.19	3 (10%)
1	PSU	S2	823	1	18,21,22	4.39	8 (44%)	21,30,33	2.46	6 (28%)
1	PSU	S2	822	1	18,21,22	4.41	8 (44%)	21,30,33	2.18	5 (23%)
1	6MZ	S2	1832	1	22,25,26	2.64	6 (27%)	29,36,39	2.24	7 (24%)
1	OMC	S2	1703	1	19,22,23	3.45	7 (36%)	25,31,34	0.72	0
1	E3C	S2	568	1	19,23,24	3.40	7 (36%)	21,33,36	2.57	5 (23%)
1	PSU	S2	119	1	18,21,22	4.32	7 (38%)	21,30,33	1.92	4 (19%)
1	M7A	S2	1806	1	19,25,26	1.60	2 (10%)	25,37,40	3.85	9 (36%)
1	OMC	S2	1710	1	19,22,23	3.51	8 (42%)	25,31,34	0.67	0
1	A2M	S2	159	1	22,25,26	4.10	9 (40%)	30,36,39	3.00	15 (50%)
1	PSU	S2	1243	1	18,21,22	4.24	8 (44%)	21,30,33	2.01	4 (19%)
1	A2M	S2	668	1	22,25,26	4.12	10 (45%)	30,36,39	3.30	16 (53%)
1	A2M	S2	1678	1	22,25,26	4.05	9 (40%)	30,36,39	3.42	18 (60%)
1	A2M	S2	1031	1	22,25,26	4.06	9 (40%)	30,36,39	2.97	16 (53%)
1	OMC	S2	174	1	19,22,23	3.57	8 (42%)	25,31,34	0.76	0
1	OMU	S2	121	1	19,22,23	3.02	6 (31%)	25,31,34	1.99	5 (20%)
1	OMG	S2	644	1	23,26,27	2.41	9 (39%)	32,38,41	2.18	10 (31%)
1	MA6	S2	1850	1	23,26,27	1.48	5 (21%)	33,38,41	3.69	13 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	A2M	S2	166	1	22,25,26	4.15	9 (40%)	30,36,39	3.06	13 (43%)
1	A2M	S2	27	1	22,25,26	4.10	9 (40%)	30,36,39	2.89	13 (43%)
1	OMG	S2	683	1	23,26,27	2.36	8 (34%)	32,38,41	2.03	9 (28%)
1	4AC	S2	1842	1,85	21,24,25	3.33	9 (42%)	28,34,37	1.16	4 (14%)
1	5MC	S2	1374	1	19,22,23	3.68	8 (42%)	26,32,35	0.97	2 (7%)
1	MA6	S2	1851	1	23,26,27	1.52	5 (21%)	33,38,41	3.72	13 (39%)
1	OMG	S2	509	1	23,26,27	2.43	9 (39%)	32,38,41	2.15	9 (28%)
1	B8Q	S2	1219	1	18,22,23	4.76	7 (38%)	21,32,35	1.69	4 (19%)
1	B8N	S2	1248	1	25,29,30	3.13	6 (24%)	28,42,45	1.90	6 (21%)
1	PSU	S2	1081	1	18,21,22	4.42	8 (44%)	21,30,33	2.11	5 (23%)
1	PSU	S2	612	1	18,21,22	4.26	8 (44%)	21,30,33	2.08	6 (28%)
1	A2M	S2	484	1	22,25,26	4.10	9 (40%)	30,36,39	3.05	17 (56%)

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
1	OMU	S2	116	1	-	4/9/27/28	0/2/2/2
1	5MU	S2	814	1	-	0/7/25/26	0/2/2/2
1	UR3	S2	1830	1	-	5/7/25/26	0/2/2/2
1	OMC	S2	517	1	-	0/9/27/28	0/2/2/2
1	4AC	S2	1337	1	-	1/11/29/30	0/2/2/2
1	PSU	S2	823	1	-	2/7/25/26	0/2/2/2
1	PSU	S2	822	1	-	0/7/25/26	0/2/2/2
1	6MZ	S2	1832	1	-	2/9/27/28	0/3/3/3
1	OMC	S2	1703	1	-	2/9/27/28	0/2/2/2
1	E3C	S2	568	1	-	5/9/44/45	0/2/2/2
1	PSU	S2	119	1	-	0/7/25/26	0/2/2/2
1	M7A	S2	1806	1	-	1/7/37/38	0/3/3/3
1	OMC	S2	1710	1	-	1/9/27/28	0/2/2/2
1	A2M	S2	159	1	-	3/9/27/28	0/3/3/3
1	PSU	S2	1243	1	-	2/7/25/26	0/2/2/2
1	A2M	S2	668	1	-	5/9/27/28	0/3/3/3
1	A2M	S2	1678	1	-	3/9/27/28	0/3/3/3
1	A2M	S2	1031	1	-	0/9/27/28	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMC	S2	174	1	-	0/9/27/28	0/2/2/2
1	OMU	S2	121	1	-	2/9/27/28	0/2/2/2
1	OMG	S2	644	1	-	3/9/27/28	0/3/3/3
1	MA6	S2	1850	1	-	5/11/29/30	0/3/3/3
1	A2M	S2	166	1	-	3/9/27/28	0/3/3/3
1	A2M	S2	27	1	-	1/9/27/28	0/3/3/3
1	OMG	S2	683	1	-	2/9/27/28	0/3/3/3
1	4AC	S2	1842	1,85	-	0/11/29/30	0/2/2/2
1	5MC	S2	1374	1	-	0/7/25/26	0/2/2/2
1	MA6	S2	1851	1	-	6/11/29/30	0/3/3/3
1	OMG	S2	509	1	-	1/9/27/28	0/3/3/3
1	B8Q	S2	1219	1	-	0/7/42/43	0/2/2/2
1	B8N	S2	1248	1	-	2/16/34/35	0/2/2/2
1	PSU	S2	1081	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	612	1	-	0/7/25/26	0/2/2/2
1	A2M	S2	484	1	-	0/9/27/28	0/3/3/3

All (258) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	814	5MU	C4-C5	22.82	1.82	1.44
1	S2	814	5MU	C6-N1	17.11	1.67	1.38
1	S2	814	5MU	C6-C5	-11.92	1.15	1.34
1	S2	1219	B8Q	C4-N3	11.46	1.66	1.48
1	S2	1081	PSU	C6-C5	11.41	1.47	1.35
1	S2	823	PSU	C6-C5	11.35	1.47	1.35
1	S2	1243	PSU	C6-C5	11.16	1.47	1.35
1	S2	822	PSU	C6-C5	11.15	1.47	1.35
1	S2	119	PSU	C6-C5	11.08	1.47	1.35
1	S2	814	5MU	C4-N3	-10.84	1.18	1.38
1	S2	1219	B8Q	C6-C5	10.80	1.55	1.33
1	S2	668	A2M	C2'-C1'	-10.69	1.26	1.53
1	S2	612	PSU	C6-C5	10.67	1.47	1.35
1	S2	159	A2M	C2'-C1'	-10.57	1.27	1.53
1	S2	484	A2M	C2'-C1'	-10.51	1.27	1.53
1	S2	27	A2M	C2'-C1'	-10.51	1.27	1.53
1	S2	1031	A2M	C2'-C1'	-10.47	1.27	1.53
1	S2	166	A2M	C2'-C1'	-10.44	1.27	1.53
1	S2	1678	A2M	C2'-C1'	-10.28	1.27	1.53
1	S2	1031	A2M	C3'-C4'	-10.24	1.27	1.53
1	S2	668	A2M	C3'-C4'	-10.19	1.27	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	27	A2M	C3'-C4'	-10.14	1.27	1.53
1	S2	484	A2M	C3'-C4'	-10.13	1.27	1.53
1	S2	166	A2M	C3'-C4'	-10.05	1.27	1.53
1	S2	159	A2M	C3'-C4'	-9.78	1.28	1.53
1	S2	1219	B8Q	C2-N1	9.45	1.51	1.38
1	S2	116	OMU	C2-N1	9.42	1.53	1.38
1	S2	1832	6MZ	C6-N6	9.36	1.44	1.34
1	S2	822	PSU	C2-N1	9.28	1.48	1.36
1	S2	612	PSU	C2-N1	9.16	1.48	1.36
1	S2	823	PSU	C2-N1	9.15	1.48	1.36
1	S2	1678	A2M	C3'-C4'	-9.01	1.30	1.53
1	S2	1081	PSU	C2-N1	8.99	1.48	1.36
1	S2	1374	5MC	C6-C5	8.99	1.49	1.34
1	S2	119	PSU	C2-N1	8.85	1.48	1.36
1	S2	1243	PSU	C2-N1	8.77	1.48	1.36
1	S2	1830	UR3	C2-N1	8.57	1.50	1.38
1	S2	517	OMC	C4-N4	8.47	1.54	1.33
1	S2	174	OMC	C4-N4	8.40	1.54	1.33
1	S2	1710	OMC	C4-N4	8.35	1.54	1.33
1	S2	1248	B8N	C4-N3	-8.17	1.26	1.40
1	S2	1703	OMC	C4-N4	8.16	1.53	1.33
1	S2	568	E3C	C6-C5	8.08	1.50	1.33
1	S2	1842	4AC	C4-N3	8.05	1.46	1.32
1	S2	823	PSU	C2-N3	7.89	1.50	1.37
1	S2	1337	4AC	C4-N3	7.78	1.45	1.32
1	S2	1248	B8N	C6-N1	7.54	1.54	1.36
1	S2	568	E3C	C2-N1	7.42	1.48	1.38
1	S2	119	PSU	C2-N3	7.36	1.49	1.37
1	S2	121	OMU	C2-N1	7.29	1.49	1.38
1	S2	822	PSU	C2-N3	7.13	1.49	1.37
1	S2	1081	PSU	C2-N3	7.03	1.49	1.37
1	S2	568	E3C	C2-N3	7.01	1.46	1.37
1	S2	612	PSU	C2-N3	7.00	1.49	1.37
1	S2	174	OMC	C2-N3	6.85	1.49	1.36
1	S2	116	OMU	C2-N3	6.83	1.49	1.38
1	S2	1703	OMC	C2-N3	6.81	1.49	1.36
1	S2	517	OMC	C2-N3	6.74	1.49	1.36
1	S2	1248	B8N	C4-C5	6.72	1.62	1.47
1	S2	1243	PSU	C2-N3	6.72	1.48	1.37
1	S2	1710	OMC	C6-C5	6.71	1.50	1.35
1	S2	517	OMC	C6-C5	6.71	1.50	1.35
1	S2	174	OMC	C6-C5	6.66	1.50	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	1710	OMC	C2-N3	6.63	1.49	1.36
1	S2	1703	OMC	C6-C5	6.50	1.50	1.35
1	S2	1374	5MC	C4-N3	6.49	1.44	1.34
1	S2	1337	4AC	C6-C5	6.38	1.49	1.35
1	S2	121	OMU	C2-N3	6.31	1.49	1.38
1	S2	1678	A2M	C6-N6	6.29	1.50	1.34
1	S2	683	OMG	C4-N3	6.27	1.48	1.34
1	S2	644	OMG	C4-N3	6.25	1.48	1.34
1	S2	1678	A2M	O4'-C1'	6.24	1.56	1.42
1	S2	121	OMU	C6-C5	6.21	1.49	1.35
1	S2	1374	5MC	C5-C4	6.20	1.48	1.44
1	S2	509	OMG	C4-N3	6.19	1.48	1.34
1	S2	1842	4AC	C2-N3	6.17	1.48	1.36
1	S2	174	OMC	C4-N3	6.13	1.46	1.34
1	S2	1337	4AC	C2-N3	6.13	1.48	1.36
1	S2	116	OMU	C6-C5	6.11	1.49	1.35
1	S2	1678	A2M	C3'-C2'	6.06	1.66	1.53
1	S2	517	OMC	C4-N3	6.05	1.46	1.34
1	S2	166	A2M	O4'-C1'	6.01	1.55	1.42
1	S2	1703	OMC	C4-N3	6.00	1.46	1.34
1	S2	1374	5MC	C2-N3	5.98	1.48	1.36
1	S2	27	A2M	O4'-C1'	5.94	1.55	1.42
1	S2	159	A2M	O4'-C1'	5.92	1.55	1.42
1	S2	159	A2M	C3'-C2'	5.90	1.65	1.53
1	S2	166	A2M	C3'-C2'	5.88	1.65	1.53
1	S2	1710	OMC	C4-N3	5.87	1.46	1.34
1	S2	484	A2M	O4'-C1'	5.78	1.55	1.42
1	S2	1031	A2M	O4'-C1'	5.70	1.55	1.42
1	S2	484	A2M	C3'-C2'	5.70	1.65	1.53
1	S2	668	A2M	O4'-C1'	5.63	1.55	1.42
1	S2	1842	4AC	C6-C5	5.62	1.48	1.35
1	S2	166	A2M	C6-N6	5.57	1.48	1.34
1	S2	484	A2M	C6-N6	5.53	1.48	1.34
1	S2	668	A2M	C3'-C2'	5.53	1.65	1.53
1	S2	27	A2M	C6-N6	5.49	1.48	1.34
1	S2	159	A2M	C6-N6	5.43	1.48	1.34
1	S2	668	A2M	C6-N6	5.42	1.48	1.34
1	S2	1031	A2M	C6-N6	5.42	1.48	1.34
1	S2	1248	B8N	C2-N1	5.40	1.55	1.39
1	S2	1219	B8Q	C2-N3	-5.38	1.25	1.35
1	S2	509	OMG	C2-N3	5.35	1.46	1.33
1	S2	644	OMG	C2-N3	5.32	1.46	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	1081	PSU	O2-C2	-5.27	1.12	1.23
1	S2	822	PSU	O2-C2	-5.22	1.12	1.23
1	S2	1830	UR3	C2-N3	5.17	1.49	1.39
1	S2	27	A2M	C3'-C2'	5.17	1.64	1.53
1	S2	814	5MU	C2-N3	5.15	1.46	1.38
1	S2	1243	PSU	O2-C2	-5.14	1.12	1.23
1	S2	683	OMG	C2-N3	5.12	1.45	1.33
1	S2	568	E3C	C4-N3	5.09	1.56	1.48
1	S2	1031	A2M	C3'-C2'	5.08	1.64	1.53
1	S2	119	PSU	O2-C2	-5.07	1.12	1.23
1	S2	1678	A2M	O4'-C4'	5.04	1.56	1.45
1	S2	823	PSU	O2-C2	-4.94	1.12	1.23
1	S2	1337	4AC	C7-N4	4.94	1.47	1.37
1	S2	166	A2M	O4'-C4'	4.93	1.56	1.45
1	S2	1248	B8N	C6-C5	4.93	1.42	1.35
1	S2	612	PSU	O2-C2	-4.92	1.12	1.23
1	S2	159	A2M	O4'-C4'	4.87	1.55	1.45
1	S2	1842	4AC	C7-N4	4.85	1.47	1.37
1	S2	1337	4AC	C4-N4	4.85	1.47	1.39
1	S2	1081	PSU	O4-C4	-4.83	1.14	1.23
1	S2	116	OMU	C4-N3	4.82	1.46	1.38
1	S2	644	OMG	C2-N2	4.80	1.45	1.34
1	S2	612	PSU	O4-C4	-4.78	1.14	1.23
1	S2	1219	B8Q	C4-C5	-4.77	1.39	1.49
1	S2	121	OMU	C4-N3	4.77	1.46	1.38
1	S2	509	OMG	C2-N2	4.77	1.45	1.34
1	S2	27	A2M	O4'-C4'	4.76	1.55	1.45
1	S2	1243	PSU	O4-C4	-4.76	1.14	1.23
1	S2	119	PSU	O4-C4	-4.75	1.14	1.23
1	S2	822	PSU	O4-C4	-4.69	1.14	1.23
1	S2	1806	M7A	C6-N6	4.69	1.46	1.34
1	S2	683	OMG	C2-N2	4.66	1.45	1.34
1	S2	1830	UR3	C6-C5	4.65	1.45	1.35
1	S2	484	A2M	O4'-C4'	4.64	1.55	1.45
1	S2	1337	4AC	C2-N1	4.58	1.49	1.40
1	S2	1842	4AC	C4-N4	4.56	1.46	1.39
1	S2	1031	A2M	O4'-C4'	4.55	1.55	1.45
1	S2	1832	6MZ	C5-C4	-4.48	1.31	1.39
1	S2	1842	4AC	C2-N1	4.45	1.49	1.40
1	S2	1337	4AC	C5-C4	4.35	1.50	1.41
1	S2	668	A2M	O4'-C4'	4.32	1.54	1.45
1	S2	1374	5MC	C4-N4	4.30	1.45	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	174	OMC	C2-N1	4.19	1.48	1.40
1	S2	1374	5MC	C6-N1	4.16	1.45	1.38
1	S2	814	5MU	C2-N1	4.10	1.44	1.38
1	S2	822	PSU	C6-N1	4.07	1.43	1.36
1	S2	1081	PSU	C6-N1	4.00	1.42	1.36
1	S2	517	OMC	C6-N1	3.98	1.47	1.38
1	S2	1337	4AC	C6-N1	3.92	1.47	1.38
1	S2	119	PSU	C6-N1	3.90	1.42	1.36
1	S2	1710	OMC	C2-N1	3.84	1.48	1.40
1	S2	517	OMC	C2-N1	3.82	1.48	1.40
1	S2	1806	M7A	C5-N7	3.79	1.48	1.39
1	S2	1374	5MC	C2-N1	3.77	1.48	1.40
1	S2	1842	4AC	C5-C4	3.77	1.49	1.41
1	S2	1703	OMC	C2-N1	3.76	1.47	1.40
1	S2	612	PSU	C6-N1	3.75	1.42	1.36
1	S2	174	OMC	C6-N1	3.72	1.47	1.38
1	S2	1710	OMC	C6-N1	3.69	1.46	1.38
1	S2	1832	6MZ	C8-N9	-3.68	1.31	1.37
1	S2	823	PSU	O4-C4	-3.57	1.16	1.23
1	S2	823	PSU	C4-N3	3.52	1.45	1.38
1	S2	509	OMG	C5-N7	-3.51	1.32	1.39
1	S2	1850	MA6	C5-C4	-3.50	1.32	1.39
1	S2	1851	MA6	C5-C4	-3.50	1.32	1.39
1	S2	823	PSU	C6-N1	3.48	1.42	1.36
1	S2	1842	4AC	C6-N1	3.47	1.46	1.38
1	S2	1243	PSU	C6-N1	3.47	1.42	1.36
1	S2	668	A2M	C5-C4	-3.45	1.32	1.39
1	S2	1703	OMC	C6-N1	3.41	1.46	1.38
1	S2	1832	6MZ	C5-N7	-3.39	1.32	1.39
1	S2	683	OMG	C5-N7	-3.28	1.32	1.39
1	S2	1081	PSU	O4'-C1'	-3.27	1.39	1.43
1	S2	822	PSU	O4'-C1'	-3.21	1.39	1.43
1	S2	27	A2M	C5-C4	-3.20	1.33	1.39
1	S2	119	PSU	C4-N3	3.18	1.44	1.38
1	S2	27	A2M	C5-N7	-3.15	1.33	1.39
1	S2	1031	A2M	C5-N7	-3.07	1.33	1.39
1	S2	1851	MA6	C6-N6	3.04	1.45	1.36
1	S2	1850	MA6	C5-N7	-3.03	1.33	1.39
1	S2	612	PSU	C4-N3	3.02	1.44	1.38
1	S2	1851	MA6	C5-N7	-3.01	1.33	1.39
1	S2	166	A2M	C5-C4	-3.00	1.33	1.39
1	S2	1219	B8Q	C31-N3	3.00	1.52	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	644	OMG	C5-N7	-3.00	1.33	1.39
1	S2	484	A2M	C5-N7	-3.00	1.33	1.39
1	S2	822	PSU	C4-N3	2.94	1.44	1.38
1	S2	1031	A2M	C5-C4	-2.93	1.33	1.39
1	S2	683	OMG	O6-C6	-2.91	1.18	1.23
1	S2	1850	MA6	C6-N6	2.90	1.44	1.36
1	S2	568	E3C	C6-N1	2.90	1.45	1.38
1	S2	668	A2M	C5-N7	-2.89	1.33	1.39
1	S2	1081	PSU	C4-N3	2.88	1.44	1.38
1	S2	166	A2M	C5-N7	-2.86	1.33	1.39
1	S2	484	A2M	C5-C4	-2.84	1.34	1.39
1	S2	159	A2M	C5-C4	-2.80	1.34	1.39
1	S2	159	A2M	C5-N7	-2.77	1.34	1.39
1	S2	1851	MA6	C8-N9	-2.74	1.32	1.37
1	S2	668	A2M	C8-N9	-2.74	1.32	1.37
1	S2	644	OMG	O6-C6	-2.72	1.18	1.23
1	S2	1374	5MC	O2-C2	-2.72	1.18	1.23
1	S2	509	OMG	C2-N1	2.71	1.44	1.37
1	S2	568	E3C	C31-N3	2.70	1.54	1.47
1	S2	612	PSU	O4'-C1'	-2.67	1.40	1.43
1	S2	1850	MA6	C8-N9	-2.67	1.33	1.37
1	S2	116	OMU	C6-N1	2.63	1.44	1.38
1	S2	1219	B8Q	C6-N1	-2.62	1.31	1.38
1	S2	509	OMG	O6-C6	-2.61	1.18	1.23
1	S2	1031	A2M	C8-N9	-2.59	1.33	1.37
1	S2	121	OMU	C6-N1	2.58	1.44	1.38
1	S2	1832	6MZ	C9-N6	2.53	1.49	1.45
1	S2	166	A2M	C8-N9	-2.53	1.33	1.37
1	S2	27	A2M	C8-N9	-2.50	1.33	1.37
1	S2	1851	MA6	C4-N9	-2.48	1.32	1.37
1	S2	644	OMG	C2-N1	2.47	1.43	1.37
1	S2	1830	UR3	C6-N1	2.45	1.43	1.38
1	S2	1710	OMC	O2-C2	-2.42	1.19	1.23
1	S2	159	A2M	C8-N9	-2.42	1.33	1.37
1	S2	683	OMG	C2-N1	2.41	1.43	1.37
1	S2	1678	A2M	C5-C4	-2.41	1.34	1.39
1	S2	568	E3C	C4-C5	-2.41	1.44	1.49
1	S2	1830	UR3	O2-C2	-2.41	1.18	1.22
1	S2	1243	PSU	C4-N3	2.40	1.43	1.38
1	S2	644	OMG	C4-N9	-2.38	1.32	1.38
1	S2	644	OMG	C5-C6	2.30	1.53	1.44
1	S2	517	OMC	O2-C2	-2.30	1.19	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	1830	UR3	C4-N3	2.29	1.45	1.40
1	S2	121	OMU	C5-C4	2.28	1.48	1.43
1	S2	174	OMC	O2-C2	-2.27	1.19	1.23
1	S2	1248	B8N	O4-C4	-2.24	1.18	1.23
1	S2	517	OMC	C5-C4	2.24	1.48	1.42
1	S2	509	OMG	C4-N9	-2.24	1.32	1.38
1	S2	823	PSU	O4'-C1'	-2.21	1.40	1.43
1	S2	814	5MU	O2-C2	-2.19	1.19	1.23
1	S2	1703	OMC	O2-C2	-2.18	1.19	1.23
1	S2	509	OMG	C6-N1	2.15	1.42	1.38
1	S2	1710	OMC	C5-C4	2.14	1.47	1.42
1	S2	174	OMC	C5-C4	2.13	1.47	1.42
1	S2	484	A2M	C8-N9	-2.13	1.33	1.37
1	S2	668	A2M	C4-N9	-2.09	1.33	1.37
1	S2	1842	4AC	O2-C2	-2.09	1.19	1.23
1	S2	1832	6MZ	C6-N1	-2.09	1.31	1.35
1	S2	1243	PSU	O4'-C1'	-2.07	1.41	1.43
1	S2	1850	MA6	C4-N9	-2.06	1.33	1.37
1	S2	814	5MU	O4-C4	-2.06	1.19	1.23
1	S2	1678	A2M	C5'-C4'	2.06	1.57	1.51
1	S2	509	OMG	C5-C6	2.05	1.52	1.44
1	S2	1678	A2M	C5-N7	-2.05	1.35	1.39
1	S2	683	OMG	C5-C6	2.03	1.52	1.44
1	S2	116	OMU	O4-C4	-2.02	1.20	1.24
1	S2	644	OMG	C6-N1	2.01	1.42	1.38
1	S2	683	OMG	C4-N9	-2.01	1.33	1.38
1	S2	1337	4AC	O2-C2	-2.00	1.20	1.23

All (263) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	1851	MA6	N1-C6-N6	-13.43	100.49	116.86
1	S2	1850	MA6	N1-C6-N6	-12.74	101.34	116.86
1	S2	1806	M7A	C5-C6-N6	10.81	142.11	123.75
1	S2	814	5MU	C5-C4-N3	10.06	124.07	115.32
1	S2	1806	M7A	N6-C6-N1	-9.46	97.30	118.38
1	S2	1851	MA6	C5-C6-N6	9.20	139.89	125.33
1	S2	1850	MA6	C5-C6-N6	8.18	138.28	125.33
1	S2	1806	M7A	C4-N9-C1'	-8.06	107.85	126.63
1	S2	668	A2M	C4-N9-C1'	-7.91	108.13	126.63
1	S2	1678	A2M	C4-N9-C1'	-7.63	108.79	126.63
1	S2	1830	UR3	C1'-N1-C2	7.58	129.45	117.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	668	A2M	C1'-N9-C8	7.44	143.62	127.09
1	S2	814	5MU	C5-C6-N1	-7.20	115.49	123.31
1	S2	166	A2M	C4-N9-C1'	-7.15	109.92	126.63
1	S2	814	5MU	C4-N3-C2	-7.04	118.11	127.34
1	S2	568	E3C	O2-C2-N3	-6.96	113.19	122.10
1	S2	484	A2M	C4-N9-C1'	-6.96	110.36	126.63
1	S2	1678	A2M	C1'-N9-C8	6.86	142.32	127.09
1	S2	484	A2M	C1'-N9-C8	6.85	142.29	127.09
1	S2	159	A2M	C4-N9-C1'	-6.59	111.22	126.63
1	S2	166	A2M	C1'-N9-C8	6.49	141.51	127.09
1	S2	1830	UR3	C6-N1-C2	-6.46	116.52	121.80
1	S2	568	E3C	C1'-N1-C2	6.41	127.53	117.04
1	S2	159	A2M	C1'-N9-C8	6.11	140.65	127.09
1	S2	121	OMU	C4-N3-C2	-6.06	119.09	126.61
1	S2	1031	A2M	C4-N9-C1'	-5.90	112.82	126.63
1	S2	668	A2M	N3-C2-N1	-5.89	119.66	128.58
1	S2	1678	A2M	N3-C2-N1	-5.88	119.68	128.58
1	S2	27	A2M	N3-C2-N1	-5.87	119.69	128.58
1	S2	1850	MA6	N1-C2-N3	-5.87	119.70	128.58
1	S2	1850	MA6	C1'-N9-C8	-5.87	114.07	127.09
1	S2	1806	M7A	N3-C2-N1	-5.86	119.72	128.58
1	S2	668	A2M	N6-C6-N1	-5.85	105.34	118.38
1	S2	1851	MA6	N1-C2-N3	-5.83	119.76	128.58
1	S2	166	A2M	N3-C2-N1	-5.76	119.87	128.58
1	S2	1830	UR3	C4-N3-C2	-5.67	120.01	124.58
1	S2	27	A2M	C5-C4-N3	-5.61	118.99	126.72
1	S2	1031	A2M	N3-C2-N1	-5.60	120.11	128.58
1	S2	116	OMU	C1'-N1-C2	5.58	127.62	117.59
1	S2	1031	A2M	C1'-N9-C8	5.57	139.46	127.09
1	S2	1678	A2M	C2'-C1'-N9	-5.56	104.61	113.75
1	S2	1031	A2M	C5-C4-N3	-5.54	119.09	126.72
1	S2	1832	6MZ	N1-C2-N3	-5.53	120.21	128.58
1	S2	1031	A2M	N6-C6-N1	-5.48	106.17	118.38
1	S2	484	A2M	N3-C2-N1	-5.46	120.31	128.58
1	S2	27	A2M	C4-N9-C1'	-5.43	113.94	126.63
1	S2	509	OMG	C5-C4-N3	-5.41	119.77	128.39
1	S2	27	A2M	N6-C6-N1	-5.41	106.33	118.38
1	S2	823	PSU	O2-C2-N1	-5.40	117.22	122.79
1	S2	683	OMG	C5-C4-N3	-5.40	119.80	128.39
1	S2	159	A2M	N3-C2-N1	-5.38	120.44	128.58
1	S2	159	A2M	C5-C4-N3	-5.30	119.42	126.72
1	S2	166	A2M	N6-C6-N1	-5.30	106.58	118.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	568	E3C	C6-N1-C2	-5.26	117.50	121.80
1	S2	823	PSU	N1-C2-N3	5.24	120.70	115.17
1	S2	484	A2M	N6-C6-N1	-5.22	106.75	118.38
1	S2	1850	MA6	C5-C4-N3	-5.21	119.54	126.72
1	S2	814	5MU	N3-C2-N1	5.18	121.63	114.89
1	S2	644	OMG	C5-C4-N3	-5.13	120.22	128.39
1	S2	822	PSU	C4-N3-C2	-5.11	119.34	126.37
1	S2	27	A2M	C1'-N9-C8	5.07	138.34	127.09
1	S2	159	A2M	N6-C6-N1	-5.05	107.13	118.38
1	S2	1832	6MZ	C5-C4-N3	-5.00	119.84	126.72
1	S2	1081	PSU	N1-C2-N3	4.97	120.41	115.17
1	S2	1678	A2M	C5-C4-N3	-4.97	119.88	126.72
1	S2	484	A2M	C5-C4-N3	-4.91	119.95	126.72
1	S2	1248	B8N	C5-C4-N3	4.89	125.03	116.15
1	S2	1851	MA6	C1'-N9-C8	-4.88	116.26	127.09
1	S2	1243	PSU	N1-C2-N3	4.88	120.31	115.17
1	S2	644	OMG	C1'-N9-C4	-4.87	112.09	126.49
1	S2	1851	MA6	N9-C8-N7	-4.81	107.11	113.94
1	S2	166	A2M	C5-C4-N3	-4.81	120.10	126.72
1	S2	822	PSU	N1-C2-N3	4.79	120.22	115.17
1	S2	612	PSU	C4-N3-C2	-4.79	119.77	126.37
1	S2	116	OMU	C4-N3-C2	-4.75	120.72	126.61
1	S2	814	5MU	C5M-C5-C6	-4.74	116.43	122.85
1	S2	1830	UR3	O2-C2-N3	-4.73	114.79	121.33
1	S2	823	PSU	C6-N1-C2	-4.72	118.31	122.69
1	S2	1243	PSU	C6-N1-C2	-4.69	118.34	122.69
1	S2	668	A2M	C5-C4-N3	-4.64	120.33	126.72
1	S2	1081	PSU	C4-N3-C2	-4.57	120.07	126.37
1	S2	1850	MA6	N9-C8-N7	-4.52	107.53	113.94
1	S2	1219	B8Q	C31-N3-C4	4.52	122.58	114.76
1	S2	668	A2M	N9-C8-N7	-4.49	107.56	113.94
1	S2	166	A2M	N9-C8-N7	-4.44	107.63	113.94
1	S2	612	PSU	N1-C2-N3	4.44	119.85	115.17
1	S2	119	PSU	C4-N3-C2	-4.43	120.26	126.37
1	S2	1678	A2M	N9-C8-N7	-4.43	107.66	113.94
1	S2	1851	MA6	C5-C4-N3	-4.41	120.64	126.72
1	S2	1832	6MZ	C4-C5-C6	4.41	120.44	116.78
1	S2	1850	MA6	C4-N9-C1'	4.41	136.94	126.63
1	S2	509	OMG	C2-N3-C4	4.39	119.86	112.30
1	S2	668	A2M	C5-C6-N6	4.39	134.15	123.29
1	S2	1678	A2M	N6-C6-N1	-4.36	108.66	118.38
1	S2	823	PSU	C4-N3-C2	-4.35	120.37	126.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	823	PSU	C6-C5-C4	4.33	121.10	118.17
1	S2	644	OMG	C2-N3-C4	4.32	119.74	112.30
1	S2	121	OMU	N3-C2-N1	4.30	120.49	114.89
1	S2	683	OMG	C2-N3-C4	4.26	119.64	112.30
1	S2	644	OMG	C1'-N9-C8	4.24	138.78	126.73
1	S2	1243	PSU	C4-N3-C2	-4.17	120.63	126.37
1	S2	1248	B8N	C4-N3-C2	-4.15	120.51	125.62
1	S2	1081	PSU	C6-N1-C2	-4.15	118.84	122.69
1	S2	1850	MA6	C4-C5-C6	4.12	120.17	115.91
1	S2	1806	M7A	N3-C4-N9	4.10	132.01	126.88
1	S2	159	A2M	N9-C8-N7	-4.10	108.12	113.94
1	S2	1830	UR3	O4-C4-N3	4.10	124.65	119.66
1	S2	119	PSU	N1-C2-N3	4.09	119.48	115.17
1	S2	814	5MU	O4-C4-C5	-4.08	120.25	124.92
1	S2	1031	A2M	C5-C6-N6	4.07	133.37	123.29
1	S2	814	5MU	C5M-C5-C4	4.07	123.12	118.78
1	S2	484	A2M	C5-C6-N6	4.02	133.23	123.29
1	S2	27	A2M	C5-C6-N6	4.01	133.21	123.29
1	S2	1031	A2M	N9-C8-N7	-3.99	108.27	113.94
1	S2	1219	B8Q	N3-C2-N1	3.99	122.72	117.16
1	S2	509	OMG	C1'-N9-C4	-3.96	114.78	126.49
1	S2	1851	MA6	C4-C5-C6	3.95	119.99	115.91
1	S2	166	A2M	C5-C6-N6	3.94	133.05	123.29
1	S2	119	PSU	C6-N1-C2	-3.93	119.05	122.69
1	S2	1832	6MZ	N9-C8-N7	-3.87	108.44	113.94
1	S2	822	PSU	C6-C5-C4	3.85	120.77	118.17
1	S2	159	A2M	C5-C6-N6	3.82	132.74	123.29
1	S2	27	A2M	N9-C8-N7	-3.81	108.54	113.94
1	S2	121	OMU	C5-C4-N3	3.78	120.09	114.80
1	S2	27	A2M	N3-C4-N9	3.75	133.55	127.17
1	S2	484	A2M	N9-C8-N7	-3.75	108.62	113.94
1	S2	1806	M7A	C71-N7-C5	-3.74	107.86	123.44
1	S2	1678	A2M	C5-C6-N6	3.70	132.46	123.29
1	S2	1850	MA6	N3-C4-N9	3.70	133.46	127.17
1	S2	683	OMG	C1'-N9-C4	-3.66	115.67	126.49
1	S2	116	OMU	N3-C2-N1	3.64	119.64	114.89
1	S2	1248	B8N	N3-C2-N1	3.63	121.15	116.72
1	S2	27	A2M	C2-N3-C4	3.63	120.69	111.83
1	S2	612	PSU	C6-C5-C4	3.63	120.62	118.17
1	S2	1678	A2M	C2-N3-C4	3.62	120.67	111.83
1	S2	119	PSU	O2-C2-N1	-3.61	119.07	122.79
1	S2	683	OMG	N9-C4-N3	3.60	133.14	125.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	509	OMG	C1'-N9-C8	3.58	136.91	126.73
1	S2	1031	A2M	C2-N3-C4	3.58	120.57	111.83
1	S2	121	OMU	O2-C2-N1	-3.57	118.16	122.80
1	S2	1850	MA6	C2-N3-C4	3.56	120.52	111.83
1	S2	1851	MA6	C2-N1-C6	3.52	120.44	111.83
1	S2	509	OMG	N9-C4-N3	3.51	132.97	125.95
1	S2	1678	A2M	O2'-C2'-C1'	3.45	115.53	108.99
1	S2	1678	A2M	O3'-C3'-C2'	-3.45	101.54	111.19
1	S2	1678	A2M	N3-C4-N9	3.44	133.02	127.17
1	S2	509	OMG	C2-N1-C6	-3.42	118.92	125.11
1	S2	1851	MA6	C4-N9-C8	3.41	109.32	105.74
1	S2	668	A2M	C2-N3-C4	3.41	120.16	111.83
1	S2	1806	M7A	C2-N3-C4	3.38	120.09	111.83
1	S2	612	PSU	C6-N1-C2	-3.38	119.55	122.69
1	S2	166	A2M	C2-N3-C4	3.36	120.05	111.83
1	S2	159	A2M	C2-N3-C4	3.36	120.04	111.83
1	S2	159	A2M	N3-C4-N9	3.34	132.84	127.17
1	S2	1851	MA6	C4-N9-C1'	3.33	134.41	126.63
1	S2	1031	A2M	N3-C4-N9	3.30	132.79	127.17
1	S2	116	OMU	C5-C4-N3	3.30	119.43	114.80
1	S2	644	OMG	C2-N1-C6	-3.30	119.12	125.11
1	S2	1832	6MZ	C2-N3-C4	3.29	119.86	111.83
1	S2	644	OMG	N9-C8-N7	-3.28	107.31	113.40
1	S2	484	A2M	C2-N3-C4	3.27	119.82	111.83
1	S2	1850	MA6	C2-N1-C6	3.22	119.70	111.83
1	S2	1830	UR3	C1'-N1-C6	-3.18	113.99	120.78
1	S2	644	OMG	N9-C4-N3	3.17	132.29	125.95
1	S2	683	OMG	C1'-N9-C8	3.17	135.73	126.73
1	S2	1851	MA6	C2-N3-C4	3.17	119.56	111.83
1	S2	822	PSU	C6-N1-C2	-3.16	119.76	122.69
1	S2	1374	5MC	C5-C6-N1	-3.13	119.92	123.31
1	S2	1248	B8N	C1'-C5-C4	3.12	122.34	117.61
1	S2	1081	PSU	O2-C2-N1	-3.09	119.60	122.79
1	S2	1850	MA6	C4-N9-C8	3.09	108.98	105.74
1	S2	1337	4AC	C6-C5-C4	3.08	120.71	117.00
1	S2	683	OMG	C2-N1-C6	-3.07	119.55	125.11
1	S2	1832	6MZ	N3-C4-N9	3.06	132.36	127.17
1	S2	1219	B8Q	O2-C2-N3	-3.06	118.66	122.95
1	S2	822	PSU	O2-C2-N1	-3.04	119.65	122.79
1	S2	116	OMU	O2-C2-N3	-3.01	115.94	121.49
1	S2	116	OMU	O4-C4-C5	-3.01	119.98	125.16
1	S2	1678	A2M	C2'-C3'-C4'	3.00	108.44	101.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	1678	A2M	C4-N9-C8	3.00	108.88	105.74
1	S2	668	A2M	C3'-C2'-C1'	2.99	108.54	102.81
1	S2	166	A2M	N3-C4-N9	2.97	132.21	127.17
1	S2	166	A2M	C5-N7-C8	2.96	108.11	103.45
1	S2	612	PSU	O2-C2-N1	-2.95	119.75	122.79
1	S2	683	OMG	N9-C8-N7	-2.95	107.93	113.40
1	S2	568	E3C	C4-N3-C2	-2.95	116.69	122.00
1	S2	814	5MU	C6-C5-C4	2.94	120.44	118.02
1	S2	1678	A2M	C5-N7-C8	2.91	108.02	103.45
1	S2	668	A2M	C5-N7-C8	2.90	108.01	103.45
1	S2	1851	MA6	N3-C4-N9	2.89	132.09	127.17
1	S2	116	OMU	C1'-N1-C6	-2.89	114.60	120.78
1	S2	814	5MU	O3'-C3'-C2'	2.89	121.08	111.82
1	S2	1851	MA6	C5-N7-C8	2.87	107.97	103.45
1	S2	1248	B8N	C31-N3-C4	2.86	121.23	117.18
1	S2	1243	PSU	O2-C2-N1	-2.85	119.84	122.79
1	S2	159	A2M	C5-N7-C8	2.85	107.93	103.45
1	S2	1031	A2M	C5-N7-C8	2.85	107.93	103.45
1	S2	509	OMG	O6-C6-C5	-2.80	119.15	126.53
1	S2	121	OMU	O4-C4-C5	-2.77	120.39	125.16
1	S2	509	OMG	N9-C8-N7	-2.76	108.28	113.40
1	S2	27	A2M	O4'-C1'-C2'	-2.76	101.83	106.59
1	S2	1337	4AC	C5-C4-N3	-2.74	118.31	122.60
1	S2	484	A2M	O4'-C1'-C2'	-2.74	101.87	106.59
1	S2	1806	M7A	C5-C4-N3	-2.73	120.24	126.56
1	S2	568	E3C	C1'-N1-C6	-2.73	114.95	120.78
1	S2	1850	MA6	C5-N7-C8	2.73	107.73	103.45
1	S2	644	OMG	C5-C6-N1	2.73	120.19	113.25
1	S2	484	A2M	N3-C4-N9	2.70	131.76	127.17
1	S2	166	A2M	C4-N9-C8	2.70	108.57	105.74
1	S2	116	OMU	C6-N1-C2	-2.67	117.75	121.00
1	S2	509	OMG	C5-C6-N1	2.67	120.04	113.25
1	S2	1081	PSU	C6-C5-C4	2.66	119.97	118.17
1	S2	484	A2M	C5-N7-C8	2.65	107.61	103.45
1	S2	1219	B8Q	C31-N3-C2	2.64	121.85	117.70
1	S2	1248	B8N	O4-C4-C5	-2.64	118.02	122.58
1	S2	683	OMG	O6-C6-C5	-2.63	119.59	126.53
1	S2	27	A2M	C5-N7-C8	2.63	107.58	103.45
1	S2	1832	6MZ	C5-N7-C8	2.62	107.57	103.45
1	S2	644	OMG	O6-C6-C5	-2.60	119.67	126.53
1	S2	668	A2M	C4-C5-N7	-2.58	107.64	110.58
1	S2	1842	4AC	O7-C7-CM7	-2.57	117.48	122.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	683	OMG	C5-C6-N1	2.56	119.78	113.25
1	S2	159	A2M	O4'-C1'-C2'	-2.52	102.25	106.59
1	S2	668	A2M	C5-C4-N9	2.51	108.55	105.81
1	S2	668	A2M	C2'-C3'-C4'	2.50	107.37	101.99
1	S2	1842	4AC	C5-C4-N3	-2.48	118.72	122.60
1	S2	1842	4AC	C6-C5-C4	2.47	119.98	117.00
1	S2	159	A2M	C6-C5-C4	2.45	120.52	117.18
1	S2	484	A2M	C2'-C1'-N9	-2.43	109.75	113.75
1	S2	668	A2M	C4-N9-C8	2.39	108.25	105.74
1	S2	1374	5MC	CM5-C5-C6	-2.37	119.64	122.85
1	S2	814	5MU	O4-C4-N3	-2.36	115.67	120.11
1	S2	668	A2M	N3-C4-N9	2.32	131.12	127.17
1	S2	1031	A2M	C4-C5-N7	-2.29	107.96	110.58
1	S2	1031	A2M	C3'-C2'-C1'	2.29	107.19	102.81
1	S2	27	A2M	C6-C5-C4	2.28	120.29	117.18
1	S2	159	A2M	C4-N9-C8	2.27	108.12	105.74
1	S2	484	A2M	C5-C4-N9	2.27	108.28	105.81
1	S2	166	A2M	C4-C5-N7	-2.26	108.00	110.58
1	S2	668	A2M	C5'-C4'-C3'	-2.22	107.21	115.21
1	S2	1031	A2M	C6-C5-C4	2.20	120.19	117.18
1	S2	823	PSU	O4'-C1'-C2'	2.20	108.20	105.15
1	S2	1337	4AC	O7-C7-CM7	-2.20	118.14	122.05
1	S2	159	A2M	C4-C5-N7	-2.18	108.09	110.58
1	S2	1842	4AC	N4-C4-N3	2.18	117.40	113.87
1	S2	1678	A2M	CM3'-O2'-C2'	2.15	119.98	114.47
1	S2	484	A2M	C6-C5-C4	2.15	120.11	117.18
1	S2	1031	A2M	O4'-C1'-C2'	-2.14	102.91	106.59
1	S2	484	A2M	C4-C5-N7	-2.13	108.15	110.58
1	S2	484	A2M	O4'-C1'-N9	2.12	112.16	108.09
1	S2	1031	A2M	C5-C4-N9	2.12	108.12	105.81
1	S2	1031	A2M	C4'-O4'-C1'	-2.10	104.83	109.47
1	S2	159	A2M	C3'-C2'-C1'	2.09	106.81	102.81
1	S2	27	A2M	C4'-O4'-C1'	-2.09	104.86	109.47
1	S2	166	A2M	C4'-O4'-C1'	-2.07	104.89	109.47
1	S2	1678	A2M	C3'-C2'-C1'	2.07	106.77	102.81
1	S2	1806	M7A	N9-C8-N7	2.06	106.29	103.37
1	S2	612	PSU	O4'-C1'-C2'	2.06	108.00	105.15
1	S2	814	5MU	O3'-C3'-C4'	2.04	116.95	111.08
1	S2	1678	A2M	C6-C5-C4	2.03	119.94	117.18
1	S2	644	OMG	C8-N7-C5	2.02	107.87	104.26
1	S2	814	5MU	O2-C2-N1	-2.01	120.17	122.80
1	S2	484	A2M	C4'-O4'-C1'	-2.01	105.02	109.47

There are no chirality outliers.

All (61) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	S2	27	A2M	C1'-C2'-O2'-CM'
1	S2	116	OMU	O4'-C4'-C5'-O5'
1	S2	159	A2M	O4'-C4'-C5'-O5'
1	S2	166	A2M	C1'-C2'-O2'-CM'
1	S2	509	OMG	C1'-C2'-O2'-CM2
1	S2	568	E3C	O4'-C1'-N1-C2
1	S2	568	E3C	O4'-C1'-N1-C6
1	S2	823	PSU	O4'-C4'-C5'-O5'
1	S2	1678	A2M	O4'-C4'-C5'-O5'
1	S2	1678	A2M	C1'-C2'-O2'-CM'
1	S2	1703	OMC	O4'-C4'-C5'-O5'
1	S2	1830	UR3	O4'-C4'-C5'-O5'
1	S2	1830	UR3	O4'-C1'-N1-C6
1	S2	1830	UR3	O4'-C1'-N1-C2
1	S2	1832	6MZ	C5-C6-N6-C9
1	S2	1832	6MZ	N1-C6-N6-C9
1	S2	1850	MA6	O4'-C4'-C5'-O5'
1	S2	1850	MA6	C5-C6-N6-C9
1	S2	1851	MA6	O4'-C4'-C5'-O5'
1	S2	1851	MA6	C3'-C4'-C5'-O5'
1	S2	1851	MA6	C5-C6-N6-C10
1	S2	116	OMU	C3'-C4'-C5'-O5'
1	S2	121	OMU	O4'-C4'-C5'-O5'
1	S2	159	A2M	C3'-C4'-C5'-O5'
1	S2	166	A2M	O4'-C4'-C5'-O5'
1	S2	166	A2M	C3'-C4'-C5'-O5'
1	S2	568	E3C	C3'-C4'-C5'-O5'
1	S2	568	E3C	O4'-C4'-C5'-O5'
1	S2	668	A2M	O4'-C4'-C5'-O5'
1	S2	668	A2M	C3'-C4'-C5'-O5'
1	S2	683	OMG	C3'-C4'-C5'-O5'
1	S2	823	PSU	C3'-C4'-C5'-O5'
1	S2	1678	A2M	C3'-C4'-C5'-O5'
1	S2	1703	OMC	C3'-C4'-C5'-O5'
1	S2	1850	MA6	C3'-C4'-C5'-O5'
1	S2	644	OMG	C3'-C4'-C5'-O5'
1	S2	683	OMG	O4'-C4'-C5'-O5'
1	S2	1243	PSU	C3'-C4'-C5'-O5'
1	S2	1243	PSU	O4'-C4'-C5'-O5'
1	S2	1850	MA6	N1-C6-N6-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	S2	1851	MA6	N1-C6-N6-C10
1	S2	1830	UR3	C3'-C4'-C5'-O5'
1	S2	644	OMG	O4'-C4'-C5'-O5'
1	S2	121	OMU	C3'-C4'-C5'-O5'
1	S2	1830	UR3	C2'-C1'-N1-C6
1	S2	1850	MA6	C5-C6-N6-C10
1	S2	668	A2M	C2'-C1'-N9-C8
1	S2	1248	B8N	N3-C31-C32-C33
1	S2	1337	4AC	O4'-C4'-C5'-O5'
1	S2	159	A2M	C4'-C5'-O5'-P
1	S2	644	OMG	C4'-C5'-O5'-P
1	S2	1806	M7A	C4'-C5'-O5'-P
1	S2	568	E3C	C4'-C5'-O5'-P
1	S2	1851	MA6	C4'-C5'-O5'-P
1	S2	116	OMU	C2'-C1'-N1-C6
1	S2	1710	OMC	C1'-C2'-O2'-CM2
1	S2	116	OMU	C2'-C1'-N1-C2
1	S2	668	A2M	C2'-C1'-N9-C4
1	S2	668	A2M	O4'-C1'-N9-C8
1	S2	1851	MA6	C5-C6-N6-C9
1	S2	1248	B8N	C32-C33-C34-O35

There are no ring outliers.

12 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	S2	814	5MU	2	0
1	S2	1830	UR3	2	0
1	S2	517	OMC	1	0
1	S2	1243	PSU	2	0
1	S2	644	OMG	1	0
1	S2	1850	MA6	1	0
1	S2	166	A2M	3	0
1	S2	27	A2M	1	0
1	S2	683	OMG	1	0
1	S2	1851	MA6	1	0
1	S2	509	OMG	2	0
1	S2	1219	B8Q	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 38 ligands modelled in this entry, 37 are monoatomic - leaving 1 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
86	MVM	t	5112	-	35,35,35	1.90	7 (20%)	44,49,49	2.68	13 (29%)

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
86	MVM	t	5112	-	-	4/20/28/28	0/5/5/5

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	t	5112	MVM	N4-N5	-6.71	1.31	1.38
86	t	5112	MVM	C5-N1	6.17	1.46	1.37
86	t	5112	MVM	C6-N1	2.50	1.45	1.39
86	t	5112	MVM	C12-C5	2.34	1.54	1.50
86	t	5112	MVM	C2-CL	2.15	1.78	1.73
86	t	5112	MVM	O1-C5	-2.14	1.18	1.22
86	t	5112	MVM	C7-C3	-2.02	1.48	1.53

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
86	t	5112	MVM	N7-C22-N4	7.52	134.33	125.88
86	t	5112	MVM	C15-N4-N5	6.74	125.32	119.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
86	t	5112	MVM	C15-N4-C22	-6.53	124.75	130.55
86	t	5112	MVM	C6-N1-C5	-5.54	116.30	122.94
86	t	5112	MVM	C18-C22-N7	-5.09	120.19	127.18
86	t	5112	MVM	C1-C9-N1	-4.53	104.78	116.16
86	t	5112	MVM	C19-C18-N6	3.76	135.39	130.50
86	t	5112	MVM	C21-N7-C22	3.49	122.96	115.05
86	t	5112	MVM	C8-N3-C6	3.30	122.53	115.05
86	t	5112	MVM	C7-C3-C9	2.92	116.36	110.81
86	t	5112	MVM	C6-N1-C9	2.79	122.54	118.40
86	t	5112	MVM	N3-C6-N1	2.13	118.63	116.35
86	t	5112	MVM	C20-C21-N7	-2.00	120.25	123.42

There are no chirality outliers.

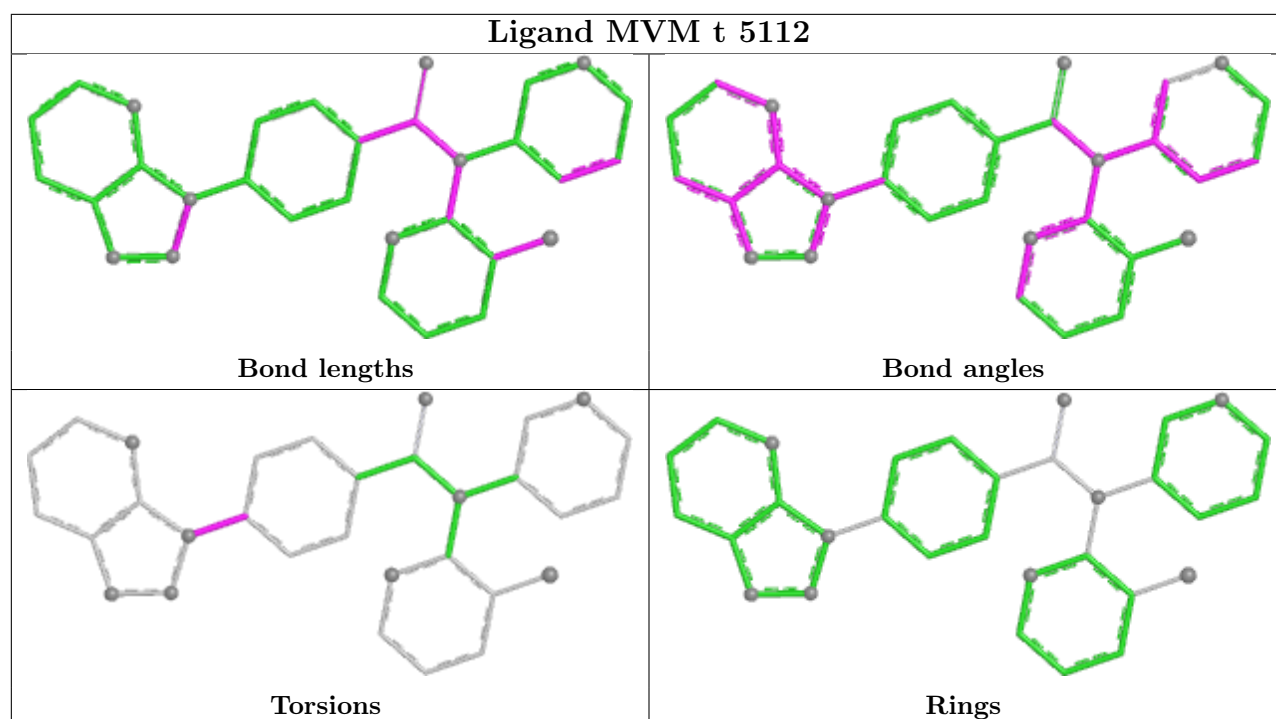
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
86	t	5112	MVM	C16-C15-N4-C22
86	t	5112	MVM	C14-C15-N4-C22
86	t	5112	MVM	C14-C15-N4-N5
86	t	5112	MVM	C16-C15-N4-N5

There are no ring outliers.

No monomer is involved in short contacts.

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	S2	17
79	t	16
80	v	4
6	SF	2
5	SE	2
23	SC	2
10	SL	2
7	SH	1
63	c	1
35	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	S2	1677:U	O3'	1678:A2M	P	61.26

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	S2	1353:A	O3'	1354:G	P	60.55
1	SF	55:ARG	C	56:TYR	N	60.24
1	S2	503:C	O3'	504:G	P	59.86
1	S2	1357:A	O3'	1358:U	P	59.41
1	S2	110:U	O3'	111:A	P	58.86
1	S2	798:A	O3'	799:U	P	58.85
1	S2	1680:G	O3'	1681:U	P	58.80
1	SF	64:ALA	C	65:GLN	N	58.56
1	SH	103:LYS	C	104:PRO	N	58.48
1	SE	67:GLN	C	68:ARG	N	58.35
1	S2	500:A	O3'	501:C	P	58.28
1	SC	192:LEU	C	193:VAL	N	58.27
1	S2	863:U	O3'	864:A	P	58.14
1	S2	859:G	O3'	860:G	P	58.11
1	SC	185:THR	C	186:GLY	N	57.74
1	SE	65:CYS	C	66:MET	N	57.71
1	SL	37:TYR	C	38:LYS	N	56.63
1	SL	47:PRO	C	48:LYS	N	56.57
1	S2	797:C	O3'	798:A	P	56.52
1	S2	115:U	O3'	116:OMU	P	55.93
1	S2	753:C	O3'	785:C	P	26.57
1	t	1680:C	O3'	1699:C	P	18.72
1	t	3919:C	O3'	4035:G	P	17.96
1	t	517:C	O3'	629:G	P	17.78
1	t	750:G	O3'	890:C	P	17.53
1	t	976:U	O3'	1047:G	P	17.42
1	t	2881:G	O3'	3569:C	P	17.40
1	S2	1752:C	O3'	1779:G	P	16.56
1	t	2093:C	O3'	2228:C	P	16.30
1	t	1253:A	O3'	1256:G	P	15.47
1	t	4737:G	O3'	4815:C	P	15.25
1	t	1089:A	O3'	1145:G	P	15.04
1	t	1202:G	O3'	1216:G	P	14.01
1	S2	739:C	O3'	746:C	P	13.28
1	S2	698:G	O3'	730:C	P	12.37
1	S2	225:G	O3'	287:U	P	10.20
1	v	17:A	O3'	18:G	P	7.00
1	t	945:G	O3'	946:G	P	6.50
1	c	119:CYS	C	120:ARG	N	6.26
1	v	10:G	O3'	11:C	P	4.33
1	t	4734:C	O3'	4735:C	P	4.12
1	t	4817:G	O3'	4818:G	P	4.04

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	v	21:A	O3'	22:G	P	3.65
1	t	964:C	O3'	965:G	P	3.39
1	t	1938:U	O3'	1939:A	P	3.39
1	v	41:C	O3'	42:C	P	3.19
1	A	220:GLY	C	221:LYS	N	1.16

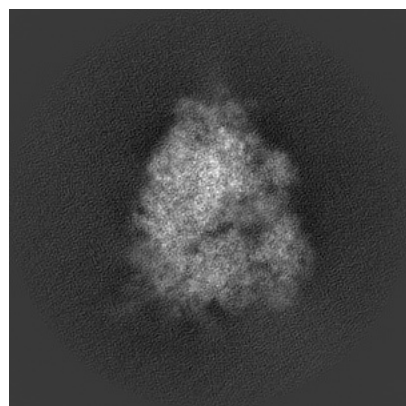
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0597. These allow visual inspection of the internal detail of the map and identification of artifacts.

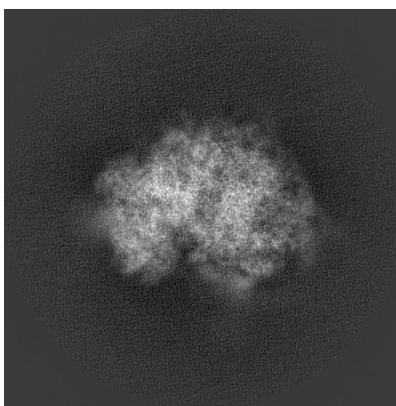
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

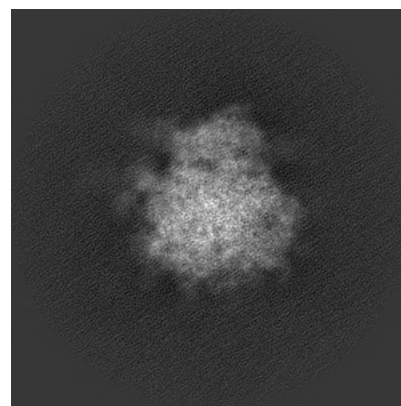
6.1.1 Primary map



X

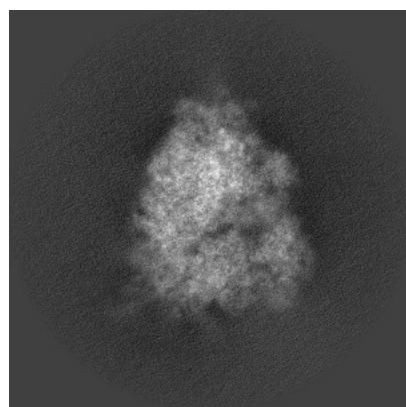


Y

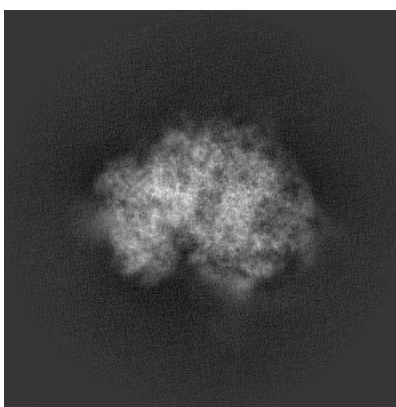


Z

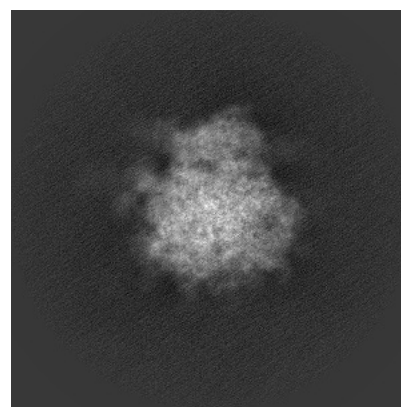
6.1.2 Raw map



X



Y

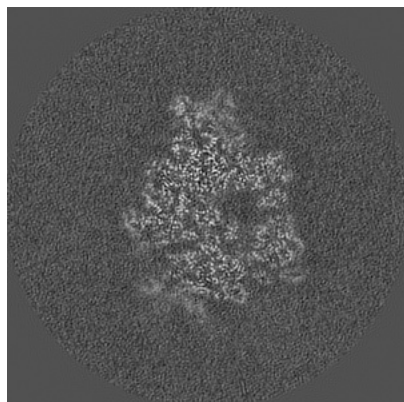


Z

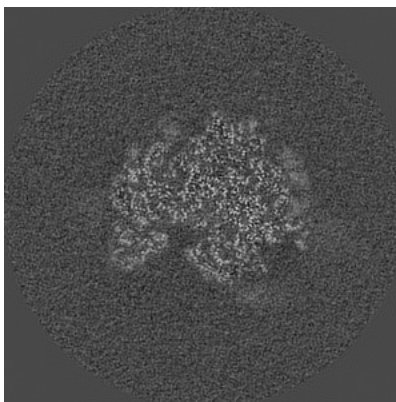
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

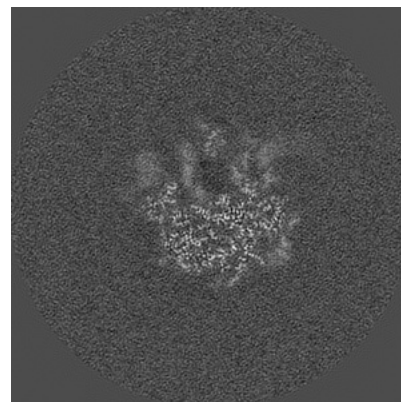
6.2.1 Primary map



X Index: 215

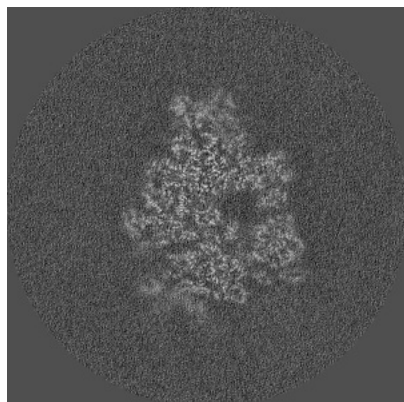


Y Index: 215

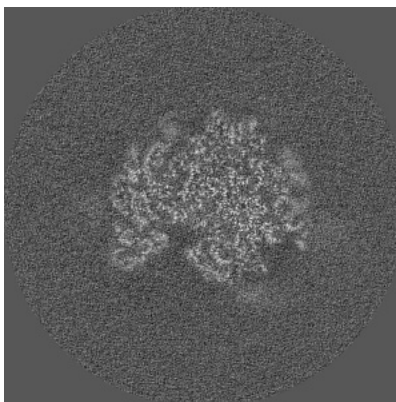


Z Index: 215

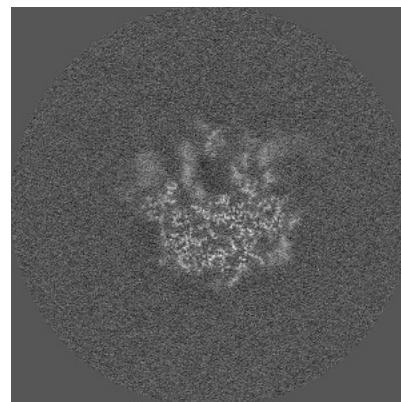
6.2.2 Raw map



X Index: 215



Y Index: 215

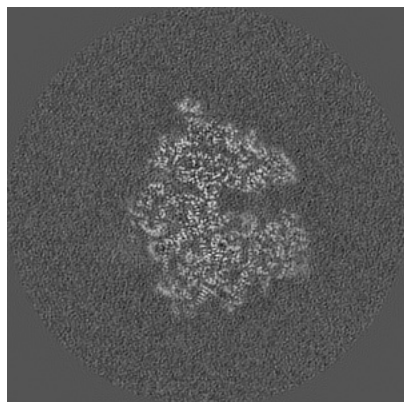


Z Index: 215

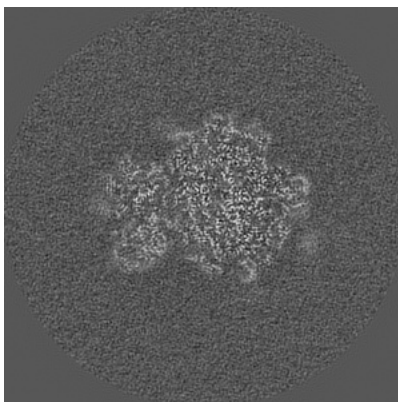
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

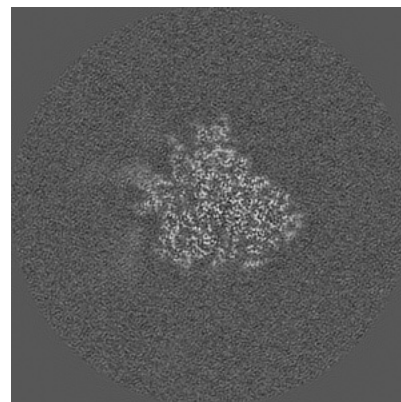
6.3.1 Primary map



X Index: 232

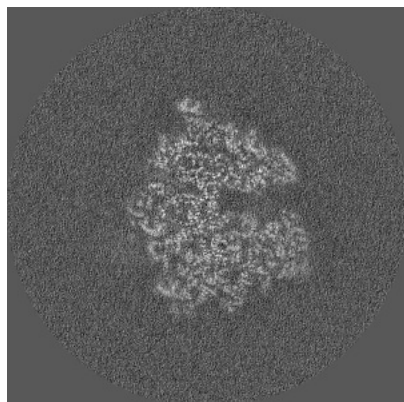


Y Index: 205

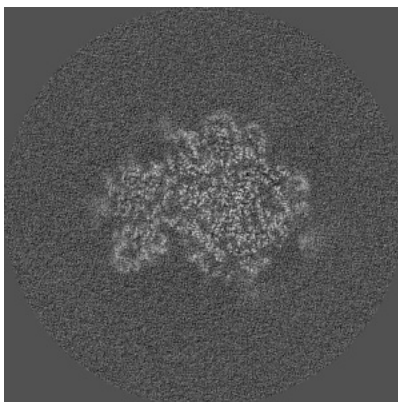


Z Index: 242

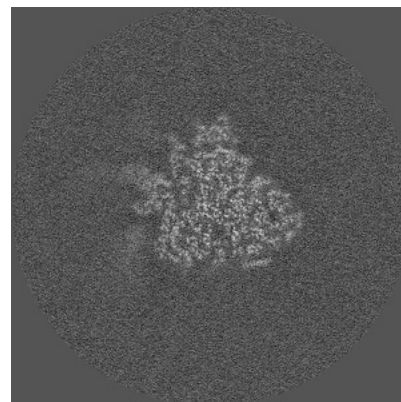
6.3.2 Raw map



X Index: 232



Y Index: 207

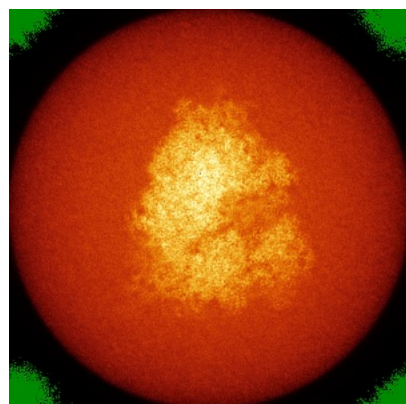


Z Index: 243

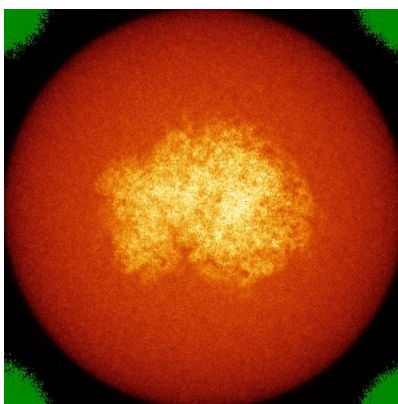
The images above show the largest variance slices of the map in three orthogonal directions.

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

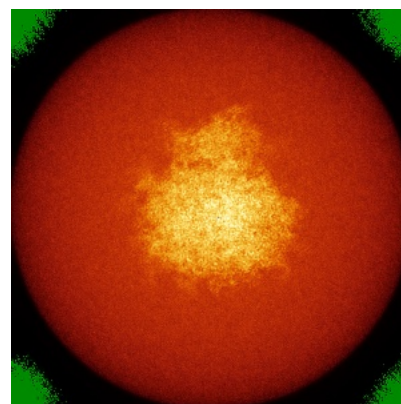
6.4.1 Primary map



X

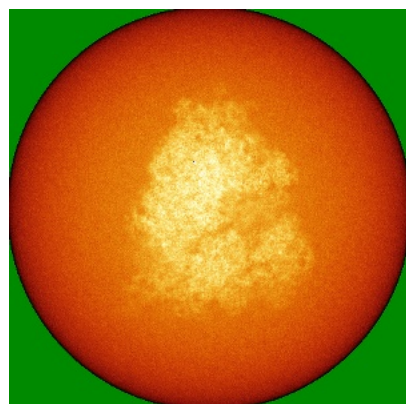


Y

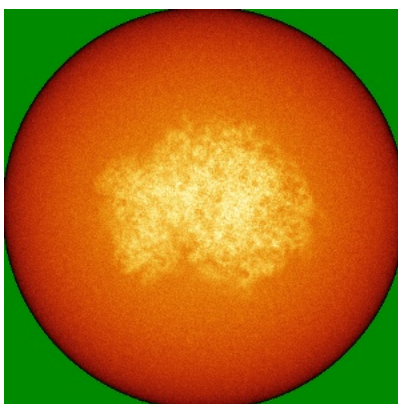


Z

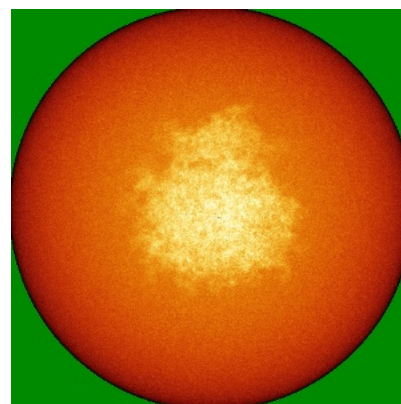
6.4.2 Raw map



X



Y

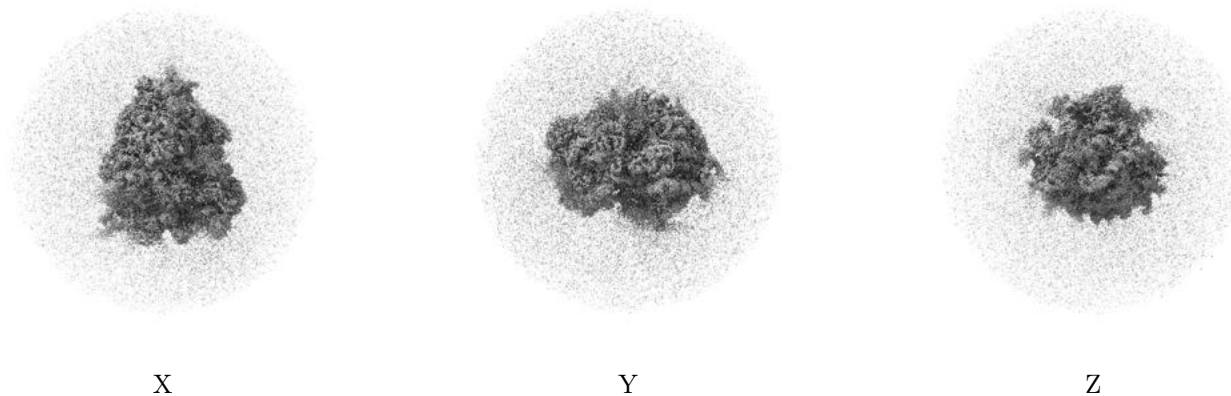


Z

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.

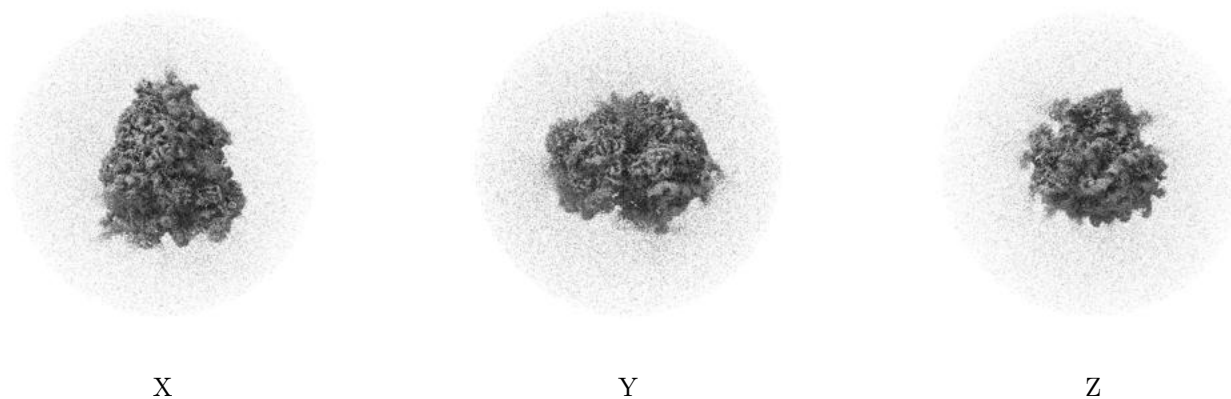
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.022. 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



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.

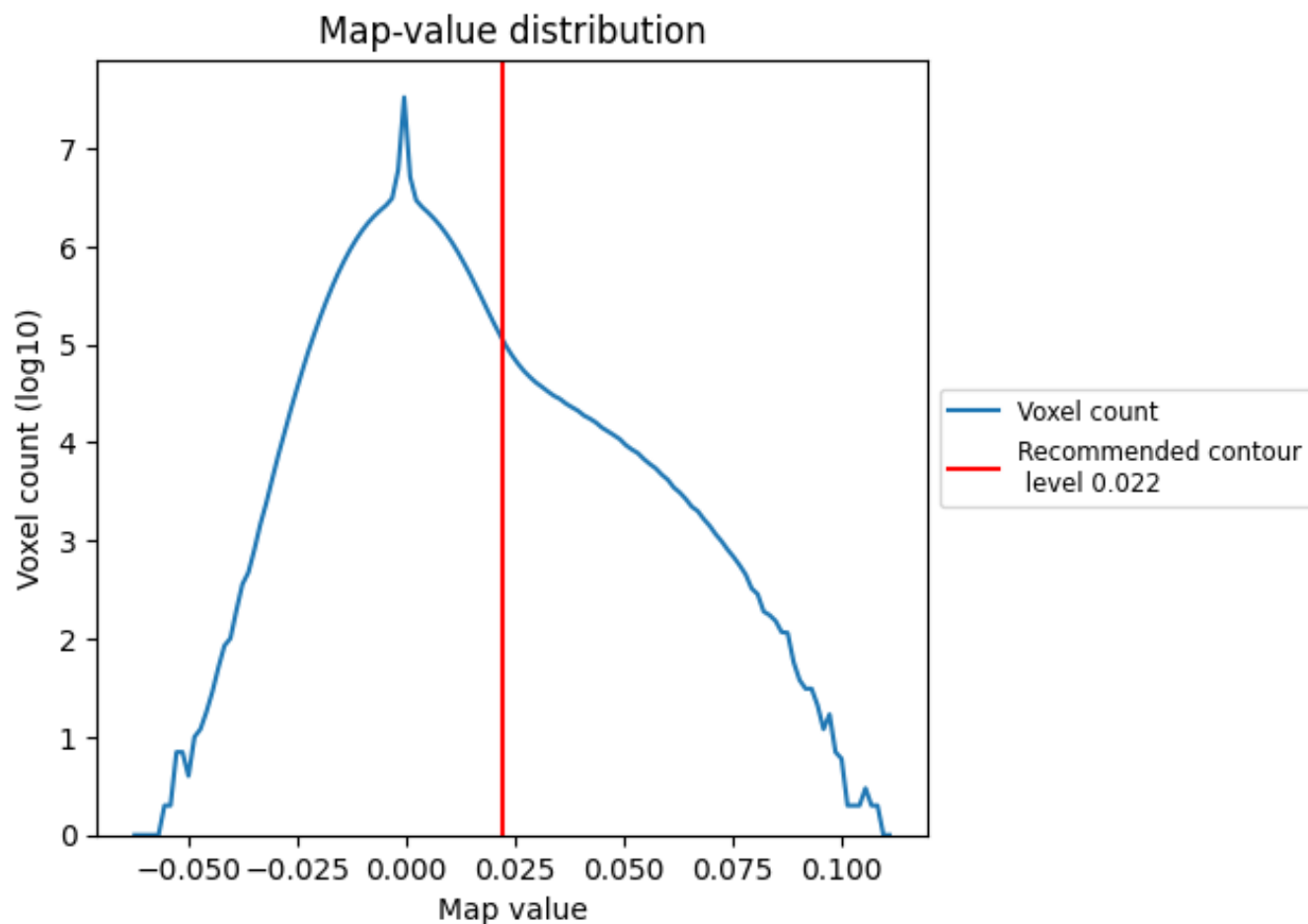
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

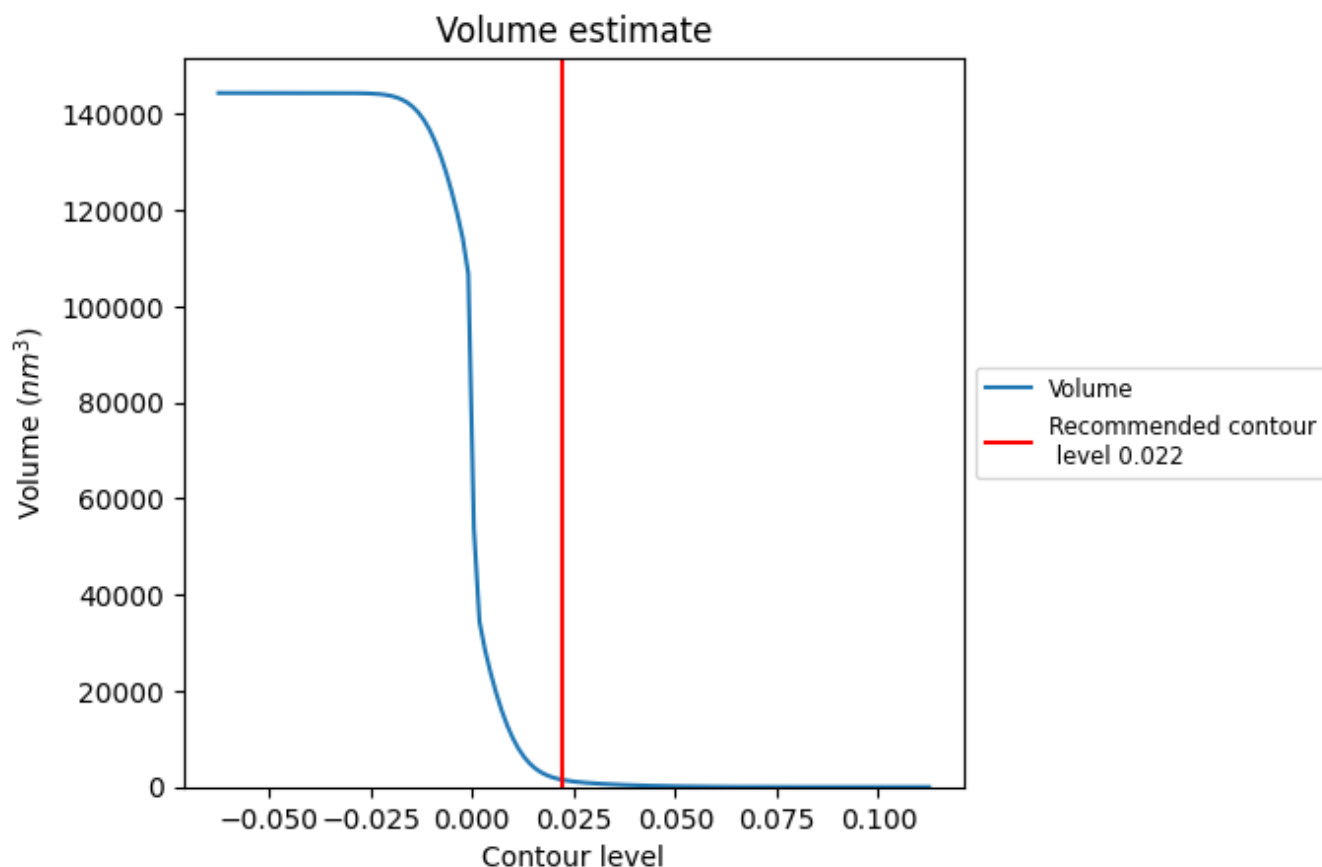
This section contains the results of statistical analysis of the map.

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.

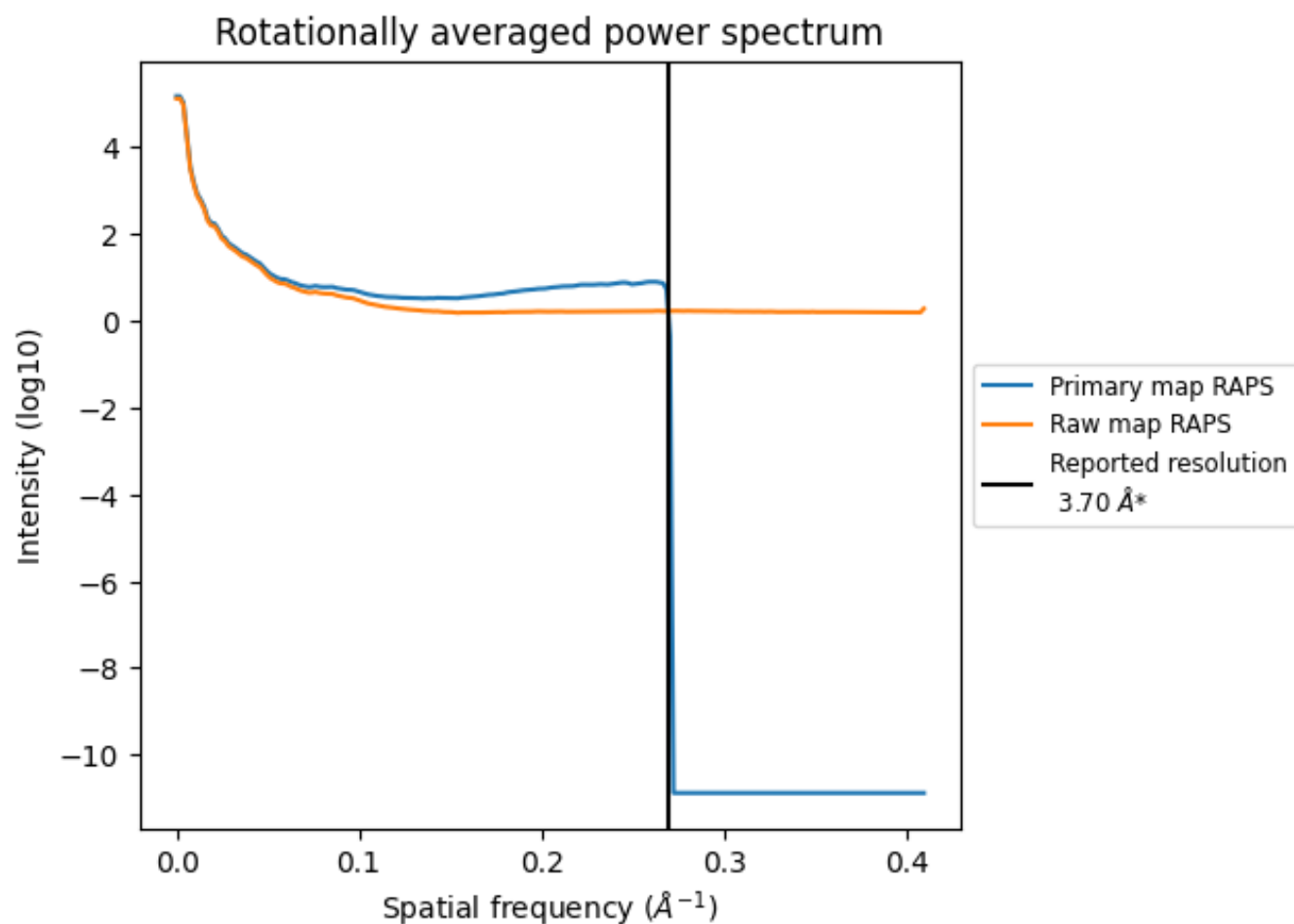
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1529 nm³; this corresponds to an approximate mass of 1381 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 ⓘ

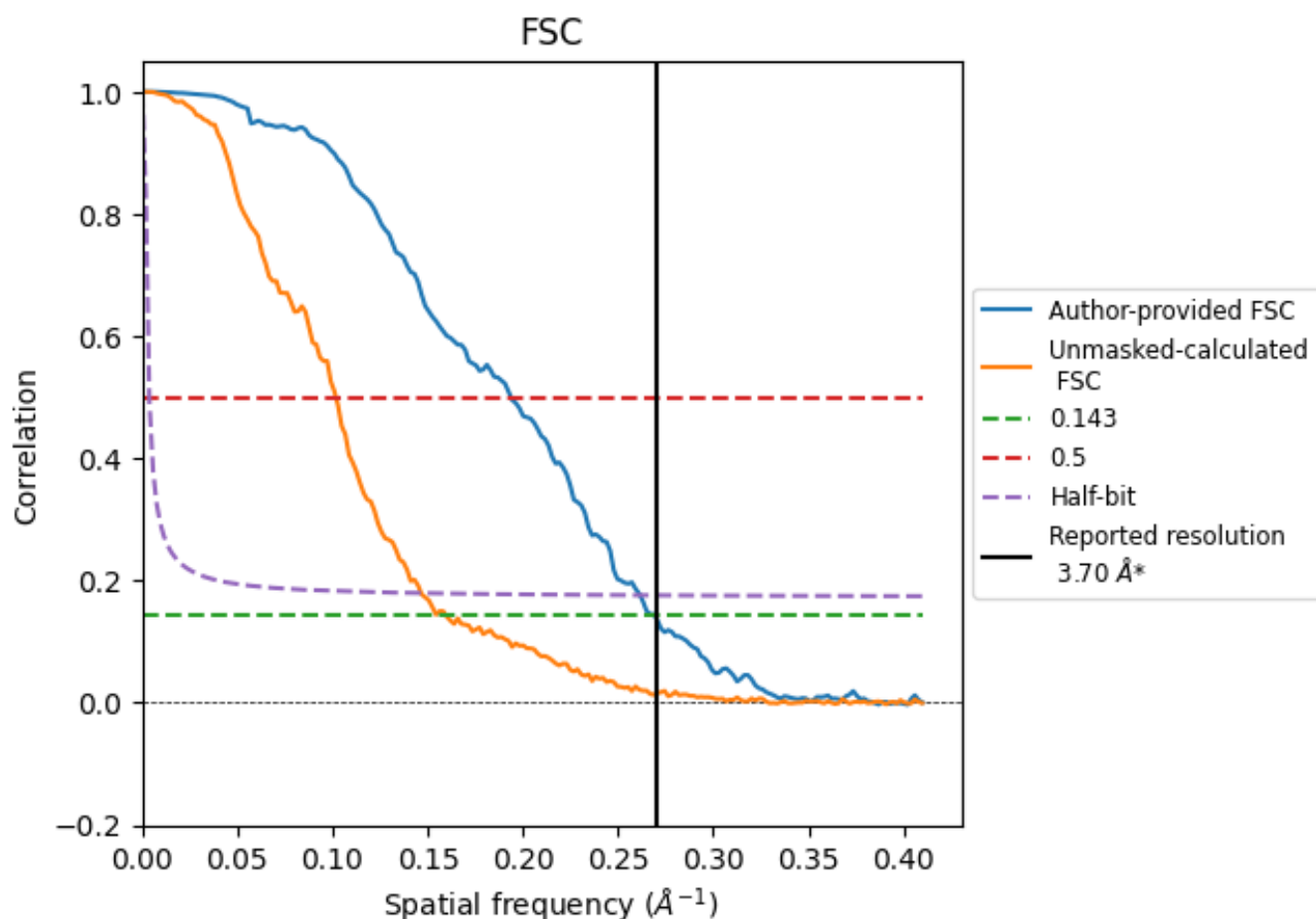


*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

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 0.270 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

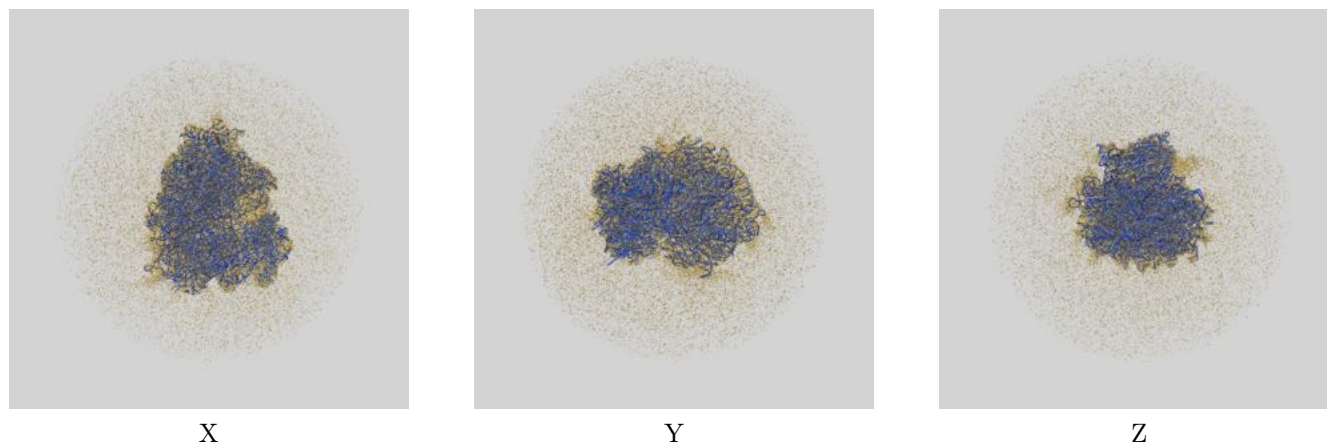
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.72	5.16	3.82
Unmasked-calculated*	6.27	9.82	6.83

*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 6.27 differs from the reported value 3.7 by more than 10 %

9 Map-model fit [i](#)

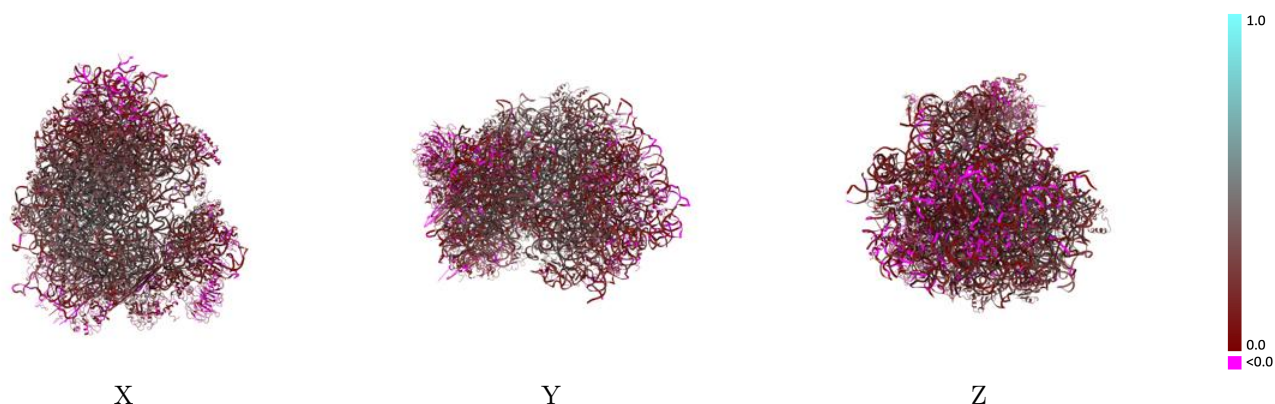
This section contains information regarding the fit between EMDB map EMD-0597 and PDB model 6OM7. Per-residue inclusion information can be found in section 3 on page 21.

9.1 Map-model overlay [i](#)



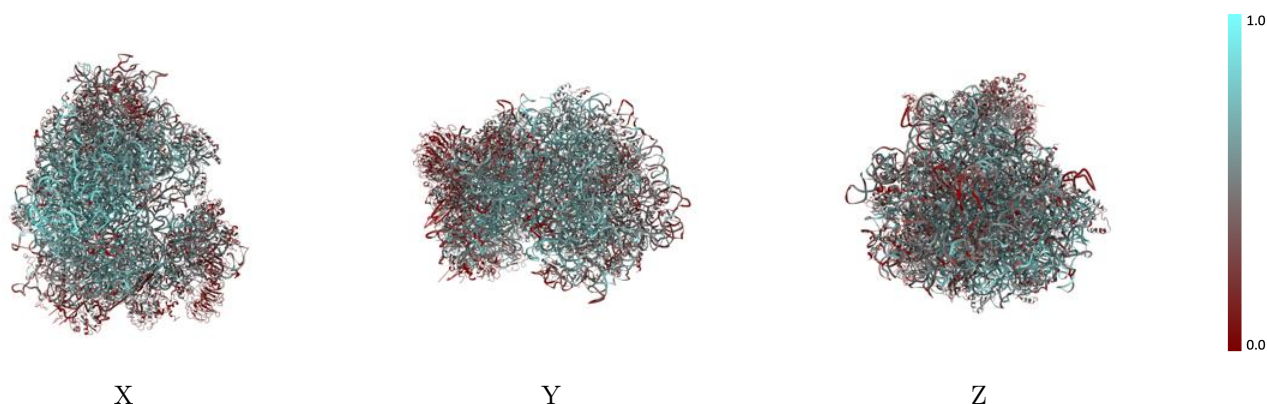
The images above show the 3D surface view of the map at the recommended contour level 0.022 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



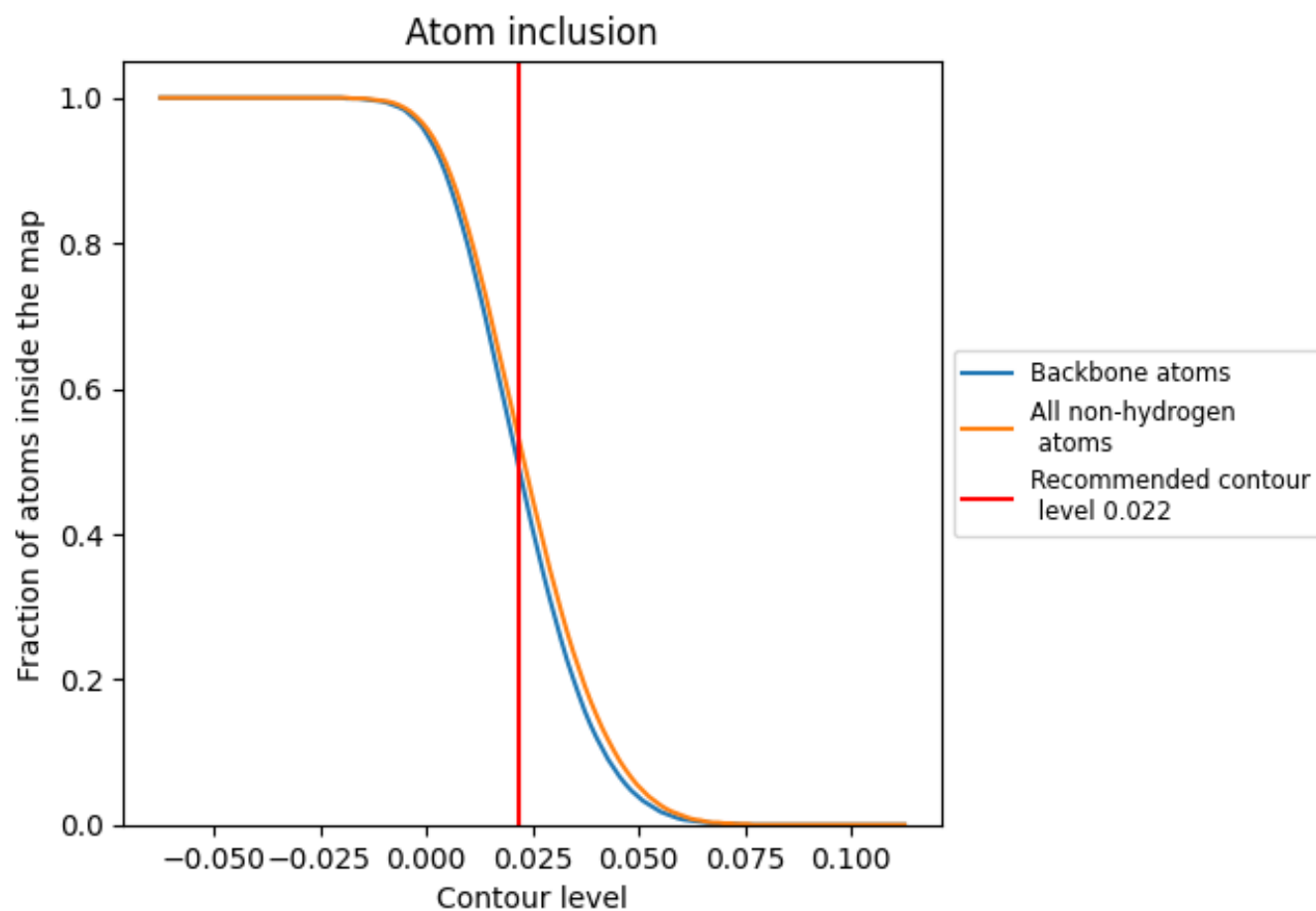
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.022).

9.4 Atom inclusion [i](#)



At the recommended contour level, 48% of all backbone atoms, 52% 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 (0.022) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5250	 0.2340
A	 0.6450	 0.4200
B	 0.4430	 0.2080
C	 0.3920	 0.1470
D	 0.6640	 0.2810
E	 0.6340	 0.2190
F	 0.3890	 0.1480
G	 0.2630	 0.0490
H	 0.3920	 0.1460
I	 0.5100	 0.3120
J	 0.4310	 0.2230
K	 0.5180	 0.3110
L	 0.4370	 0.2240
M	 0.4270	 0.1930
N	 0.3540	 0.1060
O	 0.5910	 0.3280
P	 0.4390	 0.1810
Q	 0.4650	 0.2140
R	 0.3930	 0.1580
S	 0.5250	 0.2890
S2	 0.6070	 0.2560
SA	 0.3140	 0.1730
SB	 0.4640	 0.3020
SC	 0.4150	 0.2360
SD	 0.3230	 0.1990
SE	 0.3410	 0.1810
SF	 0.3150	 0.1710
SG	 0.2930	 0.1350
SH	 0.2650	 0.1320
SI	 0.3870	 0.1930
SJ	 0.4470	 0.2410
SK	 0.3230	 0.1900
SL	 0.3750	 0.2150
SM	 0.1240	 0.1550
SN	 0.4630	 0.2780



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
SO	0.4720	0.2960
SP	0.3710	0.2460
SQ	0.2560	0.1050
SR	0.2930	0.1600
SS	0.3610	0.1940
ST	0.2910	0.0980
SU	0.2450	0.1310
SV	0.3760	0.2110
SW	0.4510	0.2450
SX	0.5590	0.3640
SY	0.3780	0.1960
SZ	0.2620	0.1340
Sa	0.4880	0.3140
Sb	0.3410	0.2250
Sc	0.2260	0.1510
Sd	0.4560	0.2260
Se	0.3890	0.2550
Sf	0.1550	0.1690
Sg	0.1620	0.0460
T	0.4700	0.2200
U	0.4190	0.1970
V	0.4350	0.1910
W	0.5620	0.3490
X	0.2620	0.1390
Y	0.5620	0.3370
Z	0.4320	0.1860
a	0.5950	0.3570
b	0.4380	0.1860
c	0.3360	0.1390
d	0.5130	0.3250
e	0.4750	0.2240
f	0.3660	0.1430
g	0.3790	0.1290
h	0.5850	0.3740
i	0.4880	0.2440
j	0.4740	0.2350
k	0.6320	0.3540
l	0.4700	0.2820
m	0.5600	0.3180
n	0.5790	0.3170
o	0.6030	0.3880
p	0.4550	0.2660

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
q	 0.6240	 0.4000
r	 0.3340	 0.0750
t	 0.6250	 0.2490
u	 0.4410	 0.2310
v	 0.5250	 0.2470
w	 0.6620	 0.3480
y	 0.3050	 0.2710